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Research Article

Quantum Composites: A Review, and New Results for Models for Condensed Matter Nuclear Science

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Abstract

A composite is made up of constituent particles; the center of mass dynamics is that of a single particle, and the composite can have many internal states and degrees of freedom. The notion of a quantum composite is foundational to atomic, molecular, nuclear and particle physics; in our view it is also foundational to condensed matter nuclear science. It comes as a surprise that there do not appear to be review papers that discuss quantum composites. Here we consider elementary particles models, which are used to model composites; the most widely used example is that of the Dirac phenomenology for protons and neutrons. Quantum composite models can be developed from many-particle models, in some cases simply by rewriting in terms of center of mass and relative operators, and in other cases through a reduction or transformation. We have proposed models for anomalies in condensed matter nuclear science which rely heavily on the notion of a relativistic quantum composite. In the nonrelativistic case there is a clean separation of center of mass and internal degrees of freedom, so that any coupling between them must occur through external field interactions. The relativistic composite has a sizeable coupling between the center of mass motion and internal degrees of freedom, which we have proposed is responsible for the anomalies in condensed matter nuclear science. We have developed a new model in which the center of mass dynamics is modeled as nonrelativistic, but the internal structure is kept relativistic; this kind of model is much better adapted to problems in condensed matter nuclear science. Our approach has been strongly criticized, since in a Poincaré invariant theory the center of mass motion separates from the internal degrees of freedom in free space. We are able to rotate out the strongest part of this coupling in free space, consistent with Poincaré invariance. However, in the lattice the problem is in general much more complicated, and more powerful tools are required to diagonalize this relativistic coupling. The spin-boson type of models that we have considered previously for this are the simplest idealized models that can be diagonalized; they describe rich dynamics not present in the free-space version of the problem.

Keywords: Center of mass, Foldy–Wouthuysen transformation, Phonon–nuclear coupling, Quantum composite

1. Introduction

Ever since the announcement by Fleischmann and Pons of the observation of excess heat in a heavy water electrochemical experiment involving the loading of deuterium into Pd [1,2], people working in the resulting field have been

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interested in understanding how such an effect might occur. The development of condensed matter physics and nuclear physics over the previous century led to basic theories for each discipline independently, and in neither case was there any basis for understanding how nuclear energy might be released cleanly in an electrochemistry experiment. Although it is possible for a condensed matter environment to provide additional screening between deuterons not present in molecular D_2, it is hard to see how other atoms on an atomic scale might lead to unexpected interactions on a much smaller nuclear scale. And in nuclear physics there is simply no previous experimental observations that suggest a large nuclear energy quantum might result in measurable thermal energy in the absence of commensurate energetic nuclear radiation. The many subsequent experimental observations of anomalies has largely supported the claims of Fleischmann and Pons, and in addition continues to contribute to a growing list of anomalies (low-level nuclear emissions, elemental anomalies, collimated X-ray emission) suggesting that there is a major problem with our understanding of how the world works. The response of mainstream science has not been interested, sympathetic, or supportive of this line of inquiry; consequently the field has largely been decimated over the past quarter century.

In our view there are two basic theoretical issues to be faced in the development of a theory for the anomalies. The first concerns what happens to the large nuclear quanta when energy is generated, such that no commensurate energetic products are seen. If this large quantum can be down-converted, then this part of the theoretical problem can be resolved. Theories that have been put forth for the most part over the years have not addressed this issue, instead focusing on other parts of the problem. We have found a relatively simple mechanism implemented in a model involving equivalent two-level systems, a highly excited oscillator, and loss, which appears to be capable of coherent energy exchange under conditions of massive up-conversion and down-conversion [3,4]. However, for this mechanism to work there needs to be a reasonably strong coupling between vibrations (or plasmons or magnons) and the internal nuclear degrees of freedom, much stronger than conventional indirect electric and magnetic dipole interactions.

This brings us to the second of the basic theoretical issues to be faced, which involves whether there can be some new mechanism that allows for a substantial interaction between the condensed matter system on the atomic and macroscopic scales, and the internal nuclear system on the fermi scale. The strongest argument against such an effect is the absence of such an interaction in the literature in either condensed matter physics, or nuclear physics; fields which are considered at this point to be mature, and hence well-studied. The chances that such a substantial interaction has gone unnoticed over the tens of thousands of studies in the literature is epsilonic.

Nevertheless, we have proposed that such an interaction not only exists, but is required in a relativistic model based on a many-particle Dirac Hamiltonian [5]. It may be useful here to review the basic argument initially associated with the proposal. In the nonrelativistic problem there is a clean separation between the center of mass and relative degrees of freedom in free space, and the weak coupling that comes about in the presence of external fields is insufficient. In the relativistic version of the problem when the many-particle Dirac model is written in terms of center of mass and relative operators then there is an explicit coupling. The intuition at the time was that there are (relativistic) changes in the nucleus itself associated with the motion, which can be described by a superposition of rest frame states; consequently, one should expect there to be a coupling between the center of mass motion and the internal states required to modify the nuclear states to be consistent with relativity.

If so, then this solves the problem. The interaction between the center of mass and internal degrees of freedom in this relativistic interaction is much stronger than (conventional) electric or magnetic dipole coupling. Moreover, the associated phonon exchange matrix element for a $D_2/^4He$ transition based on this coupling is sufficiently large that it is consistent with the experimentally observed rate of excess heat production in the Fleischmann-Pons experiment, in a model where the down-conversion of the large quantum is not limiting the reaction rate.

This approach generally has received a large amount of criticism over the years. For example, it is generally not accepted that a large quantum can be fractionated as the models predict. It has been argued that such a down-conversion process must be of very high order so that the rate in perturbation theory is vanishingly small. Other arguments have been made that the incoherent decay involves reaction products moving away near the speed of light, which must make the incoherent channels much faster than the proposed coherent ones.

The proposal for a strong relativistic coupling has been met with a particularly devastating criticism. In this case the argument is that the proposed coupling itself doesn't exist; since in a Poincaré invariant theory the center of mass and relative degrees of freedom separate in the sense that the free space Hamiltonian can be written in the form

$$\hat{H} \;=\; \sqrt{(\hat{M}c^2)^2 + c^2|\hat{\mathbf{P}}|^2}, \tag{1}$$

where $\hat{\mathbf{P}}$ is the center of mass momentum operator, and where $\hat{M}$ is the mass operator that depends on internal degrees of freedom. According to this line of thought, there is no anomalously strong coupling as proposed, and the resulting theory is simply (and obviously) in error [6].

The original plan for the study reported in this work was to examine simple models for composites, and to make the case for the relativistic model that we have been using; there was no plan initially to respond to this devastating argument. In the process of documenting the work it seemed like a good idea to begin making a connection with the relevant literature. A colleague had suggested that it would be helpful to note that finite basis models for composites something like what we have proposed are used in the particle physics literature [6]. Since our models rely so heavily on the notion of a quantum composite, we presumed that there would be standard reviews and references that we could make use of. After some effort tracking down the relevant literature it became clear that the notion of a quantum composite is foundational to atomic, molecular, nuclear and particle physics; however, there are no review papers and no universally accepted standard references. This came as a surprise.

Consequently, it seemed to be useful to attempt to develop a systematic discussion of quantum composites. The simplest models used for composites are elementary particle models, perhaps with modifications. The most widely used model of this kind is the Dirac phenomenology for protons and neutrons. However, more complicated elementary particle models are also used, and these are certainly related to the models we have been working with.

Composite models with realistic internal structure can be developed based on many-particle Hamiltonians. In the simplest case this involves simply writing the model in terms of center of mass and relative operators; in more complicated cases reductions or transformations are involved. In retrospect the development of a systematic review for composites seems like an obvious thing to do; the resulting composite models discussed in what follows are in a sense "simple," even when they involve lots of terms.

There is a strong connection between the coupling terms we have used (for coupling between vibrations and internal nuclear degrees of freedom), and the spin–orbit interaction; this motivated us to see whether others had noticed the same coupling terms, and perhaps provide support for our approach. As it turns out quite a lot has been written about the center of mass coupling terms, but these terms have been treated differently from other interactions in the literature. Most of the papers which include a discussion of these terms are interested in the issue of Poincaré invariance, which perhaps should have been expected. Consequently, our study was expanded to include this additional topic, and associated arguments. It became clear that the coupling terms that we have focused on are present in the models as a requirement of Poincaré invariance.

What we did not expect was to be able to address the above-mentioned devastating criticism. It is clear from the literature that the coupling term we have been working with can be rotated out in free space, and we are able to construct a rotation that does this for a reasonably general potential model. However, it is not clear at all that the generalization of the rotation for nuclei in a condensed matter environment will always be helpful. Instead, the lattice problem is much harder than the free space problem, and in general will need to be analyzed with more powerful tools. The models that we have studied which show coherent energy exchange under conditions of massive up-conversion and down-conversion are idealized and simplified versions of the more general analysis that is needed.

There are quite a few other kinds of models that have used for composite systems as well; including models based on Majorana infinite component wave functions, on many-time formalisms, on a proper time formalism, and based on the Bethe-Salpeter equation. We have included a brief survey of some of these approaches. There are a very large number of works which treat composites based on field theory; in order to keep this review within a manageable scope, and also to try to make it more accessible to the diverse audience of our condensed matter nuclear science community, we have included only a minimal set of comments concerning this large body of work.

We have found it useful to exploit the finite basis approximation for detailed calculations, so this approach is described as well.

Several hundred papers have been cited in this review, which might seem to be excessive. However, as remarked above quantum composite models are fundamental to many fields and consequently widely used, which means that a large number of papers have been written which are relevant to the topics and issues discussed in this work. A more complete review of quantum composites and associated issues could easily include between one and two thousand references. In the course of writing things up, it seemed useful to cite a few of the most relevant papers, and more in the case of issues that are potentially contentious. As a result, there is much more relevant literature than what is included in the references; however, if a reader is interested in a particular topic it should be possible to track down more papers with modern search tools on a particular topic given the references included.

2. Dirac's Spin 1/2 Model and Electrons

Dirac's equation [7] was developed initially for modeling relativistic electrons, and often appears as a standard topic in textbooks. Our interest in it here is because it is widely used to model relativistic composites, specifically the proton and neutron (to be discussed subsequently). Our purpose here is both to provide a brief introduction to the model, and to examine some of the lowest-order relativistic effects.

2.1. Hamiltonian in free space

In free space we can write

$$\hat{H} \ = \ \beta mc^2 + \boldsymbol{\alpha} \cdot c\hat{\mathbf{p}}, \tag{2}$$

where β is a 4×4 matrix, and $\boldsymbol{\alpha}$ is a vector ($\boldsymbol{\alpha} \ = \ \hat{\mathbf{i}}_x\alpha_x + \hat{\mathbf{i}}_y\alpha_y + \hat{\mathbf{i}}_z\alpha_z$) of 4×4 matrices

$$\beta = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \qquad \alpha_x = \begin{bmatrix} \mathbf{0} & \sigma_x \\ \sigma_x & \mathbf{0} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix},$$

$$\alpha_y = \begin{bmatrix} \mathbf{0} & \sigma_y \\ \sigma_y & \mathbf{0} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}, \qquad \alpha_z = \begin{bmatrix} \mathbf{0} & \sigma_z \\ \sigma_z & \mathbf{0} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}. \tag{3}$$

2.2. Relativistic energy and momentum relation

The time-independent Dirac equation in free space is

$$E\psi = \beta mc^2\psi + \boldsymbol{\alpha} \cdot c\hat{\mathbf{p}}\psi, \tag{4}$$

where the wave function ψ is a 4-component vector

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}. \tag{5}$$

We can square the energy on the left and square the Hamiltonian operator on the right to obtain

$$E^2\psi = \left[(\beta mc^2)^2 + (\beta mc^2)(\boldsymbol{\alpha} \cdot c\hat{\mathbf{p}}) + (\boldsymbol{\alpha} \cdot c\hat{\mathbf{p}})(\beta mc^2) + (\boldsymbol{\alpha} \cdot c\hat{\mathbf{p}})^2 \right] \psi. \tag{6}$$

In free space the relativistic energy momentum relation of a free electron satisfies

$$E = \sqrt{(mc^2)^2 + c^2|\mathbf{p}|^2}. \tag{7}$$

For consistency we would like

$$\beta^2 = \mathbf{I}, \qquad \boldsymbol{\alpha}\beta + \beta\boldsymbol{\alpha} = 0, \qquad (\boldsymbol{\alpha} \cdot c\hat{\mathbf{p}})^2 = c^2|\hat{\mathbf{p}}|^2. \tag{8}$$

Dirac arrived at the expressions given above as a solution for these consistency relations. In Dirac's spin 1/2 model these relations are satisfied algebraically (we will find this is not the case in other models to be discussed).

2.3. Minimal coupling

Dirac proposed that the electromagnetic field could be included through the replacement

$$p_\mu \;\rightarrow\; p_\mu + eA_\mu = p_\mu - qA_\mu, \tag{9}$$

which began to be referred to as minimal coupling in the 1960s. The charge q for an electron is negative with a value of $-e$. We can rewrite this in connection with the energy and vector momentum operators as

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \;\rightarrow\; \hat{E} - q\Phi = i\hbar\frac{\partial}{\partial t} - q\Phi,$$

$$\hat{\mathbf{p}} = -i\hbar\nabla \;\rightarrow\; \hat{\mathbf{p}} - q\mathbf{A} = -i\hbar\nabla - q\mathbf{A}, \tag{10}$$

where Φ is the scalar electric potential and $\mathbf{A}$ is the vector potential which in the Coulomb gauge satisfies

$$\mathbf{E} = -\nabla\Phi - \frac{\partial}{\partial t}\mathbf{A},$$

$$\mu_0\mathbf{H} = \nabla \times \mathbf{A}. \tag{11}$$

The Dirac Hamiltonian including interactions with the electromagnetic field becomes

$$\hat{H} = \beta mc^2 + \boldsymbol{\alpha} \cdot c(\hat{\mathbf{p}} - q\mathbf{A}) + q\Phi. \tag{12}$$

2.4. Positive and negative energy sectors

Next we consider the time-independent Dirac equation for a particle in a static electric and magnetic field

$$E\psi = \beta mc^2\psi + \boldsymbol{\alpha}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})\psi + q\Phi\psi. \tag{13}$$

This eigenvalue equation describes two different energy channels that are coupled. This can be seen by expressing the 4-component wave function as

$$\psi = \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} u_\uparrow \\ u_\downarrow \\ v_\uparrow \\ v_\downarrow \end{bmatrix}, \tag{14}$$

where u and v are 2-component spinors. Plugging into the Dirac equation leads to two coupled equations

$$\begin{aligned} Eu &= mc^2 u + \boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})v + q\Phi u, \\ Ev &= -mc^2 v + \boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})u + q\Phi v. \end{aligned} \tag{15}$$

The first of these appears to describe a particle in states with positive energy mc^2, the second describes a particle in states with negative energy $-mc^2$, with coupling between the two.

2.5. Pauli reduction and nonrelativistic limit

We are interested in examining some of the lowest-order relativistic corrections of the Dirac model for the electron to the nonrelativistic limit. The spinor v associated with the negative energy sector can be written in terms of the spinor u associated with the positive energy sector according to

$$v = \frac{1}{E + mc^2 - V}\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})u. \tag{16}$$

We can use this to write a single more complicated equation for the positive energy channel alone as

$$Eu = mc^2 u + [\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})]\frac{1}{E + mc^2 - q\Phi}[\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})]u + q\Phi u. \tag{17}$$

If the potential is small compared to the mass energy we might expand the sandwiched term according to

$$\frac{1}{E + mc^2 - q\Phi} \rightarrow \frac{1}{E + mc^2} + \frac{q\Phi}{(E + mc^2)^2} + \cdots \tag{18}$$

If the energy eigenvalue is not very different from mc^2 then we might approximate further

$$\frac{1}{E + mc^2 - q\Phi} \rightarrow \frac{1}{2mc^2} + \frac{q\Phi}{4(mc^2)^2} + \cdots \tag{19}$$

With this approximation the eigenvalue equation for the positive energy channel reduces to

$$Eu = mc^2 u + [\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})] \left[\frac{1}{2mc^2} + \frac{q\Phi}{4(mc^2)^2} + \cdots\right] [\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})]u + q\Phi u. \tag{20}$$

This can be simplified to

$$(E - mc^2)u = \left\{\frac{|\hat{\mathbf{p}}|^2}{2m} + \left(q\Phi + \frac{q^2|\hat{\mathbf{A}}|^2}{2m}\right) - \frac{q}{2m}\left(\hat{\mathbf{p}}\cdot\mathbf{A} + \mathbf{A}\cdot\hat{\mathbf{p}}\right) - i\frac{(\hat{\mathbf{p}}\times q\mathbf{A} + q\mathbf{A}\times\hat{\mathbf{p}})\cdot\sigma}{2m}\right\} u$$
$$+ [\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})] \left[\frac{q\Phi}{4(mc^2)^2} + \cdots\right] [\boldsymbol{\sigma}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})]u. \tag{21}$$

On the right hand side we recognize the nonrelativistic kinetic energy operator $|\hat{\mathbf{p}}|^2/2m$ as well as terms corresponding to the electrostatic potential $q\Phi$ and ponderomotive potential $q^2|\hat{\mathbf{A}}|^2/2m$. We see a term normally used for the interaction with the transvere electromagnetic radiation field

$$\hat{H}_{\text{int}} = -\frac{q}{2m}\left(\hat{\mathbf{p}}\cdot\mathbf{A} + \mathbf{A}\cdot\hat{\mathbf{p}}\right). \tag{22}$$

2.6. Magnetic dipole interaction

The next term accounts for the magnetic dipole interaction

$$-i\frac{(\hat{\mathbf{p}}\times q\mathbf{A} + q\mathbf{A}\times\hat{\mathbf{p}})\cdot\sigma}{2m} = -\frac{\hbar q}{2m}\sigma\cdot\nabla\times\mathbf{A} = -\hat{\boldsymbol{\mu}}_s\cdot\mathbf{B}, \tag{23}$$

where the magnetic dipole operator in Dirac's model is

$$\hat{\boldsymbol{\mu}}_s = \frac{\hbar q}{2m}\boldsymbol{\sigma} = \frac{q}{m}\hat{\mathbf{s}} = -\frac{e}{m}\hat{\mathbf{s}}. \tag{24}$$

Dirac's model for the electron yields a magnetic dipole interaction which is very close to experiment; we can write

$$\hat{\boldsymbol{\mu}}_s = -g_s\frac{e}{2m}\hat{\mathbf{s}}, \tag{25}$$

where from Dirac's mode $g_s = 2$ and from the NIST reference on fundamental constants

$$g_s = 2.00231930436182. \tag{26}$$

We regard the magnetic dipole interaction in this discussion as the lowest-order relativistic effect involving the vector potential not included in $\hat{H}_{\text{int}}$. If we are interested in how well a relativistic model describes a particle or composite, the magnetic dipole interaction provides a good test.

2.7. Spin–orbit interaction

The reduction of the terms in the second line of Eq. (21) produces a great many terms and corresponding effects; one of them is the spin–orbit term in a central field potential

$$\hat{H}_{\rm SO} = \frac{q}{2m^2c^2}\frac{1}{r}\frac{{\rm d}\Phi}{{\rm d}r}\hat{\mathbf{L}}\cdot\hat{\mathbf{s}} \tag{27}$$

with $q = -e$. Our interest in this discussion is focused on this term as one of the lowest-order relativistic effects involving the scalar potential.

3. Dirac Spin 1/2 Models for the Proton and Neutron

The proton and neutron are composite particles with spin 1/2; however, the Dirac equation is routinely used to model them both. This seems useful to us for a variety of reasons: both composites are well studied; corrections to the Dirac model are recognized; the structure of the nucleon as a composite has been studied.

3.1. Magnetic dipole interaction

Both the proton and neutron have magnetic moments that differ from the Dirac model. For the proton we can write

$$\hat{\boldsymbol{\mu}}_s = \frac{g_{\rm p}e}{2M_{\rm p}}\hat{\mathbf{s}} \tag{28}$$

with the NIST listed value of $g_{\rm p} = 5.585694702$ (the Dirac model would predict a value of 2). For the neutron we have

$$\hat{\boldsymbol{\mu}}_s = \frac{g_{\rm n}e}{2M_{\rm n}}\hat{\mathbf{s}} \tag{29}$$

with the NIST listed value of $g_{\rm n} = -3.82608545$ (the Dirac model would predict a value of 0).

The lowest-order relativistic effect involving the transverse electromagnetic field is the magnetic dipole interaction. For both the proton and neutron the basic Dirac spin 1/2 model results in a magnetic dipole interaction which is not in good agreement with experiment.

3.2. Pauli interaction Hamiltonian

Pauli proposed a covariant interaction that describes coupling between an anomalous magnetic moment and the radiation field [8,9], which has been widely used subsequently in addition to minimal coupling to describe proton interactions with photons [10–13]. The associated interaction Hamiltonian can be written as

$$\begin{aligned}\hat{H}_{\rm Pauli} &= \left(\frac{g_{\rm p}}{2}-1\right)\frac{e\hbar}{2M_{\rm p}}\begin{bmatrix} -(\boldsymbol{\sigma}\cdot\mathbf{B}) & i(\boldsymbol{\sigma}\cdot\mathbf{E}) \\ -i(\boldsymbol{\sigma}\cdot\mathbf{E}) & (\boldsymbol{\sigma}\cdot\mathbf{B})\end{bmatrix} \\ &= -\left(\frac{g_{\rm p}}{2}-1\right)\frac{e\hbar}{2M_{\rm p}}\beta\bigg(\boldsymbol{\sigma}\cdot\mathbf{B} - i\boldsymbol{\alpha}\cdot\mathbf{E}\bigg).\end{aligned} \tag{30}$$

In the nonrelativistic limit this model results in a magnetic dipole interaction that agrees with experiment, and a spin–orbit coupling term with the proton magnetic moment

$$\hat{H}_{\rm SO} = \frac{(g_{\rm p}-1)e}{2m^2c^2}\frac{1}{r}\frac{{\rm d}\Phi}{{\rm d}r}\hat{\mathbf{L}}\cdot\hat{s}. \tag{31}$$

The Lagrangian associated with the Pauli interaction appears in many papers [14,15].

3.3. Dirac–Pauli Hamiltonian for the proton

The resulting Dirac–Pauli Hamiltonian is

$$\hat{H} = \beta M_{\rm p}c^2 + \boldsymbol{\alpha}\cdot c(\hat{\mathbf{p}} - e\mathbf{A}) - \left(\frac{g_{\rm p}}{2}-1\right)\frac{e\hbar}{2M_{\rm p}}\beta\left(\boldsymbol{\sigma}\cdot\mathbf{B} - i\boldsymbol{\alpha}\cdot\mathbf{E}\right). \tag{32}$$

This model describes a spin 1/2 particle with an additional (anomalous) magnetic dipole moment, and coupling to the electromagnetic field through minimal (Dirac) coupling and through the Pauli interaction. The anomalous spin in this model is an added magnetic dipole unconnected with the relativistic kinetic energy part of the Hamiltonian, while there is a magnetic dipole moment in addition present due to the spin 1/2 that is a consequence of the relativistic kinetic energy part of the Hamiltonian.

Nonrelativistic Hamiltonians derived from the Dirac–Pauli Hamiltonian have been discussed in [16–18].

3.4. Proton Compton scattering below the pion threshold

The interaction of light with protons can be studied experimentally in scattering experiments with gamma rays. Elastic scattering of gammas and protons occurs below the threshold for pion production ($m_{\pi^\pm}c^2 = 139.57$ MeV, and $m_{\pi^0}c^2 = 134.98$ MeV), which is very closely related to elastic scattering between gammas and electrons below the pair production threshold [19]. In this case it is possible to use standard diagrammatic methods to compute the scattering cross section, leading to results algebraically similar at low order to those obtained in electron Compton scattering. Proton Compton scattering has been frequently reviewed [20–22].

In early proton Compton experiments that explored the dependence of the cross section on the scattering angle, minor deviations were found relative to predictions based on Dirac (minimal coupling) and Pauli photon interactions [23]; these were attributed to the polarizability of the proton. It is possible to extract accurate estimates for the polarizability of the proton from experiment [24–27], which can be compared to theoretical models [28–30] and nucleon models [31–33].

At higher energy an additional correction to the Dirac and Pauli interactions needs to be included to take into account the fact that the proton is not a point particle. This is done through the introduction of form factors [34,35].

The situation becomes more complicated above the pion threshold, where additional physics is required to model pion production. At even higher energies excitation of the proton to internal excited states is possible, which complicates things further.

The good agreement between the Dirac spin 1/2 model (with relatively minor corrections) for the proton in connection with proton Compton scattering below the pion threshold provides confidence in the model.

3.5. Dirac–Pauli equation for the neutron

The Dirac equation is widely used to model neutrons as well. Since the neutron has no net electric charge, there is no Dirac minimal coupling present. Since the neutron has an anomalous magnetic moment, it would be appropriate to include the Pauli interaction. The resulting Dirac equation is [36–38]

$$\hat{H} = \boldsymbol{\alpha} \cdot c\hat{\mathbf{p}} + \beta M_{\rm n} c^2 - \left(\frac{g_{\rm n}}{2}\right) \frac{e\hbar}{2M_{\rm n}} \beta \bigg(\boldsymbol{\sigma} \cdot \mathbf{B} - i\boldsymbol{\alpha} \cdot \mathbf{E} \bigg). \tag{33}$$

Li et al. [15] have discussed a neutron Dirac equation that models an electric dipole moment; however, experiments so far have not detected one [39,40].

3.6. Dirac phenomenology for nuclear models

A major application of Dirac spin 1/2 models for neutrons and protons is for the computation of nuclear structure and reaction processes [41–44]. These models have proven to be very successful when combined with modern nucleon–nucleon interaction models [45].

4. Higher Spin Models

In this section we are interested in relativistic models for elementary particles with a spin greater than 1/2, and the application of these models to composite systems (higher spin baryons). There is a very substantial associated literature, most of which is not well known outside of particle physics. Our purpose here is not to provide a systematic review; instead we would like to focus on a small number of basic issues appropriate to an introduction for the nonspecialist, and discuss briefly the application to composite systems. We will focus mostly on the spin 3/2 case since this is more interesting, and there are more papers; but we will point out some applications of a spin 1 model.

4.1. Spin 3/2 model of Dirac

Dirac was one of the first to consider the development of wave equations for higher spin systems [46]. He argued that such equations could be constructed from wave equations much like the spin 1/2 case, but with more indices. In the spin 3/2 case the resulting wave equation is written in a form probably not appropriate for the discussion; however, with some work we can write it in the much less elegant form

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} A^{\dot{\beta}}_{1\lambda} \\ A^{\dot{\beta}}_{2\lambda} \\ B^{\dot{1}\dot{\beta}}_{\lambda} \\ B^{\dot{2}\dot{\beta}}_{\lambda} \end{bmatrix} = mc^2 \begin{bmatrix} 0\,0\,1\,0 \\ 0\,0\,0\,1 \\ 1\,0\,0\,0 \\ 0\,1\,0\,0 \end{bmatrix} \begin{bmatrix} A^{\dot{\beta}}_{1\lambda} \\ A^{\dot{\beta}}_{2\lambda} \\ B^{\dot{1}\dot{\beta}}_{\lambda} \\ B^{\dot{2}\dot{\beta}}_{\lambda} \end{bmatrix} + c \begin{bmatrix} \hat{p}_z & \hat{p}_x + i\hat{p}_y & 0 & 0 \\ \hat{p}_x - i\hat{p}_y & -\hat{p}_z & 0 & 0 \\ 0 & 0 & -\hat{p}_z & -(\hat{p}_x + i\hat{p}_y) \\ 0 & 0 & -(\hat{p}_x - i\hat{p}_y) & \hat{p}_z \end{bmatrix} \begin{bmatrix} A^{\dot{\beta}}_{1\lambda} \\ A^{\dot{\beta}}_{2\lambda} \\ B^{\dot{1}\dot{\beta}}_{\lambda} \\ B^{\dot{2}\dot{\beta}}_{\lambda} \end{bmatrix}. \tag{34}$$

The appearance of dotted indices is important to the notation used by Dirac, which helps to keep track of which indices are raised in the different components. The indices $\dot{\beta}$ and λ each go between 1 and 2, so this wave equation is for a 16-component system. The eigenvalues for the associated Hamiltonian are

$$E = \pm\sqrt{(2mc^2)^2 + c^2|\hat{\mathbf{p}}|^2}. \tag{35}$$

Dirac argued that by imposing a symmetry condition on the components such that $A^{\dot{\beta}}_{12} = A^{\dot{\beta}}_{21}$ and $B^{\dot{1}\dot{2}}_{\lambda} = B^{\dot{2}\dot{1}}_{\lambda}$, it was possible to obtain a 12-component wave equation for a spin 3/2 system.

Dirac proposed to make use of minimal coupling to include interactions with the radiation field.

4.2. Dirac–Fierz–Pauli spin 3/2 model in free space

This was pursued by Fierz and Pauli [47], who considered both spin 3/2 and spin 2 wave equations. In the spin 3/2 case the free-space Hamiltonian was written in a compact notation that we have avoided, which with some effort we can rewrite in the form

$$\hat{H} = mc^2\beta + \boldsymbol{\alpha} \cdot c\hat{\mathbf{p}} \tag{36}$$

with the following definitions for the 12×12 $\boldsymbol{\alpha}$ and β matrices

$$\beta = \left[\begin{array}{cccccc|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right], \qquad
\alpha_x = \left[\begin{array}{cccccc|cccccc}
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{array}\right],$$

$$\alpha_y = i\left[\begin{array}{cccccc|cccccc}
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{array}\right], \qquad
\alpha_z = \left[\begin{array}{cccccc|cccccc}
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1
\end{array}\right] \tag{37}$$

in connection with a wave function of the form

$$\psi = \begin{bmatrix} a_{11}^{\dot{1}} \\ a_{11}^{\dot{2}} \\ a_{12}^{\dot{1}} \\ a_{12}^{\dot{2}} \\ a_{22}^{\dot{1}} \\ a_{22}^{\dot{2}} \\ b_1^{\dot{1}\dot{1}} \\ b_2^{\dot{1}\dot{1}} \\ b_1^{\dot{1}\dot{2}} \\ b_2^{\dot{1}\dot{2}} \\ b_1^{\dot{2}\dot{2}} \\ b_2^{\dot{2}\dot{2}} \end{bmatrix}, \tag{38}$$

where the $a^{\dot{\alpha}}_{\rho\gamma}$ and $b^{\dot{\rho}\dot{\gamma}}_{\beta}$ components correspond to the definitions of Fierz and Pauli. The Dirac–Fierz–Pauli spin 3/2 model is not written out in this form explicitly in the literature, in part because this form is not useful for understanding the important properties of the model; however, it is useful in the context of our discussion since we can see what the model looks like; and because it provides and example of a many-component Dirac equation that is of a form somewhat similar to what we will encounter much later in this paper when we discuss the finite basis approximation for more complicated composites.

The eigenvalues of this Hamiltonian are

$$E = \pm\sqrt{(mc^2)^2 + c^2|\mathbf{p}|^2}, \pm\sqrt{(2mc^2)^2 + c^2|\mathbf{p}|^2}. \tag{39}$$

There are eight eigenvalues with mass $\pm m$ and four with mass $\pm 2m$. The set of eight are connected with a spin 3/2 particle, and the other set of four describe a spin 1/2 particle; to describe a spin 3/2 particle with mass m the part of the solution that is for the mass $2m$ spin 1/2 particle must be eliminated. This is accomplished through compact constraints (which eliminate antisymmetric solutions) that Fierz and Pauli found; which we can rewrite in the form

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} a_{11}^{\dot{1}} \\ a_{11}^{\dot{2}} \\ a_{12}^{\dot{1}} \\ a_{12}^{\dot{2}} \\ a_{22}^{\dot{1}} \\ a_{22}^{\dot{2}} \end{bmatrix} = -c\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -(p_x - ip_y) & p_z & p_z & p_x + ip_y & 0 & 0 \\ 0 & 0 & -(p_x - ip_y) & p_z & p_z & p_x + ip_y \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} a_{11}^{\dot{1}} \\ a_{11}^{\dot{2}} \\ a_{12}^{\dot{1}} \\ a_{12}^{\dot{2}} \\ a_{22}^{\dot{1}} \\ a_{22}^{\dot{2}} \end{bmatrix}, \tag{40}$$

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} b_1^{\dot{1}\dot{1}} \\ b_2^{\dot{1}\dot{1}} \\ b_1^{\dot{1}\dot{2}} \\ b_2^{\dot{1}\dot{2}} \\ b_1^{\dot{2}\dot{2}} \\ b_2^{\dot{2}\dot{2}} \end{bmatrix} = -c\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ -(p_x - ip_y) & p_z & p_z & p_x + ip_y & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -(p_x - ip_y) & p_z & p_z & p_x + ip_y \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} b_1^{\dot{1}\dot{1}} \\ b_2^{\dot{1}\dot{1}} \\ b_1^{\dot{1}\dot{2}} \\ b_2^{\dot{1}\dot{2}} \\ b_1^{\dot{2}\dot{2}} \\ b_2^{\dot{2}\dot{2}} \end{bmatrix}. \tag{41}$$

A further discussion of this model can be found in [48].

4.3. Coupling with the electromagnetic field

Dirac proposed that minimal coupling could be used to describe interactions with the electromagnetic field [46]. This implies a higher-spin Hamiltonian of the form

$$\hat{H} = mc^2\beta + \boldsymbol{\alpha} \cdot c(\hat{\mathbf{p}} - q\mathbf{A}) + q\Phi. \tag{42}$$

Pauli and Fierz showed that adding minimal coupling in this way led to an inconsistency. The resolution of this involved adding additional fields (two simple spinor fields c_α and $d^{\dot{\beta}}$) to develop a Lagrangian, from which wave equations and constraints could be developed; both without an electromagnetic field present (in which case the additional fields are constrained to vanish), and also with an electromagnetic field present (where they do not). In this case minimal coupling with the electromagnetic field requires additional degrees of freedom to be added to the wave equation for the model to be consistent.

4.4. Rarita–Schwinger spin 3/2 model in free space

Rarita and Schwinger developed a Lagrangian for a spin 3/2 elementary particle [49], from which follows the wave equation

$$i\hbar\frac{\partial}{\partial t}\Psi_\mu = \beta mc^2\Psi_\mu + \boldsymbol{\alpha} \cdot c\hat{\mathbf{p}}\Psi_\mu, \tag{43}$$

where Ψ_μ is a 4-vector made up of spinors, so that there are 16 complex elements (the μ index refers to the 4-vector construction, and the spinor index is suppressed). The β and $\boldsymbol{\alpha}$ matrices in this equation operate on the (suppressed) spinor indices, so that this equation implies four sets of 4×4 matrix equations, or 16 equations in all.

We can think of this as a direct product of a spin 1/2 spinor and a vector with spin 0 and spin 1, which we would expect to lead to spin 1/2 and spin 3/2 components; we might write for the rest frame [50]

$$\frac{1}{2} \otimes (0+1) = \frac{1}{2} + \frac{1}{2} + \frac{3}{2}. \tag{44}$$

The Rarita–Schwinger wave function has 16 elements (and hence 16 degrees of freedom in this context); only eight degrees of freedom are required for the spin 3/2 part of Ψ_μ, and consequently eight constraints are needed to eliminate the two spin 1/2 degrees of freedom. These constraints follow from their Lagrangian, and are usually written compactly as [51]

$$\gamma^\mu\Psi_\mu = 0, \tag{45}$$

$$\partial^\mu\Psi_\mu = 0. \tag{46}$$

4.5. Free-space Hamiltonian with eight degrees of freedom

A free-space Hamiltonian for an 8-component wavefunction specific to the spin 3/2 degrees of freedom (associated with the Rarita–Schwinger model, and also the Dirac–Pauli–Fierz model) was constructed by Moldauer and Case [52]; this Hamiltonian is nonlinear in the momentum. It can be written as

$$\hat{H} = mc^2 \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{bmatrix} \left(1 + \frac{1}{2} \frac{|\hat{\mathbf{p}}|^2 - (\mathbf{\Sigma}_{3/2} \cdot \hat{\mathbf{p}})^2}{\frac{4}{9}|\hat{\mathbf{p}}|^2 + (mc)^2} \right) + \begin{bmatrix} \mathbf{0} & \mathbf{\Sigma}_{3/2} \cdot c\hat{\mathbf{p}} \\ \mathbf{\Sigma}_{3/2} \cdot c\hat{\mathbf{p}} & \mathbf{0} \end{bmatrix} \left(1 + \frac{|\hat{\mathbf{p}}|^2 - (\mathbf{\Sigma}_{3/2} \cdot \hat{\mathbf{p}})^2}{\frac{4}{9}|\hat{\mathbf{p}}|^2 + (mc)^2} \right) \tag{47}$$

with

$$(\Sigma_{3/2})_x = \begin{bmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{3} & 0 \\ 0 & \frac{2}{3} & 0 & \frac{1}{\sqrt{3}} \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \end{bmatrix}, \quad (\Sigma_{3/2})_y = i \begin{bmatrix} 0 & -\frac{1}{\sqrt{3}} & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & -\frac{2}{3} & 0 \\ 0 & \frac{2}{3} & 0 & -\frac{1}{\sqrt{3}} \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \end{bmatrix}, \quad (\Sigma_{3/2})_z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \tag{48}$$

where the $\mathbf{\Sigma}_{3/2}$ matrices here are recognized as spin 3/2 generalizations of the $\boldsymbol{\sigma}$ matrices. The eigenvalues are

$$E = \pm\sqrt{(mc^2)^2 + c^2|\mathbf{p}|^2}. \tag{49}$$

We can see from this an interesting feature of the Rarita–Schwinger model. When all 16 degrees of freedom are included the associated Hamiltonian is linear in the momentum; however, the implementation of constraints that remove the spin 1/2 degrees of freedom lead to a more complicated model for the degrees of freedom that remain.

4.6. Minimal coupling

Minimal coupling is often used in connection with the Rarita–Schwinger model, which is implemented using a higher-spin wave equation of the form

$$i\hbar\frac{\partial}{\partial t}\Psi_\mu = \beta mc^2\Psi_\mu + \boldsymbol{\alpha}\cdot c(\hat{\mathbf{p}} - q\mathbf{A})\Psi_\mu + q\Phi\Psi_\mu. \tag{50}$$

The nonrelativistic limit of the model is discussed by Moldauer and Case, and also in [53]; the Foldy–Wouthuysen transformation is considered in [54].

Massive higher-spin models in general seem to suffer from all kinds of maladies. Johnson and Sudarshan showed that an inconsistency in the commutation relations appeared when higher spin models are quantized [55]. Velo and Zwanziger showed that wave propagation faster than the speed of light occurs for the coupled electromagnetic and Rarita–Schwinger system [56]. There are issues with causality associated with the constraints [57]. Further discussion of these issues can be found in [58–62]. There has been much interest in the possibility of developing an acceptable field theory for spin 3/2 models that continues up to the present day [63–66]. In a recent paper by Adler [67] it is suggested that a suitable field theory for the massless case can be constructed, and that mass can be brought in afterward through a Higgs coupling.

4.7. Higher spin models used for modeling composites

Our interest in these models in this section is motivated by their application to physical composite systems. For example, the Rarita–Schwinger model has been used early on for excited states of the nucleon [68–70], for the $\Delta(1232)$ and other baryon resonances [71–73]. Elementary spin 1 models have been used for modeling the deuteron as a composite in collisions with heavier nuclei [74–76].

5. Bargmann–Wigner Models and Applications

Following the introduction of the quark model in 1964 [77] there was great interest in developing simple models for mesons and baryons based on collinear propagating quarks. These early models were based a the Bargmann–Wigner construction, which was developed to describe elementary particles with higher spin. Consistent with the discussion in Section 4, this provides us with examples of models for composite systems based on wave equations for elementary particles.

5.1. Simple product wave function model

Since our discussion here is introductory, the place to start may be with a simple product approximation (which is very much not what Bargmann and Wigner started with). Consider the construction of a simple product wave function written as

$$\Psi_{\mu_1,\ldots,\mu_N}(\mathbf{r}_1,t_1,\ldots,\mathbf{r}_N,t_N) = \psi_{\mu_1}(\mathbf{r}_1,t_1)\cdots\psi_{\mu_N}(\mathbf{r}_N,t_N), \tag{51}$$

where each single particle wave function satisfies

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \beta mc^2\psi(\mathbf{r},t) + \boldsymbol{\alpha}\cdot c\hat{\mathbf{p}}\psi(\mathbf{r},t). \tag{52}$$

The subscripts μ_j are spinor subscripts associated with particle j, with associated space-time coordinates $\mathbf{r}_j, t_j$. It would follow that the product wave function satisfies a set of wave equations of the form

$$\left[i\hbar\frac{\partial}{\partial t_1} - \beta mc^2 - \boldsymbol{\alpha}\cdot c\hat{\mathbf{p}}_1\right]_{\mu_1,\nu_1}\Psi_{\nu_1,\cdots,\mu_N}(\mathbf{r}_1,t_1,\ldots,\mathbf{r}_N,t_N) = 0,$$

$$\vdots$$

$$\left[i\hbar\frac{\partial}{\partial t_N} - \beta mc^2 - \boldsymbol{\alpha}\cdot c\hat{\mathbf{p}}_N\right]_{\mu_N,\nu_N}\Psi_{\mu_1,\cdots,\nu_N}(\mathbf{r}_1,t_1,\ldots,\mathbf{r}_N,t_N) = 0. \tag{53}$$

We might think of this as a Dirac equation for each particle individually, with all of the other particle wave functions simply multiplying the one acted upon by the Dirac operator.

5.2. Bargmann–Wigner model

If we start with the simple model above, and then require that spatial coordinates of all of the particles are the same

$$\mathbf{r}_1 \;\rightarrow\; \mathbf{r} \quad \cdots \quad \mathbf{r}_N \;\rightarrow\; \mathbf{r} \tag{54}$$

and similarly for the time coordinates

$$t_1 \;\rightarrow\; t \quad \cdots \quad t_N \;\rightarrow\; t, \tag{55}$$

we would end up with a model that describes noninteracting particles that travel together. The wave function in this case would satisfy a set of wave equations of the form

$$\left[i\hbar\frac{\partial}{\partial t} - \beta mc^2 - \boldsymbol{\alpha}\cdots c\hat{\mathbf{p}}\right]_{\mu_1,\nu_1} \Psi_{\nu_1,\dots,\mu_N}(\mathbf{r},t) = 0,$$

$$\vdots$$

$$\left[i\hbar\frac{\partial}{\partial t} - \beta mc^2 - \boldsymbol{\alpha}\cdot c\hat{\mathbf{p}}\right]_{\mu_N,\nu_N} \Psi_{\mu_1,\dots,\nu_N}(\mathbf{r},t) = 0. \tag{56}$$

This provides a nonrigorous argument for the Bargmann–Wigner model.

It is possible to add additional structure to the model. For example, if the particles are identical then we would adopt initially an anti-symmetric wave function

$$\Psi_{\mu_1,\dots,\mu_N}(\mathbf{r}_1,t_1,\dots,\mathbf{r}_N,t_N) = \mathcal{A}\left\{\psi_{\mu_1}(\mathbf{r}_1,t_1)\cdots\psi_{\mu_N}(\mathbf{r}_N,t_N)\right\} \tag{57}$$

Doing so leads to a Bargmann–Wigner wave function that is antisymmetric in the spinor indices

$$\Psi_{\dots,\mu_r,\dots,\mu_s,\dots}(\mathbf{r},t) = -\Psi_{\dots,\mu_s,\dots,\mu_r,\dots}(\mathbf{r},t). \tag{58}$$

We might also be interested in a superposition of product wave functions in order to describe some group of interest; doing so leads to an imposition of the same group structure in the Bargmann–Wigner wave function.

5.3. Application to SU(6)

Perhaps the most important application of the Bargmann–Wigner model was in connection with QCD when first developed. Bargmann–Wigner wave functions adapted to SU(6) were proposed to for simple models describing mesons and baryons as collinear noninteracting quarks [79–81] following the development of the quark model. These were used with success to describe interactions between baryons and mesons [82]

5.4. Bargmann–Wigner Hamiltonian

Because of the need for a covariant description in particle physics generally, one does not often encounter a Hamiltonian for the Bargmann–Wigner model. Nevertheless, the associated arguments are straightforward, and it is of interest in this discussion to pursue the issue. We might consider a wave function made up of a product of single particle wave functions in a Hamiltonian type of model according to

$$\Psi_{\mu_1,\dots,\mu_N}(\mathbf{r}_1,\dots,\mathbf{r}_N,t) = \psi_{\mu_1}(\mathbf{r}_1,t)\cdots\psi_{\mu_N}(\mathbf{r}_N,t), \tag{59}$$

where the single particle wave functions satisfy

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \beta mc^2\psi(\mathbf{r},t) + \boldsymbol{\alpha}\cdot c\hat{\mathbf{p}}\psi(\mathbf{r},t). \tag{60}$$

Associated with the many-particle product wave function above is a separable free space Hamiltonian of the form

$$\hat{H} = \beta_1 mc^2 + \boldsymbol{\alpha}_1 \cdot c\hat{\mathbf{p}}_1 + \cdots + \beta_N mc^2 + \boldsymbol{\alpha}_N \cdot c\hat{\mathbf{p}}_N. \tag{61}$$

We can define the total momentum

$$\hat{\mathbf{P}} = \hat{\mathbf{p}}_1 + \cdots + \hat{\mathbf{p}}_N \tag{62}$$

and relative momenta defined according to

$$\hat{\boldsymbol{\pi}}_1 = \hat{\mathbf{p}}_1 - \frac{\hat{\mathbf{P}}}{N} \quad \cdots \quad \hat{\boldsymbol{\pi}}_N = \hat{\mathbf{p}}_N - \frac{\hat{\mathbf{P}}}{N}. \tag{63}$$

Although we have defined N relative momenta here, there are only $N-1$ independent operators since

$$\hat{\boldsymbol{\pi}}_1 + \cdots + \hat{\boldsymbol{\pi}}_N = 0. \tag{64}$$

The free space Hamiltonian above can then be written as

$$\hat{H} = (\beta_1 + \cdots + \beta_N)mc^2 + \frac{1}{N}(\boldsymbol{\alpha}_1 + \cdots + \boldsymbol{\alpha}_N) \cdot c\hat{\mathbf{P}} + \boldsymbol{\alpha}_1 \cdot c\hat{\boldsymbol{\pi}}_1 + \cdots + \boldsymbol{\alpha}_N \cdot c\hat{\boldsymbol{\pi}}_N. \tag{65}$$

Now if we presume collinear propagation, such that the relative momenta can be neglected

$$\hat{\boldsymbol{\pi}}_j \;\rightarrow\; 0, \tag{66}$$

we end up with

$$\hat{H} = (\beta_1 + \cdots + \beta_N)mc^2 + \frac{1}{N}(\boldsymbol{\alpha}_1 + \cdots + \boldsymbol{\alpha}_N) \cdot c\hat{\mathbf{P}}. \tag{67}$$

This we recognize as a Hamiltonian for the Bargmann–Wigner model. This kind of Hamiltonian has been used in recent years for the high-spin Dirac oscillator [83] and applications [84,85]. The eigenvalues of this Hamiltonian are

$$E = \begin{cases} \sqrt{(Mc^2)^2 + c^2|\mathbf{P}|^2}, \\ \dfrac{N-2}{N}\sqrt{(Mc^2)^2 + c^2|\mathbf{P}|^2}, \\ \vdots \\ -\sqrt{(Mc^2)^2 + c^2|\mathbf{P}|^2}. \end{cases} \tag{68}$$

This is understood simply as a consequence of each constituent particle having the possibility of being in the positive energy sector or negative energy sector.

5.5. Square of the Hamiltonian

We recall that the square of the spin 1/2 Dirac Hamiltonian satisfies

$$\left(\beta mc^2 + \boldsymbol{\alpha} \cdot c\hat{\mathbf{p}}\right)^2 = (mc^2)^2 + c^2|\hat{\mathbf{p}}|^2 \tag{69}$$

as an algebraic identity. We are interested in whether the many-particle Hamiltonian above satisfies a similar relation. We might write the associated Hamiltonian in the form

$$\hat{H} = \mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \tag{70}$$

with

$$\mathbf{M}c^2 = (\beta_1 + \cdots + \beta_N)mc^2, \tag{71}$$

$$\mathbf{a} \cdot c\hat{\mathbf{P}} = \frac{1}{N}(\boldsymbol{\alpha}_1 + \cdots + \boldsymbol{\alpha}_N) \cdot c\hat{\mathbf{P}}. \tag{72}$$

The square of the Hamiltonian is

$$\hat{H} = (\mathbf{M}c^2)^2 + (\mathbf{M}c^2)(\mathbf{a} \cdot c\hat{\mathbf{P}}) + (\mathbf{a} \cdot c\hat{\mathbf{P}})(\mathbf{M}c^2) + (\mathbf{a} \cdot c\hat{\mathbf{P}})^2. \tag{73}$$

It can be verified that

$$\mathbf{M}\mathbf{a} + \mathbf{a}\mathbf{M} \neq 0 \tag{74}$$

and

$$(\mathbf{a} \cdot c\hat{\mathbf{P}})^2 \neq c^2|\hat{\mathbf{P}}|^2. \tag{75}$$

This is in contrast to what we had proposed previously [5]. Instead, the eigenfunctions $\Psi_{\mathbf{P}}$ of the Hamiltonian with momentum $\mathbf{P}$ satisfy

$$\left(\mathbf{M}\mathbf{a} + \mathbf{a}\mathbf{M}\right)\Psi_{\mathbf{P}} = 0. \tag{76}$$

$$(\mathbf{a} \cdot c\hat{\mathbf{P}})^2\Psi_{\mathbf{P}} = c^2|\hat{\mathbf{P}}|^2\Psi_{\mathbf{P}}. \tag{77}$$

5.6. A 20-component free space model for nucleons

The proton and neutron are made up of three quarks, so the models outline above could be relevant in the case of $N = 3$, where the free space wave function would have $4^3 = 64$ components. However, it is possible to isolate the part of the symmetric group that is relevant, which leads to a 20-component wave function. We consider first the basic symmetric group construction for an anti-symmetric three-particle state with spatial (R), flavor (F), spin (S) and color (C) degrees of freedom; the antisymmetric wavefunction can be written in terms of Yamanouchi symbols as [86,87]

$$[3\ 2\ 1]_{\mathrm{RFSC}} = [1\ 1\ 1]_{\mathrm{R}}[1\ 1\ 1]_{\mathrm{FS}}[3\ 2\ 1]_{\mathrm{C}}. \tag{78}$$

We would expect the lowest energy spatial wavefunction of a three quark system to be fully symmetric ($[1\ 1\ 1]_{\mathrm{R}}$); and the nucleon as a three-quark system is modeled as a color singlet [88] ($[3\ 2\ 1]_{\mathrm{C}}$). Consequently the flavor and spin function must be fully symmetric ($[1\ 1\ 1]_{\mathrm{FS}}$). Since there are no strange quarks involved, we are able to use a construction of the flavor part of the problem in SU(2). This can be expanded out as

$$[1\ 1\ 1]_{\mathrm{FS}} = \frac{1}{\sqrt{2}}([1\ 2\ 1]_{\mathrm{F}}[1\ 2\ 1]_{\mathrm{S}} + [2\ 1\ 1]_{\mathrm{F}}[2\ 1\ 1]_{\mathrm{S}}), \tag{79}$$

which is consistent with [89]. Note that it would be possible mathematically to form $[1\ 1\ 1]_{\mathrm{FS}}$ according to

$$[1\ 1\ 1]_{\mathrm{FS}} = [1\ 1\ 1]_{\mathrm{F}}[1\ 1\ 1]_{\mathrm{S}} \tag{80}$$

but this in inconsistent with protons and neutrons as the associated spin would be 3/2 (neutron and proton spins are 1/2), and would lead to flavor quartet states (neutrons and protons are flavor doublets). In the end we can write

$$[3\ 2\ 1]_{\mathrm{RFSC}} = [1\ 1\ 1]_{\mathrm{R}}\left(\frac{[1\ 2\ 1]_{\mathrm{F}}[1\ 2\ 1]_{\mathrm{S}} + [2\ 1\ 1]_{\mathrm{F}}[2\ 1\ 1]_{\mathrm{S}}}{\sqrt{2}}\right)[3\ 2\ 1]_{\mathrm{C}}. \tag{81}$$

We can identify two spins for a single Dirac free particle wave function, as well as positive and negative energy components. The spin degree of freedom is described by SU(2). However, in what follows we are going to be interested in the positive and negative energy degrees of freedom as well, which can also be modeled using SU(2). The generalization of the construction above to include the different energy sectors is straightforward; we may write

$$[3\ 2\ 1]_{\mathrm{RFSTC}} = [1\ 1\ 1]_{\mathrm{R}}\left(\frac{[1\ 2\ 1]_{\mathrm{F}}[1\ 2\ 1]_{\mathrm{ST}} + [2\ 1\ 1]_{\mathrm{F}}[2\ 1\ 1]_{\mathrm{ST}}}{\sqrt{2}}\right)[3\ 2\ 1]_{\mathrm{C}}, \tag{82}$$

where T refers to positive or negative energy sector.

Although this construction looks to be a completely straightforward generalization of the basic symmetric group construction above, there are some issues which are worth thinking about. At issue is what happens when the center of mass moves, or is accelerated. There can be no change in the color or flavor from a boost, so we expect the corresponding parts of the wavefunction to remain invariant. Less obvious is what happens to the spatial part of the wavefunction. After some thought, we recognize that in the simple model under construction there is no modification of the relative part of the problem when the center of mass moves since the free space Hamiltonian is totally symmetric ([1 1 1]). Hence if the relative spatial wavefunction is initially in a fully symmetric state, it remains in a fully symmetric states in the different energy sectors in this model.

Consequently, the only thing that happens is that there is a coupling between the spin degrees of freedom, and the positive and negative energy state degree of freedom.

The relevant Hamiltonian for the three noninteracting quarks of the model is

$$\hat{H} = \Big(\beta_1 + \beta_2 + \beta_3\Big) mc^2 + \left(\frac{\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2 + \boldsymbol{\alpha}_3}{3}\right) \cdot c\hat{\mathbf{P}}. \tag{83}$$

We would like to construct a reduced Hamiltonian appropriate for the mixed symmetry basis states of the quark system. This construction can be written symbolically as

$$\begin{aligned}\langle [3\ 2\ 1]_{\rm RFSTC}|\hat{H}|[3\ 2\ 1]_{\rm RFSTC}\rangle =& \langle [1\ 1\ 1]_{\rm R}|[1\ 1\ 1]_{\rm R}\rangle \langle [3\ 2\ 1]_{\rm C}|[3\ 2\ 1]_{\rm C}\rangle \\ & \bigg\{ \frac{1}{2}\langle [1\ 2\ 1]_{\rm F}|[1\ 2\ 1]_{\rm F}\rangle \langle [1\ 2\ 1]_{\rm ST}|\hat{H}|[1\ 2\ 1]_{\rm ST}\rangle \\ & + \frac{1}{2}\langle [2\ 1\ 1]_{\rm F}|[2\ 1\ 1]_{\rm F}\rangle \langle [2\ 1\ 1]_{\rm ST}|\hat{H}|[2\ 1\ 1]_{\rm ST}\rangle \bigg\} \\ =& \frac{1}{2}\langle [1\ 2\ 1]_{\rm ST}|\hat{H}|[1\ 2\ 1]_{\rm ST}\rangle + \frac{1}{2}\langle [2\ 1\ 1]_{\rm ST}|\hat{H}|[2\ 1\ 1]_{\rm ST}\rangle, \end{aligned} \tag{84}$$

where R in this refers to the relative spatial degrees of freedom. Ultimately the appropriate Hamiltonian is one that averages over the two mixed symmetry basis states. This suggests that we can write the nucleon Hamiltonian in this free-space collinear quark model as

$$\begin{aligned}\hat{H}_{\rm nuc} =& |[3\ 2\ 1]_{\rm C}\rangle |[1\ 2\ 1]_{\rm F}\rangle \hat{H}_{[1\ 2\ 1]} \langle [1\ 2\ 1]_{\rm F}|\langle [3\ 2\ 1]_{\rm C}| \\ & + |[3\ 2\ 1]_{\rm C}\rangle |[2\ 1\ 1]_{\rm F}\rangle \hat{H}_{[2\ 1\ 1]} \langle [2\ 1\ 1]_{\rm F}|\langle [3\ 2\ 1]_{\rm C}|, \end{aligned} \tag{85}$$

where the subscript for the Hamiltonian here refers the the symmetric group for flavor. The $[1\ 2\ 1]$ part of the Hamiltonian can be written

$$\hat{H}_{[1\ 2\ 1]} = \mathbf{M}c^2 + \mathbf{a} \cdot c\mathbf{P}, \tag{86}$$

where $\mathbf{M}$ and $\mathbf{a}$ are 20×20 matrices, which are given explicitly in Appendix A. The matrices are different for the $[2\ 1\ 1]$ case (since the basis states are different); however, we have found that it is possible to arrange for the basis states to be ordered so as to lead to identical matrices.

5.7. Issues with minimal coupling

We might think to apply minimal coupling directly with our Bargmann–Wigner model. For example, if we begin with

$$\hat{H} = \mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}},$$

then including the electromagnetic field would lead to

$$\hat{H} \ \rightarrow \ \mathbf{M}c^2 + \mathbf{a} \cdot c[\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})] + Q\Phi(\mathbf{R}), \tag{87}$$

where Q is the total charge

$$Q = q_1 + \cdots + q_N. \tag{88}$$

This is in essence the argument discussed briefly in [90]. However, there are issues associated with this.

Suppose that the charges of the constituent particles differ, as is the case for quarks in nucleons, and is also the case for a Dirac model for protons and neutrons in nuclei. Minimal coupling leads to a Hamiltonian of the form

$$\hat{H} = \beta_1 mc^2 + \boldsymbol{\alpha}_1 \cdot c[\hat{\mathbf{p}}_1 - q_1\mathbf{A}(\mathbf{r}_1)] + \cdots + \beta_N mc^2 + \boldsymbol{\alpha}_N \cdot c[\hat{\mathbf{p}}_N - q_N\mathbf{A}(\mathbf{r}_N)] + \sum_j q_j \Phi(\mathbf{r}_j). \tag{89}$$

The Bargmann–Wigner type of Hamiltonian that results is

$$\hat{H} = (\beta_1 + \cdots + \beta_N)mc^2 + \frac{1}{N}(\boldsymbol{\alpha}_1 + \cdots + \boldsymbol{\alpha}_N) \cdot c\hat{\mathbf{P}} + (q_1\boldsymbol{\alpha}_1 + \cdots + q_N\boldsymbol{\alpha}_N) \cdot c\mathbf{A}(\mathbf{R}) + Q\Phi(\mathbf{R}). \tag{90}$$

In matrix form we can write

$$\hat{H} = \mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} - Q\mathbf{a}_Q \cdot c\mathbf{A}(\mathbf{R}) + Q\Phi(\mathbf{R}) \tag{91}$$

with

$$\mathbf{a}_Q = \frac{q_1\boldsymbol{\alpha}_1 + \cdots + q_N\boldsymbol{\alpha}_N}{Q}. \tag{92}$$

If the charges are all the same, then $\mathbf{a}_Q = \mathbf{a}$; otherwise $\mathbf{a}_Q \neq \mathbf{a}$ and minimal coupling is inconsistent. This was noted in [5].

A possible resolution to these issues is to write the model instead as

$$\begin{aligned}\hat{H} =&(\beta_1 + \cdots + \beta_N)mc^2 + \frac{1}{N}(\boldsymbol{\alpha}_1 + \cdots + \boldsymbol{\alpha}_N) \cdot c[\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})] + Q\Phi(\mathbf{R}) \\ &- \left[\left(q_1 - \frac{Q}{N} \right) \boldsymbol{\alpha}_1 + \cdots + \left(q_N - \frac{Q}{N} \right) \boldsymbol{\alpha}_N \right] \cdot c\mathbf{A}(\mathbf{R}),\end{aligned} \tag{93}$$

where the terms on the first line can be associated with center of mass dynamics, and where terms on the second line involve internal transitions. In matrix form this is

$$\hat{H} = \mathbf{M}c^2 + \mathbf{a} \cdot c[\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})] + Q\Phi(\mathbf{R}) - (\mathbf{a}_Q - \mathbf{a}) \cdot cQ\mathbf{A}(\mathbf{R}). \tag{94}$$

These issues are perhaps more important in the case that include a realistic internal structure.

Different issues with minimal coupling for the Bargmann–Wigner model have been discussed in the literature [91,92].

6. Models for Nonrelativistic Composites

The nonrelativistic composite model is straightforward, both conceptually as well as mathematically. A big issue is the clean separation between center of mass and relative mass degrees of freedom, and there is no coupling between the total momentum and internal degrees of freedom except through external field interactions.

6.1. Equal mass model

One of the simplest models of this kind relevant to us is an equal mass Hamiltonian, which we focus on in the rest of the paper. Consider a Hamiltonian of the form

$$\hat{H} = \sum_j \frac{|\hat{\mathbf{p}}_j|^2}{2m} - \sum_j \frac{q_j}{2m} \left[\mathbf{A}(\mathbf{r}_j) \cdot \hat{\mathbf{p}}_j + \hat{\mathbf{p}}_j \cdot \mathbf{A}(\mathbf{r}_j) \right] + \sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j), \tag{95}$$

where for simplicity we have not included the ponderomotive potential. The two-particle potential terms $\hat{V}_{jk}$ are intended to include both the strong force and Coulomb/electromagnetic coupling. Some years ago people worked with empirical nuclear potentials optimized against scattering data and few nucleon bound state properties [93–100]. More recently people have moved to nucleon interaction models derived from an effective chiral field theory [45,101–103]. We note that in these models there occur interactions between three or more nucleons which are used in calculations; in what follows the interaction will be written as a two-particle potential (in an effort to simplify the equations that result) with the understanding that the same arguments apply to the higher-order terms as well.

6.2. Relative and center of mass separation

We introduce relative and center of mass coordinates according to

$$\mathbf{R} = \frac{1}{N} \sum_j \mathbf{r}_j, \qquad \hat{\mathbf{P}} = \sum_j \hat{\mathbf{p}}_j, \tag{96}$$

$$\boldsymbol{\xi}_j = \mathbf{r}_j - \mathbf{R}, \qquad \hat{\boldsymbol{\pi}}_j = \hat{\mathbf{p}}_j - \frac{\hat{\mathbf{P}}}{N}, \tag{97}$$

where N is the total number of particles. With these definitions we have the relations

$$\sum_j \boldsymbol{\xi}_j = 0, \qquad \sum_j \hat{\boldsymbol{\pi}}_j = 0. \tag{98}$$

We can make use of these to separate the Hamiltonian according to

$$\hat{H} = \hat{H}_{\boldsymbol{\xi}} + \hat{H}_{\mathbf{R}} + \hat{H}_{\text{int}}, \tag{99}$$

where $\hat{H}_{\boldsymbol{\xi}}$ is the Hamiltonian for the relative system

$$\hat{H}_{\boldsymbol{\xi}} = \sum_j \frac{|\hat{\boldsymbol{\pi}}_j|^2}{2m} + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k). \tag{100}$$

The Hamiltonian for the center of mass system $\hat{H}_{\mathbf{R}}$ is

$$\hat{H}_{\mathbf{R}} = \frac{|\hat{\mathbf{P}}|^2}{2M}, \tag{101}$$

where M is the total mass

$$M = Nm \tag{102}$$

and the interaction with the external longitudinal and transverse fields are described by the Hamiltonian $\hat{H}_{\text{int}}$

$$\begin{aligned} \hat{H}_{\text{int}} = &\sum_j \frac{q_j}{2m} \left[\mathbf{A}(\boldsymbol{\xi}_j + \mathbf{R}) \cdot \frac{\hat{\mathbf{P}}}{N} + \frac{\hat{\mathbf{P}}}{N} \cdot \mathbf{A}(\boldsymbol{\xi}_j + \mathbf{R}) \right] \\ &+ \sum_j \frac{q_j}{2m} \left[\mathbf{A}(\boldsymbol{\xi}_j + \mathbf{R}) \cdot \hat{\boldsymbol{\pi}}_j + \hat{\boldsymbol{\pi}}_j \cdot \mathbf{A}(\boldsymbol{\xi}_j + \mathbf{R}) \right] + \sum_j q_j \Phi(\boldsymbol{\xi}_j + \mathbf{R}). \end{aligned} \tag{103}$$

In the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ (hence $\hat{\mathbf{p}}_j \cdot \mathbf{A}(\mathbf{r}_j) = 0$), so that in this special case we could write

$$\hat{H}_{\text{int}} = \sum_j \frac{q_j}{m} \mathbf{A}(\boldsymbol{\xi}_j + \mathbf{R}) \cdot \left(\frac{\hat{\mathbf{P}}}{N} + \hat{\boldsymbol{\pi}}_j \right) + \sum_j q_j \Phi(\boldsymbol{\xi}_j + \mathbf{R}). \tag{104}$$

6.3. Interaction with the external scalar potential

We might assume that the potential is slowly varying in the vicinity of the center of mass, and use a Taylor series approximation

$$\Phi(\mathbf{r}_j) = \Phi(\boldsymbol{\xi}_j + \mathbf{R}) = \Phi(\mathbf{R}) + \boldsymbol{\xi}_j \cdot (\nabla\Phi)_{\mathbf{R}} + \cdots \tag{105}$$

This allows us to write

$$\begin{aligned} \sum_j q_j \Phi(\boldsymbol{\xi}_j + \mathbf{R}) &= \sum_j q_j \left[\Phi(\mathbf{R}) + \boldsymbol{\xi}_j \cdot (\nabla\Phi)_{\mathbf{R}} + \cdots \right] \\ &= Q\Phi(\mathbf{R}) + \sum_j q_j \boldsymbol{\xi}_j \cdot (\nabla\Phi) + \cdots \\ &= Q\Phi(\mathbf{R}) - \mathbf{d} \cdot \mathbf{E}_{\mathrm{L}}(\mathbf{R}) + \cdots , \end{aligned} \tag{106}$$

where Q is the total charge $\sum_j q_j$, and where $\mathbf{d}$ is the (relative) dipole operator

$$\mathbf{d} = \sum_j q_j \boldsymbol{\xi}_j . \tag{107}$$

The longitudinal electric field is related to the potential through

$$\mathbf{E}_{\mathrm{L}} = -\nabla\Phi. \tag{108}$$

Here and in what follows, the field variables without an explicit associated position are presumed to be evaluated at the composite center of mass

$$\mathbf{E}_{\mathrm{L}}(\mathbf{R}) \ \rightarrow \ \mathbf{E}_{\mathrm{L}}, \qquad \Phi(\mathbf{R}) \ \rightarrow \ \Phi. \tag{109}$$

The scalar potential interacts with the composite as a whole through the potential at the center of mass position; there is a dipole interaction which mediates transitions between the basis states of the relative problem due to coupling with the longitudinal electric field; and the $\cdots$ indicates quadrupole and higher-order multipole longitudinal field interactions.

6.4. Interaction with the external vector potential

A similar approach can be used in connection with the vector potential. We can use a Taylor series expansion and write

$$\mathbf{A}(\mathbf{r}_j) = \mathbf{A}(\boldsymbol{\xi}_j + \mathbf{R}) = \mathbf{A}(\mathbf{R}) + [(\boldsymbol{\xi}_j \cdot \nabla)\mathbf{A}] + \cdots \tag{110}$$

To make progress we write

$$
\begin{aligned}
-\sum_j \frac{q_j}{2m}\Big[\mathbf{A}(\mathbf{r}_j)\cdot\hat{\mathbf{p}}_j+\hat{\mathbf{p}}_j\cdot\mathbf{A}(\mathbf{r}_j)\Big] =& -\frac{Q}{2M}\Big[\mathbf{A}\cdot\hat{\mathbf{P}}+\hat{\mathbf{P}}\cdot\mathbf{A}\Big]-\left[\sum_j\left(q_j-\frac{Q}{N}\right)\frac{\hat{\boldsymbol{\pi}}_j}{m}\right]\cdot\mathbf{A}\\
&-\sum_j\frac{q_j}{2m}[(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{A}]\cdot\frac{\hat{\mathbf{P}}}{N}-\frac{\hat{\mathbf{P}}}{N}\cdot\sum_j\frac{q_j}{2m}[(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{A}]\\
&-\sum_j\frac{q_j}{2m}[(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{A}]\cdot\hat{\boldsymbol{\pi}}_j-\sum_j\frac{q_j}{2m}\hat{\boldsymbol{\pi}}_j\cdot[(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{A}]+\cdots
\end{aligned}
\quad (111)
$$

The first term on the right hand side describes the interaction of the composite as a whole with the vector potential, and the second term gives rise to dipole transitions coupling to the transverse electric field. The terms in the next two lines give rise to magnetic dipole interactions and second-order interactions with the transverse electric field; in the case of center of mass coupling (second line) and relative coupling (third line).

The magnetic dipole interaction is normally isolated making use of a specific vector potential for a uniform magnetic field, such as [104]

$$
\mathbf{A}(\mathbf{r})=\frac{1}{2}\mathbf{B}(\mathbf{r})\times\mathbf{r}. \quad (112)
$$

However, we would prefer a more general treatment if possible. We know that $(\boldsymbol{\xi}\cdot\nabla)\mathbf{A}$ generates terms connected with the magnetic dipole interaction, as well as others. It is possible to isolate the magnetic interactions by using

$$
(\boldsymbol{\xi}\cdot\nabla)\mathbf{A}=-\frac{1}{2}\boldsymbol{\xi}\times\mathbf{B}+\frac{1}{2}\Big[(\boldsymbol{\xi}\cdot\nabla)\mathbf{A}+\nabla(\boldsymbol{\xi}\cdot\mathbf{A})\Big], \quad (113)
$$

where it ends up that the first term can be associated with the magnetic interactions. If we make use of this we obtain

$$
\begin{aligned}
-\sum_j \frac{q_j}{2m}\Big[\mathbf{A}(\mathbf{r}_j)\cdot\hat{\mathbf{p}}_j+\hat{\mathbf{p}}_j\cdot\mathbf{A}(\mathbf{r}_j)\Big] =& -\frac{Q}{2M}\Big(\mathbf{A}\cdot\hat{\mathbf{P}}+\hat{\mathbf{P}}\cdot\mathbf{A}\Big)-\left[\sum_j\left(q_j-\frac{Q}{N}\right)\frac{\hat{\boldsymbol{\pi}}_j}{m}\right]\cdot\mathbf{A}\\
&-\frac{1}{2}\left(\sum_j q_j\boldsymbol{\xi}_j\right)\times\frac{\hat{\mathbf{P}}}{M}\cdot\mathbf{B}-\left(\sum_j\frac{q_j}{2m}\boldsymbol{\xi}_j\times\hat{\boldsymbol{\pi}}_j\right)\cdot\mathbf{B}+\cdots
\end{aligned}
\quad (114)
$$

The third term on the right hand side is the contribution of the relative angular momentum to the magnetic dipole interaction, followed by the contribution to the magnetic dipole interaction due to center of mass motion.
We can rewrite this more simply as

$$
\begin{aligned}
-\frac{q}{2m}\sum_j\Big[\mathbf{A}(\mathbf{r}_j)\cdot\hat{\mathbf{p}}_j+\hat{\mathbf{p}}_j\cdot\mathbf{A}(\mathbf{r}_j)\Big] =& -\frac{Q}{2M}\Big(\mathbf{A}\cdot\hat{\mathbf{P}}+\hat{\mathbf{P}}\cdot\mathbf{A}\Big)-\hat{\mathbf{j}}\cdot\mathbf{A}-\hat{\boldsymbol{\mu}}_l\cdot\mathbf{B}\\
&-\frac{1}{2}\mathbf{d}\times\frac{\hat{\mathbf{P}}}{M}\cdot\mathbf{B}+\cdots,
\end{aligned}
\quad (115)
$$

where we recall that $\mathbf{d}$ is the relative dipole operator $\sum_j q_j \boldsymbol{\xi}_j$, and where

$$\hat{\mathbf{j}} = \sum_j \left(q_j - \frac{Q}{N} \right) \frac{\hat{\boldsymbol{\pi}}_j}{m} \tag{116}$$

is the relative current operator, and

$$\hat{\boldsymbol{\mu}}_l = \sum_j \frac{q_j}{2m} \boldsymbol{\xi}_j \times \hat{\boldsymbol{\pi}}_j \tag{117}$$

is the relative angular momentum contribution to the magnetic dipole moment.

6.5. Resulting Hamiltonian for a nonrelativistic composite

We can assemble the results above and write

$$\begin{aligned} \hat{H} =& \frac{|\hat{\mathbf{P}}|^2}{2M} + Q\Phi - \frac{Q}{2M}\left(\mathbf{A} \cdot \hat{\mathbf{P}} + \hat{\mathbf{P}} \cdot \mathbf{A} \right) \\ &+ \sum_j \frac{|\hat{\boldsymbol{\pi}}_j|^2}{2m} + \sum_{j<k} \hat{V}_{jk}(|\boldsymbol{\xi}_j - \boldsymbol{\xi}_k|) \\ &- \mathbf{d} \cdot \mathbf{E}_L - \hat{\mathbf{j}} \cdot \mathbf{A} - \hat{\boldsymbol{\mu}}_l \cdot \mathbf{B} - \frac{1}{2} \mathbf{d} \times \frac{\hat{\mathbf{P}}}{M} \cdot \mathbf{B} + \cdots \end{aligned} \tag{118}$$

In the first line we have terms describing the composite as a particle interaction with external fields; in the second line we see the terms that describe the internal structure of the composite in terms of relative degrees of freedom. Terms that appear on the third line describes coupling between the internal degrees of freedom and the longitudinal and transverse electric fields separately, and with the magnetic field. In the last line is a term that accounts for the center of mass contribution to the magnetic dipole interaction, which couples the center of mass with internal degrees of freedom in a magnetic field.

7. Composite Model from a Many-particle Dirac Formalism

In this section we extend the development of a model for a composite particle to the many-particle Dirac formalism. This approach has the disadvantage that it is not covariant, so that the resulting relativistic composite model will not be covariant. On the other hand, we are able to carry out a construction systematically with this model, which is less straightforward with a covariant formalism. We note that in spite of its shortcomings, the Dirac formalism is widely used for atomic, molecular and nuclear physics.

7.1. Relativistic equal mass model

We consider a model based on the many-particle Dirac Hamiltonian

$$\hat{H} = \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c[\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)] + \sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j). \tag{119}$$

This kind of model has been of interest since the earliest efforts to develop a relativistic description of quantum systems with two or more particles [105–110]. Keep in mind that in this kind of model there is the possibility of both positive energy and negative energy solutions, so that bound states dissolve into the associated continuum (Brown–Ravenhall disease); in models derived from field theory, this issue is resolved through the appearance of projection operators [111–116]. In the majority of the subsequent literature the projection operators are not written out explicitly; in what follows we will also suppress the projection operators.

We are interested here in composite models for nuclei based on a Dirac phenomenology for nucleons. Consequently, it would be reasonable to use equal masses for the nucleons, and the interaction potential $\hat{V}_{jk}$ includes contributions from both the strong force and electromagnetic interactions.

7.2. Relative and center of mass variables

Relative and center of mass variables are defined once again according to

$$\mathbf{R} = \frac{1}{N}\sum_j \mathbf{r}_j, \qquad \hat{\mathbf{P}} = \sum_j \hat{\mathbf{p}}_j,$$

$$\boldsymbol{\xi}_j = \mathbf{r}_j - \mathbf{R}, \qquad \hat{\boldsymbol{\pi}}_j = \hat{\mathbf{p}}_j - \frac{\hat{\mathbf{P}}}{N}.$$

The Hamiltonian written in terms of these variables is

$$\begin{aligned}\hat{H} =& \frac{1}{N}\boldsymbol{\alpha}_j \cdot c[\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})] + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \\ &+ \sum_j q_j \Phi(\mathbf{R} + \boldsymbol{\xi}_j) - \sum_j \boldsymbol{\alpha}_j \cdot c\left[q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R})\right]. \end{aligned} \tag{120}$$

If we use Taylor series expansions of the potentials around the center of mass position, we can write for the relativistic composite a model of the form

$$\begin{aligned}\hat{H} =& \sum_j \beta_j mc^2 + \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) + Q\Phi + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk} \\ &+ \left(\sum_j q_j \boldsymbol{\xi}_j\right) \cdot \nabla\Phi - \sum_j \boldsymbol{\alpha}_j \cdot c\left(q_j - \frac{Q}{N}\right)\mathbf{A} - \sum_j \boldsymbol{\alpha}_j \cdot cq_j(\boldsymbol{\xi}_j \cdot \nabla)\mathbf{A} + \cdots \end{aligned} \tag{121}$$

In the first line we see a relativistic description of the composite interacting with external fields, and also a relativistic description of the internal problem; however, both of these models share the same mass terms. In the second line we see in the first term an electric dipole interaction with the longitudinal electric field; we see next the electric dipole interaction with the transverse electric field; and higher-order interactions are included in the terms that follow.

7.3. Rest frame model

The many-particle Dirac model above is widely used; however, from the discussion above it seems clear that for the internal relative problem in the absence of external fields we should be interested in the relative Hamiltonian

$$\hat{H} = \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}. \tag{122}$$

This model is less widely used; however, there are papers where it has been considered. In the case of the two-body problem (without external field coupling) this would be considered as a Kemmer–Fermi–Yang Hamiltonian [117,118]. This kind of model has been widely used over the years; in the case of equal mass models, to describe positronium [119–121], the deuteron and two nucleon models [122–126], mesons [127–131]. Models of this kind with nonequal masses have been used to describe the hydrogen atom [132–136]. Three-body problems Dirac models have been studied in connection with quark models for baryons [125–141]. We draw attention to the Dirac phenomenology for nuclear structure [41–44] where the rest frame is assumed, and in most cases the center of mass contributions are removed approximately at the end of the calculation.

7.4. Dirac–Pauli models

In the event that our original model includes Pauli terms, we would start out with

$$\begin{aligned} \hat{H} = & \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c[\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)] + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi(\mathbf{r}_j) \\ & - \frac{e\hbar}{2m} \sum_j \lambda_j \beta_j \Big(\boldsymbol{\Sigma}_j \cdot \mathbf{B}(\mathbf{r}_j) - i\boldsymbol{\alpha}_j \cdot \mathbf{E}(\mathbf{r}_j) \Big), \end{aligned} \tag{123}$$

where

$$\lambda_j = \begin{cases} \dfrac{g_p}{2} - 1 & \text{protons} \\ \\ \dfrac{g_n}{2} & \text{neutrons} \end{cases} \tag{124}$$

approximating the proton and neutron masses as being equal. We recall that

$$\boldsymbol{\Sigma} = \begin{bmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{bmatrix}.$$

The Pauli interaction includes an anomalous magnetic dipole interaction along with the corresponding correction to the spin–orbit interaction.

Of interest here is the composite model that results; we may write

$$\hat{H} = \sum_j \beta_j mc^2 + \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) + Q\Phi + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}$$
$$- \mathbf{d}\cdot\mathbf{E}_L - \hat{\boldsymbol{\mu}}_a \cdot \mathbf{B} - \hat{\mathbf{j}}\cdot\mathbf{A} + i\frac{e\hbar}{2m}\sum_j \lambda_j\beta_j\boldsymbol{\alpha}_j\cdot\mathbf{E} - \sum_j \boldsymbol{\alpha}_j \cdot cq_j(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{A} + \cdots, \tag{125}$$

where the relativistic relative current operator is

$$\hat{\mathbf{j}} = \sum_j \left(q_j - \frac{Q}{N}\right) c\boldsymbol{\alpha}_j \tag{126}$$

and where the anomalous magnetic dipole moment operator is

$$\hat{\boldsymbol{\mu}}_a = \frac{e\hbar}{2m}\sum_j \lambda_j \beta_j \boldsymbol{\Sigma}_j. \tag{127}$$

8. Composite Model from Elimination of Negative Energy States

In this section we will consider low-order relativistic corrections based on the elimination of negative energy states (or sometimes called Pauli reduction) from a Dirac model. We are interested in this approach since it is the simplest and most direct approximation possible which results in a model that is close to being nonrelativistic. Such an approach was used early on by Darwin [142], Breit [105], and Gaunt [143]; and it has been made use of many times subsequently [106,107,109,122–124,144–156].

8.1. Elimination of negative energy states

To make progress, we begin with the eigenvalue equation for the many-particle eigenvalue equation

$$E\Psi = \left\{\sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c[\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)] + \sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j\Phi(\mathbf{r}_j)\right\}\Psi. \tag{128}$$

The relativistic wavefunction Ψ in this case has 4^N components, which provides motivation for us to consider a nonrelativistic approximation with fewer components.

The issue we face in this discussion is that there are different sectors in which both positive energy components and negative energy components occur, and we need to keep track of them. The nonrelativistic sector is then the one containing all positive energy components; the associated part of the wave function will be denoted by $\Psi_{+\cdots+}$, where the $+$ signs are associated with different positive energy pieces associated with the different particles.

We can use this kind of notation to write coupled eigenvalue equations of the form [157]

$$
\begin{aligned}
E\Psi_{+\cdots+} = & \left[Nmc^2 + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi \right] \Psi_{+\cdots+} + \boldsymbol{\sigma}_1 \cdot c(\hat{\mathbf{p}}_1 - q_1 \mathbf{A}) \Psi_{-+\cdots+} \\
& + \cdots + \boldsymbol{\sigma}_N \cdot c(\hat{\mathbf{p}}_N - q_N \mathbf{A}) \Psi_{+\cdots+-}
\end{aligned}
$$

$$
\begin{aligned}
E\Psi_{-+\cdots+} = & \left[(N-2)mc^2 + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi \right] \Psi_{-+\cdots+} + \boldsymbol{\sigma}_1 \cdot c(\hat{\mathbf{p}}_1 - q_1 \mathbf{A}) \Psi_{++\cdots+} \\
& + \boldsymbol{\sigma}_2 \cdot c(\hat{\mathbf{p}}_2 - q_2 \mathbf{A}) \Psi_{--+\cdots+} + \cdots + \boldsymbol{\sigma}_N \cdot c(\hat{\mathbf{p}}_N - q_N \mathbf{A}) \Psi_{-\cdots+-} \\
& \vdots
\end{aligned}
\tag{129}
$$

The mass energy decreases by $2mc^2$ with each increase in the number of $-$, since we lose one positive energy particle and gain a negative energy one. Two-body versions of this approach are discussed in [122,158]. In this discussion the interaction has been taken to be the same for positive energy and negative energy sectors; modifications in the case of other potential models is straightforward.

If the problem is not overly relativistic then the channels with two or more negative energy components should have sufficiently small occupation that we might neglect them. We can develop an approximate solution for channels with a single negative energy sector according to

$$
\left[E - (N-2)mc^2 + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi \right] \Psi_{-+\cdots+} \ \rightarrow \ \boldsymbol{\sigma}_1 \cdot c(\hat{\mathbf{p}}_1 - q_1 \mathbf{A}) \Psi_{++\cdots+} \tag{130}
$$

with similar expressions for other channels. Substituting back leads to

$$
\begin{aligned}
E\Psi_{+\cdots+} \ \approx \ & \left[Nmc^2 + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi \right] \Psi_{+\cdots+} \\
& + \boldsymbol{\sigma}_1 \cdot c(\hat{\mathbf{p}}_1 - q_1 \mathbf{A}) \left[E - (N-2)mc^2 + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi \right]^{-1} \boldsymbol{\sigma}_1 \cdot c(\hat{\mathbf{p}}_1 - q_1 \mathbf{A}) \Psi_{++\cdots+} \\
& \vdots \\
& + \boldsymbol{\sigma}_N \cdot c(\hat{\mathbf{p}}_N - q_N \mathbf{A}) \left[E - (N-2)mc^2 + \sum_{j<k} \hat{V}_{jk} + \sum_j q_j \Phi \right]^{-1} \boldsymbol{\sigma}_N \cdot c(\hat{\mathbf{p}}_N - q_N \mathbf{A}) \Psi_{++\cdots+}
\end{aligned}
\tag{131}
$$

If we take $E-(N-2)mc^2$ to be $2mc^2$, then the approximate nonrelativistic Hamiltonian is

$$\begin{aligned}\hat{H} =& Mc^2 + \sum_j \frac{\Big(\boldsymbol{\sigma}_j \cdot [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)]\Big)^2}{2m} + \sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) \\ & - \frac{1}{(2mc^2)^2} \sum_l \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \left(\sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) \right) \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] + \cdots \end{aligned} \quad (132)$$

In the first line we see terms similar to those encountered in the last section where we discussed the nonrelativistic composite, and in what follows we will see that the spin contribution to the magnetic dipole interaction is now included. Spin–orbit and other relativistic corrections result from the new terms in the second line.

8.2. Keeping the Hermitian part

If we work with this model as is we encounter terms which are nonHermitian [159,160]; this is one of the reasons that this general approach is not more widely used. This problem is discussed at some length in [149]. People tend to prefer the Foldy–Wouthuysen transformation [160] instead since this issue does not arise; the F–W transformation has other advantages that will be evident later on.

If we follow the arguments of [149] we arrive at a Hamiltonian of the form

$$\begin{aligned}\hat{H} \ \rightarrow \ & Mc^2 + \sum_j \frac{\Big(\boldsymbol{\sigma}_j \cdot [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)]\Big)^2}{2m} + \sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) \\ & - \frac{1}{8m^3c^2} \left(\sum_j \Big| \boldsymbol{\sigma}_j \cdot [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)] \Big|^2 \right) \left(\sum_k \Big| \boldsymbol{\sigma}_k \cdot [\hat{\mathbf{p}}_k - q_k \mathbf{A}(\mathbf{r}_k] \Big|^2 \right) \\ & - \frac{1}{8m^2c^2} \sum_l \Big| \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \Big|^2 \left(\sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) \right) \\ & + \frac{1}{4m^2c^2} \sum_l \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \left(\sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) \right) \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \\ & - \frac{1}{8m^2c^2} \sum_l \left(\sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) \right) \Big| \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \Big|^2 . \end{aligned} \quad (133)$$

In this model we have a nonrelativistic composite model augmented with low-order relativistic corrections; however, we have some work to do to reduce it in what follows to a more standard form.

8.3. Spin magnetic dipole interaction

We can make use of the identity

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{a}) = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot \mathbf{a} \times \mathbf{b} \tag{134}$$

to expand

$$\begin{aligned}\sum_j \frac{\left(\boldsymbol{\sigma}_j \cdot [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)]\right)^2}{2m} &= \sum_j \frac{\left|\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)\right|^2}{2m} - i \sum_j q_j \left(\boldsymbol{\sigma}_j \cdot \hat{\mathbf{p}}_j \times \mathbf{A}(\mathbf{r}_j) + \boldsymbol{\sigma}_j \cdot \mathbf{A}(\mathbf{r}_j) \times \hat{\mathbf{p}}_j\right) \\ &= \sum_j \frac{\left|\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)\right|^2}{2m} - \boldsymbol{\mu}_s \cdot \mathbf{B}(\mathbf{r}_j),\end{aligned} \tag{135}$$

where

$$\boldsymbol{\mu}_s = \sum_j \frac{\hbar q_j}{2m} \boldsymbol{\sigma}_j. \tag{136}$$

8.4. Terms involving the external electrostatic potential

We can collect together higher-order terms involving the electrostatic potential Φ and write

$$\begin{aligned}&-\frac{1}{8m^2c^2} \sum_l \left|\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)]\right|^2 \left(\sum_j q_j \Phi(\mathbf{r}_j)\right) \\ &+ \frac{1}{4m^2c^2} \sum_l \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \left(\sum_j q_j \Phi(\mathbf{r}_j)\right) \boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)] \\ &- \frac{1}{8m^2c^2} \sum_l \left(\sum_j q_j \Phi(\mathbf{r}_j)\right) \left|\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)]\right|^2 \\ &= -\frac{1}{8m^2c^2} \sum_l \sum_j \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)], \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)], q_j \Phi(\mathbf{r}_j)\right]\right] \\ &= -i \frac{\hbar}{8m^2c^2} \sum_j q_j \left[\boldsymbol{\sigma}_j \cdot [\hat{\mathbf{p}}_j - q_l \mathbf{A}(\mathbf{r}_j)], \boldsymbol{\sigma}_j \cdot \mathbf{E}_L(\mathbf{r}_j)\right] \\ &= -\frac{\hbar^2}{8m^2c^2} \sum_j q_j \nabla_j \cdot \mathbf{E}_L(\mathbf{r}_j) \\ &+ \frac{\hbar}{8m^2c^2} \sum_j q_j \boldsymbol{\sigma}_j \cdot \left([\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)] \times \mathbf{E}_L(\mathbf{r}_j) - \mathbf{E}_L(\mathbf{r}_j) \times [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)]\right).\end{aligned} \tag{137}$$

We can express this in terms of center of mass and relative variables according to

$$
\begin{aligned}
&-i\frac{\hbar}{8m^2c^2}\sum_j q_j\left[\boldsymbol{\sigma}_j\cdot[\hat{\mathbf{p}}_j-q_j\mathbf{A}(\mathbf{r}_j)],\boldsymbol{\sigma}_j\cdot\mathbf{E}_L(\mathbf{r}_j)\right]\\
&=-i\frac{\hbar}{8Mmc^2}\sum_j q_j\left[\boldsymbol{\sigma}_j\cdot[\hat{\mathbf{P}}-Q\mathbf{A}(\mathbf{R})],\boldsymbol{\sigma}_j\cdot[\mathbf{E}_L(\mathbf{R})+(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{E}+\cdots]\right]\\
&\quad -i\frac{\hbar}{8m^2c^2}\sum_j q_j\left[\boldsymbol{\sigma}_j\cdot\left(\hat{\boldsymbol{\pi}}_j-q_j\mathbf{A}(\mathbf{R}+\boldsymbol{\xi}_j)+\frac{Q}{N}\mathbf{A}(\mathbf{R})\right),\boldsymbol{\sigma}_j\cdot[\mathbf{E}_L(\mathbf{R})+(\boldsymbol{\xi}_j\cdot\nabla)\mathbf{E}+\cdots]\right]\\
&=-\frac{\hbar^2Q}{8Mmc^2}\nabla\cdot\mathbf{E}_L+\frac{\hbar}{8Mmc^2}\sum_j q_j\boldsymbol{\sigma}_j\cdot\left((\hat{\mathbf{P}}-Q\mathbf{A})\times\mathbf{E}_L-\mathbf{E}_L\times(\hat{\mathbf{P}}-Q\mathbf{A})\right)\\
&\quad +\frac{\hbar}{8m^2c^2}\sum_j q_j\boldsymbol{\sigma}_j\cdot\left[\left(\hat{\boldsymbol{\pi}}_j-q_j\mathbf{A}(\mathbf{R}+\boldsymbol{\xi}_j)+\frac{Q}{N}\mathbf{A}\right)\mathbf{E}_L(\mathbf{R})-\mathbf{E}_L(\mathbf{R})\times\left(\hat{\boldsymbol{\pi}}_j-q_j\mathbf{A}(\mathbf{R}+\boldsymbol{\xi}_j)+\frac{Q}{N}\mathbf{A}\right)\right]\\
&\quad +\cdots
\end{aligned}
\tag{138}
$$

8.5. Terms involving the particle–particle interaction

Higher-order terms involving the interaction can be collected to give

$$
\begin{aligned}
&-\frac{1}{8m^2c^2}\sum_l\left|\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)]\right|^2\left(\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right)\\
&+\frac{1}{4m^2c^2}\sum_l\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)]\left(\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right)\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)]\\
&-\frac{1}{8m^2c^2}\sum_l\left(\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right)\left|\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)]\right|^2\\
=&-\frac{1}{8m^2c^2}\sum_{j<k}\sum_{l=j,k}\left[\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)],\left[\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)],\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right]\right].
\end{aligned}
\tag{139}
$$

Since the particle-particle interaction contains spin matrices, in general we cannot carry the development much further. If we express this in terms of center of mass and relative coordinates, we can write

$$
\begin{aligned}
& - \frac{1}{8m^2c^2} \sum_{j<k} \sum_{l=j,k} \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)], \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{p}}_l - q_l \mathbf{A}(\mathbf{r}_l)], \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) \right] \right] \\
= & - \frac{1}{8M^2c^2} \sum_{j<k} \sum_{l=j,k} \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})], \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})], \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right] \\
& - \frac{1}{8Mmc^2} \sum_{j<k} \sum_{l=j,k} \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})], \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N} \mathbf{A}(\mathbf{R}) \right), \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right] \\
& - \frac{1}{8Mmc^2} \sum_{j<k} \sum_{l=j,k} \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N} \mathbf{A}(\mathbf{R}) \right), \left[\boldsymbol{\sigma}_l \cdot [\hat{\mathbf{P}} - Q\mathbf{A}(\mathbf{R})], \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right] \\
& - \frac{1}{8m^2c^2} \sum_{j<k} \sum_{l=j,k} \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N} \mathbf{A}(\mathbf{R}) \right), \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N} \mathbf{A}(\mathbf{R}) \right), \right. \right. \\
& \left. \left. \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right]. \qquad (140)
\end{aligned}
$$

We see a much larger set of terms present in this case.

Included in this expression are nuclear spin–orbit terms

$$
-\frac{1}{8m^2c^2} \sum_{j<k} \sum_{l=j,k} \left[\boldsymbol{\sigma}_l \cdot \hat{\boldsymbol{\pi}}_l, \left[\boldsymbol{\sigma}_l \cdot \hat{\boldsymbol{\pi}}_l, \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right], \qquad (141)
$$

which have long been of interest in the literature [144,145,147,151–154,161,162].

Also present are terms that involve interactions between the relative degrees of freedom and the transverse electromagnetic field

$$
\begin{aligned}
& -\frac{1}{8m^2c^2} \sum_{l} \sum_{j<k} \left[\boldsymbol{\sigma}_l \hat{\boldsymbol{\pi}}_l, \left[\boldsymbol{\sigma}_l \cdot \left(-q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N} \mathbf{A}(\mathbf{R}) \right), \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right] \\
& -\frac{1}{8m^2c^2} \sum_{l} \sum_{j<k} \left[\boldsymbol{\sigma}_l \cdot \left(-q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N} \mathbf{A}(\mathbf{R}) \right), \left[\boldsymbol{\sigma}_l \cdot \hat{\boldsymbol{\pi}}_l, \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \right]. \qquad (142)
\end{aligned}
$$

These terms can contribute a correction to the magnetic moment, and is included in the analysis of Margenau [163] and subsequent authors [163–165]; and also in other analyses [10,122,158,166]. We note that exchange currents have been of interest in the literature since the observation of Siegert [167] that there should be expected additional contributions from charged meson currents. Contributions from exchange currents are beyond what is included in this formalism (see [168]).

8.6. Terms linear in $\hat{\mathbf{P}}$ with no external fields

We draw attention to terms that include the total momentum and internal nuclear transitions, the lowest order of which are

$$-\frac{1}{8Mmc^2}\sum_l\sum_{j<k}\left[\boldsymbol{\sigma}_l\cdot\hat{\mathbf{P}},\left[\boldsymbol{\sigma}_l\cdot\hat{\boldsymbol{\pi}}_l,\hat{V}_{jk}\right]\right]-\frac{1}{8Mmc^2}\sum_l\sum_{j<k}\left[\boldsymbol{\sigma}_l\cdot\hat{\boldsymbol{\pi}}_l,\left[\boldsymbol{\sigma}_l\cdot\hat{\mathbf{P}},\hat{V}_{jk}\right]\right]. \tag{143}$$

Terms of these kinds are discussed infrequently in the literature; however, a few early (and important) discussions can be found [108,161]. We will follow up on the issues in these works later on. Consequently, the majority of works involving Pauli reduction are carried out in the rest frame, and the Foldy–Wouthuysen transformation is much more widely used.

Our attention has been drawn to terms of this sort recently in connection with the development for a theory for anomalies in condensed matter nuclear science [90]. The issue in this case is that it is in general problematic to develop a sizeable coupling with the internal nuclear degrees of freedom through conventional dipole interactions with external electric and magnetic fields. These terms however provide for a very strong coupling between lattice vibrations, which in a condensed matter setting are represented in the momentum $\hat{\mathbf{P}}$, and internal nuclear states. For this reason this kind of interaction naturally drew our attention. Issues associated with this kind of coupling have ultimately provided motivation for this work.

An effort was made to evaluate numerically coupling matrix elements due to this kind of interaction [90]. Unfortunately these calculations were carried out without taking into account the issues discussed in [149], and may need to be corrected.

We will return to this kind of coupling and the associated physical significance later on in this work when we consider Poincaré invariance.

8.7. Model for a composite

We can assemble the above results and write for a Hamiltonian for a nonrelativistic composite with relativistic corrections in the form

$$\begin{aligned}\hat{H} =& Mc^2+\sum_j\frac{\left|\hat{\mathbf{p}}_j-q_j\mathbf{A}(\mathbf{r}_j)\right|^2}{2m}+\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)+\sum_j q_j\Phi(\mathbf{r}_j)\\ &-\sum_j\frac{\hbar q_j}{2m}\boldsymbol{\sigma}_j\cdot\mathbf{B}(\mathbf{r}_j)-\frac{\hbar^2}{8m^2c^2}\sum_j q_j\nabla_j\cdot\mathbf{E}_L(\mathbf{r}_j)\\ &+\frac{\hbar}{8m^2c^2}\sum_j q_j\boldsymbol{\sigma}_j\cdot\Big([\hat{\mathbf{p}}_j-q_j\mathbf{A}(\mathbf{r}_j)]\times\mathbf{E}_L(\mathbf{r}_j)-\mathbf{E}_L(\mathbf{r}_j)\times[\hat{\mathbf{p}}_j-q_j\mathbf{A}(\mathbf{r}_j)]\Big)\\ &-\frac{1}{8m^2c^2}\sum_l\sum_{j<k}\left[\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)],\left[\boldsymbol{\sigma}_l\cdot[\hat{\mathbf{p}}_l-q_l\mathbf{A}(\mathbf{r}_l)],\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right]\right].\end{aligned} \tag{144}$$

We see the nonrelativistic composite model along with low-order relativistic corrections, all in reasonably standard form.

A feature of this model is that it contains a coupling between the center of mass momentum $\hat{\mathbf{P}}$ and internal degrees of freedom of interest to us on the same footing as the nuclear spin–orbit coupling, and other interactions that are known in the literature. Also, this interaction was derived relatively simply, involving little effort in the elimination of the negative energy sectors.

A disadvantage of the model is that the longitudinal electric field appears in the model differently than the transverse electric field, which should not be the case since we started from a gauge independent model. Although it is possible to remedy this problem within the context of the approach used in this section, it will be more convenient to move on to models based on the Foldy–Wouthuysen transformation where this problem is resolved.

In terms of center of mass and relative variables we can write

$$
\begin{aligned}
\hat{H} =& Mc^2 + \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M} + Q\Phi \\
&+ \sum_j \frac{\left| \hat{\boldsymbol{\pi}}_j - q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \dfrac{Q}{N}\mathbf{A}(\mathbf{R}) \right|^2}{2m} + \sum_{j<k} \hat{V}_{jk} - \mathbf{d} \cdot \mathbf{E}_L - \boldsymbol{\mu}_s \cdot \mathbf{B} \\
&- \frac{\hbar^2 Q}{8Mmc^2} \nabla \cdot \mathbf{E}_L + \frac{\hbar}{8Mmc^2} \sum_j q_j \boldsymbol{\sigma}_j \cdot \Big((\hat{\mathbf{P}} - Q\mathbf{A}) \times \mathbf{E}_L - \mathbf{E}_L \times (\hat{\mathbf{P}} - Q\mathbf{A}) \Big) \\
&+ \frac{\hbar}{8m^2c^2} \sum_j q_j \boldsymbol{\sigma}_j \cdot \left[\left(\hat{\boldsymbol{\pi}}_j - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right) \times \mathbf{E}_L - \mathbf{E}_L \times \left(\hat{\boldsymbol{\pi}}_j - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right) \right] \\
&- \frac{1}{8m^2c^2} \sum_l \sum_{j<k} \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right), \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right), \hat{V}_{jk} \right] \right] \\
&- \frac{1}{8Mmc^2} \sum_l \sum_{j<k} \left[\boldsymbol{\sigma}_l \cdot (\hat{\mathbf{P}} - Q\mathbf{A}), \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right), \hat{V}_{jk} \right] \right] \\
&- \frac{1}{8Mmc^2} \sum_l \sum_{j<k} \left[\boldsymbol{\sigma}_l \cdot \left(\hat{\boldsymbol{\pi}}_l - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_l) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right), \left[\boldsymbol{\sigma}_l \cdot (\hat{\mathbf{P}} - Q\mathbf{A}), \hat{V}_{jk} \right] \right] \\
&- \frac{1}{8M^2c^2} \sum_l \sum_{j<k} \left[\boldsymbol{\sigma}_l \cdot (\hat{\mathbf{P}} - Q\mathbf{A}), \left[\boldsymbol{\sigma}_l \cdot (\hat{\mathbf{P}} - Q\mathbf{A}), \hat{V}_{jk} \right] \right] \\
&+ \cdots
\end{aligned}
\tag{145}
$$

Corrected Pauli reduction in this case has led to a reasonably complete model for a nonrelativistic composite with low-order relativistic corrections pretty much in standard form. The issue noted in connection with a lack of gauge invariance due to the presence of the longitudinal field will be corrected when we work with the Foldy–Wouthuysen transformation; however, the correction simply involves the replacement

$$
\mathbf{E}_L \ \rightarrow \ \mathbf{E} \tag{146}
$$

9. Model based on the Foldy–Wouthuysen Transform

We were interested in the method of elimination of negative energy states due to its simplicity; however, a major disadvantage is that it can produce nonHermitian terms. This motivates us to consider composite models based on the Foldy–Wouthuysen transformation [160] in this section, and also a closely related transform in the following section. This rotation has been very widely used for atomic problems [175–180], as well as for nuclear models [123,150,181–188].

9.1. Foldy–Wouthuysen transform

As with all unitary transformations, the basic idea is to work with a rotated wave function written as

$$\Psi' = \mathrm{e}^{i\hat{S}}\Psi. \tag{147}$$

Assuming that $\hat{S}$ is time-dependent, then the system can be modeled with the transformed Hamiltonian

$$\hat{H}' = \mathrm{e}^{i\hat{S}}\left[\hat{H} - i\hbar\frac{\partial}{\partial t}\right]\mathrm{e}^{-i\hat{S}}. \tag{148}$$

Foldy and Wouthuysen used this approach to develop transformations that allow for a nonrelativistic approximation in the case of a single particle [160,189,190]. In the case of a Dirac particle in an external field, the Dirac Hamiltonian is

$$\hat{H} = \boldsymbol{\alpha}\cdot c(\hat{p} - q\mathbf{A}) + \beta mc^2 + q\Phi. \tag{149}$$

After three successive transforms the lowest-order terms in the transformed (4×4 matrix) Hamiltonian is

$$\begin{aligned}\hat{H}' \;\rightarrow\; & \beta\left(mc^2 + \frac{|\hat{\mathbf{p}} - q\mathbf{A}|^2}{2m} - \frac{|\hat{\mathbf{p}} - q\mathbf{A}|^4}{8m^3c^2}\right) + q\Phi - \frac{\hbar q}{2m}\beta\boldsymbol{\Sigma}\cdot\mathbf{B} \\ & + \frac{\hbar q}{8m^2c^2}\left[\boldsymbol{\Sigma}\cdot(\hat{\mathbf{p}} - q\mathbf{A})\times\mathbf{E} - \boldsymbol{\Sigma}\cdot\mathbf{E}\times(\hat{\mathbf{p}} - q\mathbf{A})\right] - \frac{q\hbar^2}{8m^2c^2}\nabla\cdot\mathbf{E},\end{aligned} \tag{150}$$

where

$$\boldsymbol{\Sigma} = \begin{bmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{bmatrix}. \tag{151}$$

9.2. Many-particle model

There is a long tradition of making use of the Foldy–Wouthuysen transformation on many-particle models. F-W transformations for two interacting Dirac particles have been considered in [176,191–196]; for the many-particle case see [116,177,184,197–199]. Transformations for Hamiltonians that include Pauli interactions for the anomalous magnetic moment have been discussed in [200–204].

We begin with a many-particle model written as

$$\hat{H} = \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j\cdot c[\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)] + \sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j\Phi(\mathbf{r}_j).$$

Foldy–Wouthuysen transformations on each of the particles individually reduce all terms except for the interaction terms. We can write

$$\begin{aligned}\hat{H}' \;\rightarrow\; & mc^2\sum_j \beta_j + \sum_j \frac{\left|\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)\right|^2}{2m}\beta_j + \mathrm{e}^{i\hat{S}}\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\mathrm{e}^{-i\hat{S}} + \sum_j q_j\Phi(\mathbf{r}_j) \\ & - \sum_j \frac{\hbar q_j}{2m}\beta_j\mathbf{\Sigma}_j\cdot\mathbf{B}(\mathbf{r}_j) + \sum_j \frac{\hbar q_j}{8m^2c^2}\Big[\mathbf{\Sigma}_j\cdot[\hat{\mathbf{p}}_j - q\mathbf{A}(\mathbf{r}_j)]\times\mathbf{E}(\mathbf{r}_j) - \mathbf{\Sigma}_j\cdot\mathbf{E}(\mathbf{r}_j)\times[\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)]\Big] \\ & - \sum_j \frac{q_j\hbar^2}{8m^2c^2}\nabla\cdot\mathbf{E}(\mathbf{r}_j). \end{aligned} \tag{152}$$

Since the composite may be in motion, it is best to work in a Foldy–Wouthuysen representation rather than with a nonrelativistic approximation here since additional issues arise in the extraction of the nonrelativistic limit [200]. The Foldy–Wouthuysen transformation of the Breit interaction has been discussed in [116,176,191–196]. A Foldy–Wouthuysen transformation was considered in the case of the Bonn nuclear potential [99] by Amore et al. [208].

9.3. Lowest-order contributions to the transformed potential

We can expand the transformed potential according to

$$\mathrm{e}^{i\hat{S}}\left(\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right)\mathrm{e}^{-i\hat{S}} = \hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k) + i\Big[\hat{S},\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\Big] - \frac{1}{2}\Big[\hat{S},\Big[\hat{S},\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\Big]\Big] + \cdots \tag{153}$$

An expression for the lowest-order correction to the potential can be derived based on

$$\hat{S} = -i\frac{1}{2mc}\sum_j \beta_j\boldsymbol{\alpha}_j\cdot[\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)]. \tag{154}$$

We can use this to write

$$\begin{aligned}\mathrm{e}^{i\hat{S}}\left(\sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k)\right)\mathrm{e}^{-i\hat{S}} \;\rightarrow\; & \sum_{j<k}\hat{V}_{jk}(\mathbf{r}_j-\mathbf{r}_k) \\ & + \frac{1}{2mc}\sum_{k<l}\sum_{j=k,l}\Big[\beta_j\boldsymbol{\alpha}_j\cdot[\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)],\hat{V}_{kl}(\mathbf{r}_k-\mathbf{r}_l)\Big]. \end{aligned} \tag{155}$$

The transformed Hamiltonian can be approximated by

$$
\begin{aligned}
\hat{H}' \;\rightarrow\; & mc^2 \sum_j \beta_j + \sum_j \frac{|\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)|^2}{2m}\beta_j + \sum_{j<k} \hat{V}_{jk}(\mathbf{r}_j - \mathbf{r}_k) + \sum_j q_j \Phi(\mathbf{r}_j) - \sum_j \frac{\hbar q_j}{2m}\beta_j \boldsymbol{\Sigma}_j \cdot \mathbf{B}(\mathbf{r}_j) \\
& + \sum_j \frac{\hbar q_j}{8m^2c^2}\boldsymbol{\Sigma}_j \cdot \Big([\hat{\mathbf{p}}_j - q\mathbf{A}(\mathbf{r}_j)] \times \mathbf{E}(\mathbf{r}_j) - \mathbf{E}(\mathbf{r}_j) \times [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)] \Big) - \sum_j \frac{q_j \hbar^2}{8m^2c^2} \nabla \cdot \mathbf{E}(\mathbf{r}_j) \\
& + \frac{1}{2mc} \sum_{k<l} \sum_{j=k,l} \Big[\beta_j \boldsymbol{\alpha}_j \cdot [\hat{\mathbf{p}}_j - q_j \mathbf{A}(\mathbf{r}_j)], \hat{V}_{kl}(\mathbf{r}_k - \mathbf{r}_l) \Big].
\end{aligned} \tag{156}
$$

This model might be viewed as more or less a nonrelativistic composite model (but for a 4^N-component wave function in the F-W representation) with relativistic corrections. As such it is closely related to the composite model developed in the previous section, with the gauge invariance problem now fixed.

9.4. Model in terms of relative and center of mass operators

As before, we can make us of relative and center of mass variables defined according to

$$
\mathbf{R} = \frac{1}{N}\sum_j \mathbf{r}_j, \qquad \hat{\mathbf{P}} = \sum_j \hat{\mathbf{p}}_j,
$$

$$
\boldsymbol{\xi}_j = \mathbf{r}_j - \mathbf{R}, \qquad \hat{\boldsymbol{\pi}}_j = \hat{\mathbf{p}}_j - \frac{\hat{\mathbf{P}}}{N}.
$$

We can use these to write the transformed model as

$$
\begin{aligned}
\hat{H}' \;\to\; & mc^2 \sum_j \beta_j + \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M} \frac{1}{N} \sum_j \beta_j + Q\Phi \\
& + \sum_j \frac{\left| \hat{\boldsymbol{\pi}}_j - q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right|^2}{2m} \beta_j + \sum_{j<k} \hat{V}_{jk} - \mathbf{d} \cdot \mathbf{E}_L - \hat{\boldsymbol{\mu}}_s \cdot \mathbf{B} \\
& + \frac{1}{2mc} \sum_{k<l} \sum_{j=k,l} \left[\beta_j \boldsymbol{\alpha}_j \cdot \left(\hat{\boldsymbol{\pi}}_j - q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right), \hat{V}_{kl} \right] \\
& - \frac{Q\hbar^2}{8m^2c^2} \nabla \cdot \mathbf{E} + \sum_j \frac{\hbar q_j}{8Mmc^2} \boldsymbol{\Sigma}_j \cdot \left[\left(\hat{\mathbf{P}} - Q\mathbf{A} \right) \times \mathbf{E} - \mathbf{E} \times \left(\hat{\mathbf{P}} - Q\mathbf{A} \right) \right] \\
& + \sum_j \frac{\hbar q_j}{8m^2c^2} \boldsymbol{\Sigma}_j \cdot \left[\left(\hat{\boldsymbol{\pi}}_j - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right) \times \mathbf{E} - \mathbf{E} \times \left(\hat{\boldsymbol{\pi}}_j - q_l \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right) \right] \\
& + \sum_j \frac{(\hat{\mathbf{P}} - Q\mathbf{A}) \cdot \left(\hat{\boldsymbol{\pi}}_j - q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right)}{2M} \beta_j \\
& + \sum_j \frac{\left(\hat{\boldsymbol{\pi}}_j - q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right) \cdot (\hat{\mathbf{P}} - Q\mathbf{A})}{2M} \beta_j \\
& + \frac{1}{2Mc} \sum_{k<l} \sum_{j=k,l} \left[\beta_j \boldsymbol{\alpha}_j \cdot (\hat{\mathbf{P}} - Q\mathbf{A}), \hat{V}_{kl} \right] + \cdots
\end{aligned}
\tag{157}
$$

This composite model is more or less in a standard form, and we see the center of mass and relative Hamiltonians, couplings with external fields, electrostatic and nuclear spin–orbit terms, as well as terms that couple the center of mass to the internal degrees of freedom.

9.5. Center of mass coupling with internal degrees of freedom

One of the issues in which we are interested in particular concerns the coupling between the center of mass degrees of freedom and the internal degrees of freedom, so we are motivated to examine the associated terms further.

Since

$$
\sum_j \hat{\boldsymbol{\pi}}_j = 0, \tag{158}
$$

we can write

$$
\sum_j \frac{\hat{\mathbf{P}} \cdot \hat{\boldsymbol{\pi}}_j}{M} \beta_j = \sum_j \frac{\hat{\mathbf{P}} \cdot \hat{\boldsymbol{\pi}}_j}{M} (\beta_j - \mathbf{I}_j), \tag{159}
$$

where

$$\mathbf{I}_j = \begin{bmatrix} 1\,0\,0\,0 \\ 0\,1\,0\,0 \\ 0\,0\,1\,0 \\ 0\,0\,0\,1 \end{bmatrix}_j . \tag{160}$$

This suggests that the coupling associated with this kinetic energy term between the center of mass momentum and the internal relative momenta is of higher order in the inverse mass under conditions where the composite momentum is small.

In the absence of external fields there is a coupling between the center of mass momentum and the particle–particle potential

$$\frac{1}{2Mc}\sum_{j<k}\left[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\right]. \tag{161}$$

This term is closely related to the nonrelativistic version of the interaction we found when eliminating the contribution of the negative energy sectors above. We will consider this term further later on in this paper.

9.6. Modification in the case of Dirac–Pauli interaction

We noted above that protons and neutrons have anomalous magnetic moments, so that an additional Pauli interaction is sometimes used. In this case we would begin with

$$\begin{aligned}\hat{H} = &\sum_j \left[\beta_j mc^2 + \boldsymbol{\alpha}_j\cdot c[\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)]\right] + \sum_{j<k}\hat{V}_{jk} + \sum_j q_j\Phi(\mathbf{r}_j) \\ &- \sum_j \lambda_j \frac{e\hbar}{2m}\beta_j\left[\boldsymbol{\sigma}_j\cdot\mathbf{B}(\mathbf{r}_j) - i\boldsymbol{\alpha}_j\cdot\mathbf{E}(\mathbf{r}_j)\right].\end{aligned}$$

The nonrelativistic limit of this kind of model has been discussed numerous times in the literature [37,169–174].

If the lowest-order contributions to the magnetic dipole interaction are summed and combined with the anomalous magnetic dipole contribution, then at lowest order we can write

$$\begin{aligned}&-\sum_j \frac{q_j\boldsymbol{\xi}_k\times\hat{\boldsymbol{\pi}}_j}{2m}\cdot\mathbf{B}(\mathbf{R}) - \sum_j\frac{\hbar q_j}{2m}\boldsymbol{\sigma}_j\cdot\mathbf{B}(\mathbf{r}_j) - \sum_j\lambda_j\frac{e\hbar}{2m}\boldsymbol{\sigma}_j\cdot\mathbf{B}(\mathbf{r}_j) \\ &= -\sum_j \frac{q_j\boldsymbol{\xi}_k\times\hat{\boldsymbol{\pi}}_j}{2m}\cdot\mathbf{B}(\mathbf{R}) - \sum_j g_j\frac{e\hbar}{4m}\boldsymbol{\sigma}_j\cdot\mathbf{B}(\mathbf{r}_j) \\ &\to\ -(\hat{\boldsymbol{\mu}}_l + \boldsymbol{\mu}_s + \boldsymbol{\mu}_a)\cdot\mathbf{B}(\mathbf{R}) = -\sum_j\left(\frac{q_j}{2m}\mathbf{l}_j + \frac{e}{2m}g_j\mathbf{s}_j\right)\cdot\mathbf{B} = -\boldsymbol{\mu}\cdot\mathbf{B}.\end{aligned} \tag{162}$$

The magnetic dipole moment in this model is made up of a nonrelativistic contribution due to the internal (relative) angular momentum $\boldsymbol{\mu}_l$, a relativistic contribution due to the nucleon spin $\boldsymbol{\mu}_s$, and an extra component included through the Pauli interaction to account for the anomalous magnetic moment $\boldsymbol{\mu}_a$.

A correction also occurs for the spin–orbit terms involving the electrostatic interaction [203,204]

$$\sum_j \frac{\hbar q_j}{8m^2c^2}\mathbf{\Sigma}_j \cdot \left([\hat{\mathbf{p}}_j - q\mathbf{A}(\mathbf{r}_j)] \times \mathbf{E}(\mathbf{r}_j) - \mathbf{E}(\mathbf{r}_j) \times [\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)] \right) - \sum_j \frac{q_j\hbar^2}{8m^2c^2}\nabla \cdot \mathbf{E}(\mathbf{r}_j)$$
$$\to \sum_j \frac{\hbar(q_j + 2e\lambda_j)}{8m^2c^2}\mathbf{\Sigma}_j \cdot \left([\hat{\mathbf{p}}_j - q\mathbf{A}(\mathbf{r}_j)] \times \mathbf{E}(\mathbf{r}_j) - \mathbf{E}(\mathbf{r}_j) \times [\hat{\mathbf{p}}_j - q_j\mathbf{A}(\mathbf{r}_j)] \right)$$
$$- \sum_j \frac{\hbar^2(q_j + 2e\lambda_j)}{8m^2c^2}\nabla \cdot \mathbf{E}(\mathbf{r}_j). \tag{163}$$

10. A Partial Foldy–Wouthuysen Transformation

The motion of the nuclei in the lattice is very much nonrelativistic; however, it may be that the interior nuclear structure problem may be relativistic. It would be good to have a formulation in which the relative problem is treated relativistically, while at the same time treating the center of mass problem nonrelativistically. In this section we make use of a partial Foldy–Wouthuysen transformation to develop such a formulation.

10.1. Isolation of a center of mass Hamiltonian

We begin with the relativistic model expressed in terms of center of mass and relative variables

$$\hat{H} = \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c \left[\frac{\hat{\mathbf{P}}}{N} + \hat{\boldsymbol{\pi}}_j - q_j\mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) \right] + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) + \sum_j q_j\Phi(\mathbf{R} + \boldsymbol{\xi}_j) \tag{164}$$

and rewrite it according to

$$\hat{H} = \hat{H}_{\mathbf{R}} + \hat{H}_{\boldsymbol{\xi}} + \hat{H}_{\text{int}} \tag{165}$$

with

$$\hat{H}_{\mathbf{R}} = \sum_j \beta_j mc^2 + \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) + Q\Phi, \tag{166}$$

$$\hat{H}_{\boldsymbol{\xi}} = \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k), \tag{167}$$

$$\hat{H}_{\text{int}} = \sum_j \left[q_j\Phi(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\Phi(\mathbf{R}) \right] - \sum_j \boldsymbol{\alpha}_j \cdot c \left[q_j\mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right]. \tag{168}$$

We identify $\hat{H}_{\mathbf{R}}$ as a center of mass Hamiltonian, which will be the focus of our partial Foldy–Wouthuysen transform. The remaining terms in the Hamiltonian include $\hat{H}_{\boldsymbol{\xi}}$ which here is an incomplete version of the relative Hamiltonian, and $\hat{H}_{\text{int}}$ which includes the residual interaction with the external electromagnetic field.

10.2. Rotation of the center of mass Hamiltonian

It is possible to carry out a Foldy–Wouthuysen transformation on the center of mass Hamiltonian which leads to a model that will be of interest for us. The transformed center of mass Hamiltonian is

$$\hat{H}'_{\mathbf{R}} = \mathrm{e}^{i\hat{S}}\left(\hat{H}_{\mathbf{R}} - i\hbar\frac{\partial}{\partial t}\right)\mathrm{e}^{-i\hat{S}}.$$

We work with a transformation based on

$$\hat{S} = -i\frac{1}{2Mc^2}\sum_j \beta_j \boldsymbol{\alpha}_j \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}). \tag{169}$$

The implementation of this rotation is nontrivial, and details are provided in Appendix B. The result can be written as

$$\begin{aligned}\hat{H}'_{\mathbf{R}} \ \rightarrow\ & \sum_j \beta_j mc^2 + \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M}\frac{1}{N}\sum_j \beta_j + Q\Phi - \frac{\hbar Q}{2M}\frac{1}{N}\sum_j \beta_j \boldsymbol{\Sigma}_j \cdot \mathbf{B} \\ & - \frac{\hbar^2 Q}{8M^2c^2}\sum_j \nabla\cdot\mathbf{E} + \frac{\hbar Q}{8M^2c^2}\sum_j \boldsymbol{\Sigma}_j \cdot \left[(\hat{\mathbf{P}} - Q\mathbf{A})\times\mathbf{E} - \mathbf{E}\times(\hat{\mathbf{P}} - Q\mathbf{A})\right].\end{aligned} \tag{170}$$

10.3. Transformed Hamiltonian

We can apply the same rotation to the full Hamiltonian according to

$$\hat{H}' = \hat{H}'_{\mathbf{R}} + \mathrm{e}^{i\hat{S}}\hat{H}_{\boldsymbol{\xi}}\mathrm{e}^{-i\hat{S}} + \mathrm{e}^{i\hat{S}}\hat{H}_{\text{int}}\mathrm{e}^{-i\hat{S}}. \tag{171}$$

In the event that the external fields are relatively weak then we should be able to work with

$$\hat{H}' \ \rightarrow\ \hat{H}'_{\mathbf{R}} + \hat{H}_{\boldsymbol{\xi}} + \hat{H}_{\text{int}} + i[\hat{S}, \hat{H}_{\boldsymbol{\xi}}]. \tag{172}$$

We can evaluate

$$i[\hat{S}, \hat{H}_{\boldsymbol{\xi}}] = \frac{1}{M}\sum_j \beta_j(\hat{\mathbf{P}} - Q\mathbf{A})\cdot\hat{\boldsymbol{\pi}}_j + \frac{1}{2Mc}\sum_{k<l}\sum_{j=k,l}\left[\beta_j\boldsymbol{\alpha}_j\cdot(\hat{\mathbf{P}} - Q\mathbf{A}), \hat{V}_{kl}\right]. \tag{173}$$

We can collect terms and write

$$
\begin{aligned}
\hat{H}' \;\rightarrow\;& \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M}\frac{1}{N}\sum_j \beta_j + Q\Phi - \frac{\hbar Q}{2M}\frac{1}{N}\sum_j \beta_j \boldsymbol{\Sigma}_j \cdot \mathbf{B} - \frac{\hbar^2 Q}{8M^2c^2}\nabla\cdot\mathbf{E} \\
&+ \frac{\hbar Q}{8M^2c^2}\sum_j \boldsymbol{\Sigma}_j \cdot \bigg[(\hat{\mathbf{P}} - Q\mathbf{A})\times\mathbf{E} - \mathbf{E}\times(\hat{\mathbf{P}} - Q\mathbf{A})\bigg] \\
&+ \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk} \\
&+ \sum_j \bigg[q_j\Phi(\mathbf{R}+\boldsymbol{\xi}_j) - \frac{Q}{N}\Phi(\mathbf{R})\bigg] - \sum_j \boldsymbol{\alpha}_j\cdot c\bigg[q_j\mathbf{A}(\mathbf{R}+\boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R})\bigg] \\
&+ \frac{1}{M}\sum_j \beta_j(\hat{\mathbf{P}} - Q\mathbf{A})\cdot\hat{\boldsymbol{\pi}}_j + \frac{1}{2Mc}\sum_{j<k}\bigg[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot(\hat{\mathbf{P}} - Q\mathbf{A}), \hat{V}_{jk}\bigg].
\end{aligned}
\tag{174}
$$

The terms in the first two lines of this rotated Hamiltonian models the center of mass degrees of freedom in a nonrelativistic model interacting with the radiation field; terms in the third line models the field-free relative nuclear problem in the rest frame; terms in the fourth line account for the interaction of the internal degrees of freedom with the external electromagnetic field; and terms in the last line model the interaction of the canonical momentum of the center of mass with the internal degrees of freedom.

11. The Poincaré Group and Composite Models

In our discussions above we have considered models for composites derived from the nonrelativistic many-particle Schrödinger equation and the many-particle Dirac equation. However, the interacting many-particle Dirac model is in general not covariant, and this motivates us to consider the issue of invariance. The basic idea is that if we have a model for a composite at rest, then our model should be invariant if we translate the composite in free space, or if we rotate it, or if it moves with constant velocity [210]. Wigner considered invariance in connection with relativistic quantum mechanics in an early often-cited paper [211], and in some subsequent publications [78,212,213]. These ideas have had a fundamental impact on relativistic quantum mechanics and field theory; our interest in this section is focused only on a number of specific issues that follow from these general considerations which are of interest to us and which have been discussed in the literature.

11.1. Lie algebra of the Lorentz group

Wigner was interested in representations of what he termed the inhomogeneous Lorentz group [211], which appears in more recent literature as the Poincaré group. We are interested in the Lie algebra of the Poincaré group in connection with the discussion to follow. However, it seems worthwhile to begin with the generators and Lie algebra of the Lorentz group first.

Consider generators for infinitesimal rotations and boosts $\hat{\mathbf{J}}$ and $\hat{\mathbf{K}}$, which can be used to implement a rotation according to

$$
\Psi' = \exp\bigg(-i\theta\hat{\mathbf{n}}\cdot\hat{\mathbf{J}}\bigg)\Psi,
\tag{175}
$$

where $\hat{\mathbf{n}}$ is the axis of rotation and θ is the rotation angle; the infinitesimal boost operator can be used to implement a finite boost according to

$$\Psi' = \exp\left(i\frac{\mathbf{v}}{c}\cdot\hat{\mathbf{K}}\right)\Psi, \tag{176}$$

where $\mathbf{u}$ is the increase in velocity resulting from the boost. These are the infinitesimal operators of the Lorentz group, which satisfy the Lie algebra

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k,$$

$$[\hat{J}_i, \hat{K}_j] = i\hbar\epsilon_{ijk}\hat{K}_k,$$

$$[\hat{K}_i, \hat{K}_j] = -i\hbar\epsilon_{ijk}\frac{1}{c^2}\hat{J}_k, \tag{177}$$

where ϵ_{ijk} is the Levi-Civita symbol

$$\epsilon_{jkl} = \begin{cases} +1 \text{ if } (i,j,k) = (1,2,3),(2,3,1),(3,1,2), \\ -1 \text{ if } (i,j,k) = (3,2,1),(2,1,3),(1,3,2), \\ 0, \quad \text{otherwise.} \end{cases} \tag{178}$$

This Lie algebra is consistent with Ref. [214].

11.2. Lie algebra of the Poincaré group

Wigner understood that infinitesimal generators for translations in spacetime should be considered as well, which takes us from the Lorentz group to the inhomogeneous Lorentz group, or Poincaré group.

The momentum operator $\hat{\mathbf{P}}$ can be used as an infinitesimal generator of displacements in space according to

$$\Psi' = \exp\left(-i\frac{\mathbf{R}_0\cdot\hat{\mathbf{P}}}{\hbar}\right)\Psi, \tag{179}$$

where $\mathbf{R}_0$ is the displacement in position. The Hamiltonian operator is an infinitesimal generator of displacements in time according to

$$\Psi' = \exp\left(it_0\hat{H}\right)\Psi, \tag{180}$$

where t_0 is the displacement in time. The Lie algebra that results is the Lie algebra of the inhomogeneous Lorentz group or Poincaré group [78,215], which we can write as [216–221]

$$[\hat{P}_i, \hat{P}_j] = 0, \quad [\hat{P}_i, \hat{H}] = 0, \quad [\hat{J}_i, \hat{H}] = 0,$$

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k, \quad [\hat{J}_i, \hat{P}_j] = i\hbar\epsilon_{ijk}\hat{P}_k, \quad [\hat{J}_i, \hat{K}_j] = i\hbar\epsilon_{ijk}\hat{K}_k,$$

$$[\hat{K}_i, \hat{P}_j] = i\hbar\delta_{ij}\frac{1}{c^2}\hat{H}, \quad [\hat{K}_i, \hat{K}_j] = -i\hbar\epsilon_{ijk}\frac{1}{c^2}\hat{J}_k, \quad [\hat{K}_i, \hat{H}] = i\hbar\hat{P}_i. \tag{181}$$

If one has constructed a relativistic quantum model, one make use of this algebra to verify that it is an acceptable relativistic theory (that it is a representation of the Poincaré group) [78]. Alternatively, this algebra can be used to construct a relativistic model given a rest frame Hamiltonian [222].

11.3. Infinitesimal generators with no interaction

The many-particle Dirac Hamiltonian in the absence of an interaction, and without external fields

$$\hat{H} = \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j mc^2 \tag{182}$$

is a representation of a Hamiltonian generator of the Poincaré Lie algebra. In this case we can write for the other infinitesimal generators

$$\hat{\mathbf{P}} = \sum_j \hat{\mathbf{p}}_j, \tag{183}$$

$$\hat{\mathbf{J}} = \sum_j \mathbf{r}_j \times \hat{\mathbf{p}}_j + \frac{\hbar}{2}\boldsymbol{\Sigma}_j, \tag{184}$$

$$\hat{\mathbf{K}} = \frac{1}{2c^2}\sum_j \left[\mathbf{r}_j(\boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j mc^2) + (\boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j mc^2)\mathbf{r}_j\right]. \tag{185}$$

If a particle-particle interaction is present, then in general the resulting model will not be invariant. An exception occurs when the interaction potential is proporional to a δ-function [223]

11.4. Casimir invariant

A Casimir invariant $\hat{X}$ is an operator which commutes with the 10 Poincaré infinitesimal generators

$$\left[\hat{X}, \hat{H}\right] = 0, \quad \left[\hat{X}, \hat{P}_i\right] = 0, \quad \left[\hat{X}, \hat{J}_i\right] = 0, \quad \left[\hat{X}, \hat{K}_i\right] = 0. \tag{186}$$

With a few lines of commutator algebra it can be demonstrated that

$$\hat{M}^2c^4 = \hat{H}^2 - c^2|\hat{\mathbf{P}}|^2 \tag{187}$$

is a Casimir invariant, where $\hat{M}$ is a mass operator. This means that the energy momentum dispersion relation in a consistent relativistic model for a positive eigenvalue of a composite with no external fields must be

$$E = \sqrt{(Mc^2)^2 + c^2|\mathbf{P}|^2} \tag{188}$$

simply as a consequence of Poincaré invariance.

11.5. Separability

Poincaré invariance has numerous consequences, one of which is the separability of center of mass and relative degrees of freedom in free space. If the mass operator is a Casimir invariant, then it cannot depend on the momentum. Consequently, it should be possible to write the Hamiltonian for a Poincaré invariant model in the form [219,224]

$$\hat{H} = \sqrt{(\hat{M}c^2)^2 + c^2|\hat{\mathbf{P}}|^2}, \tag{189}$$

where $\hat{M}$ is a mass operator that depends only on relative degrees of freedom.

In the case of a two-particle Dirac model with a Breit interaction, it is possible to construct unitary transforms which separate the center of mass and relative mass terms up to $O(1/c^2)$ [209,224]. Separability in the case of more general potentials was discussed in Refs. [222,225,226]. Studies that focus on the impact on nuclear interaction models have appeared in [227–230].

11.6. Many-particle Dirac model with interaction

Our attention now turns to the issue of separability in the many-particle Dirac model when particle-particle interactions are present. We consider a model for a composite in the absence of external fields described by

$$\hat{H} = \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k). \tag{190}$$

We make use of the partial Foldy–Wouthuysen transformation of the last section to write a rotated Hamiltonian when no external fields are present

$$\begin{aligned} \hat{H}' \;\rightarrow\; & \frac{|\hat{\mathbf{P}}|^2}{2M}\frac{1}{N}\sum_j \beta_j + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk} \\ & + \frac{1}{M}\sum_j \beta_j \hat{\mathbf{P}}\cdot\hat{\boldsymbol{\pi}}_j + \frac{1}{2Mc}\sum_{j<k}\Big[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\Big]. \end{aligned} \tag{191}$$

The result of the unitary transformation is a Hamiltonian which contains separated center of mass and relative terms in the first line, and relatively small terms in the second line that provide a coupling between the center of mass and relative degrees of freedom. The coupling in the last term is consistent with the nonrelativistic reduction of a boosted composite Hamiltonian given in [231].

11.7. Interpretation for terms linear in $\hat{\mathbf{P}}$

To understand the significance of the new term we examine an example discussed some time ago in [209] which focused on the special case of the Coulomb plus Breit interaction. If we first consider the rest frame where

$$\hat{\mathbf{P}} \;\rightarrow\; 0 \tag{192}$$

then the many-particle Dirac Hamiltonian with no external field can be written as

$$\hat{H} = \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \frac{q_j q_k}{4\pi\epsilon_0} \left\{ \frac{1}{r_{jk}} - \frac{1}{2} \left[\frac{\boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k}{r_{jk}} + \frac{(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{jk})(\boldsymbol{\alpha}_k \cdot \mathbf{r}_{jk})}{r_{jk}^3} \right] \right\}. \tag{193}$$

We consider how this Hamiltonian should be modified if boosted so that the composite has a center of mass momentum $\hat{\mathbf{P}}$. For this argument we identify the $\boldsymbol{\alpha}$ matrices as equivalent normalized velocity operators (as a consequence of Ehrenfest's Theorem applied to the Dirac equation, where $\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r} \rangle = c\langle \boldsymbol{\alpha} \rangle$)

$$\boldsymbol{\alpha} \sim \frac{\hat{\mathbf{v}}}{c}. \tag{194}$$

If so, then from a naive perspective boosting the system should result in

$$\hat{\mathbf{v}} \to \hat{\mathbf{v}} + \frac{\hat{\mathbf{P}}}{M}. \tag{195}$$

Based on these simple considerations the boosted Hamiltonian should look something like

$$\hat{H} \to \frac{|\hat{\mathbf{P}}|^2}{2M} + \sum_j \beta_j mc^2 + \sum_j \left(\boldsymbol{\alpha}_j + \frac{\hat{\mathbf{P}}}{Mc} \right) \cdot c\hat{\boldsymbol{\pi}}_j$$
$$+ \sum_{j<k} \frac{q_j q_k}{4\pi\epsilon_0} \left\{ \frac{1}{r_{jk}} - \frac{1}{2} \left[\frac{\left(\boldsymbol{\alpha}_j + \frac{\hat{\mathbf{P}}}{Mc} \right) \cdot \left(\boldsymbol{\alpha}_k + \frac{\hat{\mathbf{P}}}{Mc} \right)}{r_{jk}} + \frac{\left(\boldsymbol{\alpha}_j + \frac{\hat{\mathbf{P}}}{Mc} \right) \cdot \mathbf{r}_{jk} \left(\boldsymbol{\alpha}_k + \frac{\hat{\mathbf{P}}}{Mc} \right) \cdot \mathbf{r}_{jk}}{r_{jk}^3} \right] \right\}. \tag{196}$$

We can rewrite this as

$$\hat{H} \to \frac{|\hat{\mathbf{P}}|^2}{2M} + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \frac{q_j q_k}{4\pi\epsilon_0} \left\{ \frac{1}{r_{jk}} - \frac{1}{2} \left[\frac{\boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k}{r_{jk}} + \frac{(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{jk})(\boldsymbol{\alpha}_k \cdot \mathbf{r}_{jk})}{r_{jk}^3} \right] \right\}$$
$$+ \sum_j \frac{\hat{\mathbf{P}} \cdot \hat{\boldsymbol{\pi}}_j}{M} - \frac{1}{2Mc} \frac{q_j q_k}{4\pi\epsilon_0} \left[\frac{\hat{\mathbf{P}} \cdot \boldsymbol{\alpha}_k}{r_{jk}} + \frac{\boldsymbol{\alpha}_j \cdot \hat{\mathbf{P}}}{r_{jk}} + \frac{(\hat{\mathbf{P}} \cdot \mathbf{r}_{jk})(\boldsymbol{\alpha}_k \cdot \mathbf{r}_{jk})}{r_{jk}^3} + \frac{(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{jk})(\hat{\mathbf{P}} \cdot \mathbf{r}_{jk})}{r_{jk}^3} \right]$$
$$+ \cdots \tag{197}$$

For the Coulomb plus Breit interaction the commutator that we found is evaluated to yield

$$-\frac{1}{4Mc} \frac{q_j q_k}{4\pi\epsilon_0} \sum_{j<k} \left[(\beta_j \boldsymbol{\alpha}_j + \beta_k \boldsymbol{\alpha}_k) \cdot \hat{\mathbf{P}}, \frac{\boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k}{r_{jk}} + \frac{(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{jk})(\boldsymbol{\alpha}_k \cdot \mathbf{r}_{jk})}{r_{jk}^3} \right]$$
$$= -\frac{1}{2Mc} \frac{q_j q_k}{4\pi\epsilon_0} \sum_{j<k} \left[\beta_j \frac{\hat{\mathbf{P}} \cdot \boldsymbol{\alpha}_k}{r_{jk}} + \beta_k \frac{\boldsymbol{\alpha}_j \cdot \hat{\mathbf{P}}}{r_{jk}} + \beta_j \frac{(\hat{\mathbf{P}} \cdot \mathbf{r}_{jk})(\boldsymbol{\alpha}_k \cdot \mathbf{r}_{jk})}{r_{jk}^3} + \beta_k \frac{(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{jk})(\hat{\mathbf{P}} \cdot \mathbf{r}_{jk})}{r_{jk}^3} \right]. \tag{198}$$

In this case the partial Foldy–Wouthuysen transformation gives us

$$\begin{aligned}\hat{H}' =& \frac{|\hat{\mathbf{P}}|^2}{2M}\frac{1}{N}\sum_j \beta_j + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\frac{q_j q_k}{4\pi\epsilon_0}\left\{\frac{1}{r_{jk}} - \frac{1}{2}\left[\frac{\boldsymbol{\alpha}_j\cdot\boldsymbol{\alpha}_k}{r_{jk}} + \frac{(\boldsymbol{\alpha}_j\cdot\mathbf{r}_{jk})(\boldsymbol{\alpha}_k\cdot\mathbf{r}_{jk})}{r_{jk}^3}\right]\right\} \\ &+ \sum_j \beta_j \frac{\hat{\mathbf{P}}\cdot\hat{\boldsymbol{\pi}}_j}{M} - \frac{1}{2Mc}\frac{q_j q_k}{4\pi\epsilon_0}\sum_{j<k}\left[\beta_j\frac{\hat{\mathbf{P}}\cdot\boldsymbol{\alpha}_k}{r_{jk}} + \beta_k\frac{\boldsymbol{\alpha}_j\cdot\hat{\mathbf{P}}}{r_{jk}} + \beta_j\frac{(\hat{\mathbf{P}}\cdot\mathbf{r}_{jk})(\boldsymbol{\alpha}_k\cdot\mathbf{r}_{jk})}{r_{jk}^3} + \beta_k\frac{(\boldsymbol{\alpha}_j\cdot\mathbf{r}_{jk})(\hat{\mathbf{P}}\cdot\mathbf{r}_{jk})}{r_{jk}^3}\right] \\ &+ \cdots\end{aligned} \tag{199}$$

Consequently, we understand the Hamiltonian that results from the partial Foldy–Wouthuysen transformation as generating a correction that accounts for how the interaction changes in a moving frame to first order. We see that β matrices are present in the expression that results from the evaluation of the commutator, and not present in our simple argument above; this of course complicates things, but the basic argument of [209] (and equivalent arguments given earlier by [108,161]) gives us an intuitive way to understand what the partial Foldy–Wouthuysen transformatation in this relativistic case is doing.

11.8. Terms up to second order

The nucleon-nucleon interaction models available in the literature are specified in the rest frame. We have seen that the magnetic interaction is modified in a moving composite, so we expect that parts of the nuclear interaction that are akin to the magnetic interaction will also be modified. In some nuclear physics calculations the empirical nuclear potential is corrected to account for this. For example, in [232–235] one finds

$$\hat{V}_{jk}(\mathbf{r}) \ \rightarrow \ \hat{V}_{jk}(\mathbf{r}) + \delta\hat{V}_{jk}(\mathbf{r}) \tag{200}$$

with

$$\begin{aligned}\delta\hat{V}_{jk}(\mathbf{r}_{jk}) =& \frac{1}{8m^2c^2}\left[(\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_k)\times\hat{\mathbf{P}}\cdot\hat{\mathbf{p}}_{jk}, \hat{V}_{jk}(\mathbf{r}_{jk})\right] - \frac{|\hat{\mathbf{P}}|^2}{8m^2c^2}\hat{V}_{jk}(\mathbf{r}_{jk}) \\ &+ i\frac{1}{8m^2c^2}\left[(\hat{\mathbf{P}}\cdot\mathbf{r}_{jk})(\hat{\mathbf{P}}\cdot\hat{\mathbf{p}}_{jk}), \hat{V}_{jk}(\mathbf{r}_{jk})\right].\end{aligned} \tag{201}$$

The term linear in $\hat{\mathbf{P}}$ is consistent with the first-order term from the partial Foldy–Wouthuysen transformation. The terms quadratic in $\hat{\mathbf{P}}$ are similar to second-order terms associated with

$$\hat{H}' = \hat{H} + i[\hat{S},\hat{H}] - \frac{1}{2}[\hat{S},[\hat{S},\hat{H}]] + \cdots \tag{202}$$

In this case the transformed Hamiltonian in free space is

$$\begin{aligned}\hat{H}' \rightarrow\ & \frac{|\hat{\mathbf{P}}|^2}{2M}\frac{1}{N}\sum_j \beta_j + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk} \\ & + \frac{1}{M}\sum_j \beta_j \hat{\mathbf{P}}\cdot\hat{\boldsymbol{\pi}}_j + \frac{1}{2Mc}\sum_{j<k}\left[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\right] \\ & + \frac{1}{8(Mc)^2}\sum_{j<k}\left[(\boldsymbol{\alpha}_j + \boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \left[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\right]\right].\end{aligned} \tag{203}$$

Much effort has gone into the development of chiral effective field theory [101] for the development of accurate nucleon–nucleon potential models [45]. A reduction of the potential based on a relativistic formalism has been considered [236–240], with a modification of the potential due to motion discussed in [241,242].

11.9. Elimination of the larger coupling term

Based on the discussion above a Poincaré invariant model (in free space with no external fields) is separable in the sense of a Hamiltonian with a square root as in Eq. (189); and separable as a conventional Hamiltonian at low order when the square root is linearized. The many-particle Dirac model with interactions is consistent with a separable low-order Hamiltonian in the second sense to $O(1/c^2)$ [224,225].

This suggests that we should be able to rotate out the terms linear in $\hat{\mathbf{P}}$ in $\hat{H}'$; of specific interest here is the elimination of the larger coupling term involving the commutator with the potential. We have found that it is possible to eliminate it using

$$\hat{S}' = -i\frac{1}{8Mmc^3}\sum_{j<k}\left[\beta_j + \beta_k, \left[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\right]\right] \tag{204}$$

in the event that

$$\beta_j\beta_k\hat{V}_{jk} = \hat{V}_{jk}\beta_j\beta_k \tag{205}$$

since (as can be shown with substantial algebra that)

$$i\left[\hat{S}', \sum_j \beta_j mc^2\right] = -\frac{1}{2Mc}\sum_{j<k}\left[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\right]. \tag{206}$$

The success of this rotation supports the suspicion that the many-particle Dirac model with interaction but no external fields in free space approximately separates at low order.

11.10. Impact of separability on external fields

If external fields are present, this rotation will result in terms where the external fields couple to internal states of the composite based on complicated interactions involving the particle-particle interaction. This can be illustrated by considering the lowest order terms generated with the rotation above when an electrostatic potential is present. In this case we can write

$$
\begin{aligned}
i\left[\hat{S}', Q\Phi\right] &= i\left[-i\frac{1}{8Mmc^3}\sum_{j<k}\left[\beta_j+\beta_k, \left[(\beta_j\boldsymbol{\alpha}_j+\beta_k\boldsymbol{\alpha}_k)\cdot\hat{\mathbf{P}}, \hat{V}_{jk}\right]\right], Q\Phi\right] \\
&= -\,i\frac{\hbar Q}{8Mmc^3}\sum_{j<k}(\beta_j+\beta_k)(\beta_j\boldsymbol{\alpha}_j+\beta_k\boldsymbol{\alpha}_k)\cdot\mathbf{E}_L\hat{V}_{jk}-(\beta_j+\beta_k)\hat{V}_{jk}(\beta_j\boldsymbol{\alpha}_j+\beta_k\boldsymbol{\alpha}_k)\cdot\mathbf{E}_L \\
&\quad -(\beta_j\boldsymbol{\alpha}_j+\beta_k\boldsymbol{\alpha}_k)\cdot\mathbf{E}_L\hat{V}_{jk}(\beta_j+\beta_k)+\hat{V}_{jk}(\beta_j\boldsymbol{\alpha}_j+\beta_k\boldsymbol{\alpha}_k)\cdot\mathbf{E}_L(\beta_j+\beta_k).
\end{aligned}
\tag{207}
$$

The coupling that we have rotated out now shows up reduced in magnitude in other parts of the model.

12. Many Nuclei in a Lattice

We are interested in composite models in connection with the development of a theory for anomalies in condensed matter nuclear science, where we consider the situation where many identical nuclei interact with a common highly excited vibrational model. The basis for models that we have studied has consisted of treating the nuclei as composites each with coupling terms linear in $\hat{\mathbf{P}}$, making use of a finite basis approximation, and then diagonalizing the problem that results.

If one were to naively adopt the point of view that the center of mass degrees of freedom separate from the internal degrees of freedom, then the basic program under consideration for this kind of model would be called into question. Since we are able to carry out the rotations that implement the separation, it seems useful to think about these kinds of models in terms of the rotations. Based on the discussion above, it may be best to make use of the partial Foldy–Wouthuysen transformation above in order to work with a nonrelativistic description for the center of mass degrees of freedom. Then we can consider a second rotation to implement low-order separability.

12.1. Many nuclei interacting with a common vibrational mode

Suppose that we consider a simple version of the model in which the nuclei in the lattice interact through screened Coulomb and exchange forces. In this case we could start out with an idealized Hamiltonian of the form

$$
\begin{aligned}
\hat{H} = &\sum_a\left\{\frac{1}{N_a}\sum_{j_a}\boldsymbol{\alpha}_{j_a}\cdot c\hat{\mathbf{P}}_a+\sum_{j_a}\beta_{j_a}mc^2+\sum_{j_a}\boldsymbol{\alpha}_{j_a}\cdot c\hat{\boldsymbol{\pi}}_{j_a}+\sum_{j_a<k_a}\hat{V}_{j_ak_a}(\boldsymbol{\xi}_{j_a}-\boldsymbol{\xi}_{k_a})\right\} \\
&+\sum_{a<b}\sum_{j_a,k_b}q_{j_a}q_{k_b}U_{ab}(\mathbf{r}_{j_a}-\mathbf{r}_{k_b}),
\end{aligned}
\tag{208}
$$

where $U_{ab}(\mathbf{r}_{j_a}-\mathbf{r}_{k_b})$ models the screened Coulomb interaction between nucleons in different nuclei in a Born-Oppenheimer picture. The summation over a indicates summing over the different nuclei; and the index j_a indicates a specific nucleon within nucleus a. For this model we have eliminated other external field interactions in order to simplify the notation.

12.2. First transformation

We consider now a big partial Foldy–Wouthuysen transformation which eliminates the $\boldsymbol{\alpha}_{j_a}\cdot c\hat{\mathbf{P}}_a$ coupling terms.

$$\hat{H}' = \mathrm{e}^{i\hat{S}} \left[\hat{H} - i\hbar \frac{\partial}{\partial t} \right] \mathrm{e}^{-i\hat{S}} \tag{209}$$

with

$$\hat{S} = -i \frac{1}{2mc^2} \sum_a \frac{1}{N_a} \sum_{j_a} \beta_{j_a} \alpha_{j_a} \cdot c\hat{\mathbf{P}}_a. \tag{210}$$

This leads to a transformed Hamiltonian of the form

$$\begin{aligned}
\hat{H}' \;\rightarrow\; & \sum_a \Bigg\{ \frac{|\hat{\mathbf{P}}_a|^2}{2M_a} \frac{1}{N_a} \sum_{j_a} \beta_{j_a} + \sum_{j_a} \beta_{j_a} mc^2 + \sum_{j_a} \boldsymbol{\alpha}_{j_a} \cdot c\hat{\boldsymbol{\pi}}_{j_a} + \sum_{j_a<k_a} \hat{V}_{j_a k_a} \\
& + \frac{1}{M_a} \sum_{j_a} \beta_{j_a} \hat{\mathbf{P}}_a \cdot \hat{\boldsymbol{\pi}}_{j_a} + \frac{1}{2M_a c} \sum_{j_a<k_a} \left[(\beta_{j_a} \boldsymbol{\alpha}_{j_a} + \beta_{k_a} \boldsymbol{\alpha}_{k_a}) \cdot \hat{\mathbf{P}}_a, \hat{V}_{j_a k_a} \right] \Bigg\} \\
& + \sum_{a<b} Q_a Q_b U_{ab}(\mathbf{R}_a - \mathbf{R}_b) + \sum_{a<b} \sum_{j_a, k_b} \left(q_{j_a} q_{k_b} U_{ab}(\mathbf{r}_{j_a} - \mathbf{r}_{k_b}) - \frac{Q_a}{N_a} \frac{Q_b}{N_b} U_{ab}(\mathbf{R}_a + \boldsymbol{\xi}_{j_a} - \mathbf{R}_b - \boldsymbol{\xi}_{j_b}) \right) \\
& + \sum_{b \neq a} \frac{\hbar^2 Q_a Q_b}{8M_a^2 c^2} \nabla^2 U_{ab}(\mathbf{R}_a - \mathbf{R}_b) - \sum_{a \neq b} \frac{\hbar Q_a Q_b}{8M_a^2 c^2} \sum_{j_a} \boldsymbol{\Sigma}_{j_a} \cdot \left[\hat{\mathbf{P}}_a \times (\nabla U_{ab}) - (\nabla U_{ab}) \times \hat{\mathbf{P}}_a \right] + \cdots ,
\end{aligned} \tag{211}$$

where $M_a = N_a m$ is the mass of nucleons in nucleus a. Although this rotated Hamiltonian is more complicated that the single composite equivalent that we encountered previously, we can see familiar terms; including dipole coupling terms to internal states; spin–orbit terms associated with the screened Coulomb and exchange interactions; and other coupling terms. Our inclination at this point is to neglect all minor terms not involved with the effects of immediate interest for the anomalies, and approximate the rotated Hamiltonian as

$$\begin{aligned}
\hat{H}' \;\approx\; & \sum_a \frac{|\hat{\mathbf{P}}_a|^2}{2M_a} + \sum_{a<b} Q_a Q_b U_{ab}(\mathbf{R}_a - \mathbf{R}_b) + \sum_a \Bigg\{ \sum_{j_a} \beta_{j_a} mc^2 + \sum_{j_a} \boldsymbol{\alpha}_{j_a} \cdot c\hat{\boldsymbol{\pi}}_{j_a} + \sum_{j_a<k_a} \hat{V}_{j_a k_a} \Bigg\} \\
& + \sum_a \frac{1}{2M_a c} \sum_{j_a<k_a} \left[(\beta_{j_a} \boldsymbol{\alpha}_{j_a} + \beta_{k_a} \boldsymbol{\alpha}_{k_a}) \cdot \hat{\mathbf{P}}_a, \hat{V}_{j_a k_a} \right].
\end{aligned} \tag{212}$$

What remains are center of mass kinetic and potential energy terms for the different nuclei, relative Hamiltonians for the internal nuclear states, and coupling terms which arise due to the modification of the nuclear forces when the nuclei are in motion.

12.3. Second transformation

If the nuclei were not interacting in free space, we would expect to be able to rotate out the coupling terms linear in $\hat{\mathbf{P}}_a$. For nuclei in the lattice the situation is not so clear since the nuclei interact with one another. Nevertheless, we can attempt a second Foldy–Wouthuysen transformation based on

$$\hat{S}' = -i \sum_a \frac{1}{8M_a mc^3} \sum_{j_a < k_a} \left[\beta_{j_a} + \beta_{k_a}, \left[(\beta_{j_a} \boldsymbol{\alpha}_{j_a} + \beta_{k_a} \boldsymbol{\alpha}_{k_a}) \cdot \hat{\mathbf{P}}_a, \hat{V}_{j_a k_a} \right] \right] \tag{213}$$

assuming that

$$\beta_j \beta_k \hat{V}_{jk} = \hat{V}_{jk} \beta_j \beta_k. \tag{214}$$

We can write for the doubly rotated Hamiltonian

$$\begin{aligned} \hat{H}'' \rightarrow\ & \sum_a \frac{|\hat{\mathbf{P}}_a|^2}{2M_a} + \sum_{a<b} Q_a Q_b U_{ab}(\mathbf{R}_a - \mathbf{R}_b) + \sum_a \left\{ \sum_{j_a} \beta_{j_a} mc^2 + \sum_{j_a} \boldsymbol{\alpha}_{j_a} \cdot c\hat{\boldsymbol{\pi}}_{j_a} + \sum_{j_a < k_a} \hat{V}_{j_a k_a} \right\} \\ & + i \left[\hat{S}', \sum_{a<b} Q_a Q_b U_{ab}(\mathbf{R}_a - \mathbf{R}_b) \right] - \frac{1}{2} \left[\hat{S}', \left[\hat{S}', \sum_{a<b} Q_a Q_b U_{ab}(\mathbf{R}_a - \mathbf{R}_b) \right] \right] + \cdots \end{aligned} \tag{215}$$

To lowest order the coupling term is eliminated, and all that remains is the rotation of the screened Coulomb interaction. In the first line are the lowest-order terms of the separated lattice and nuclear Hamiltonian; in the second line are some of the residual terms that remain.

The apparent simplicity of this doubly rotated Hamiltonian is probably deceptive. Operators that mediate internal transitions of one nucleus get imprinted on the screened Coulomb and exchange interaction of neighboring nuclei at lowest order. At next order these operators propagate to even more nuclei, and there appear many new terms with with products of operators involving internal transitions at different sites. If all of the nuclei are initially in the ground state, and if the lattice is unexcited or thermal then we would not expect any significant consequences associated with the neglect of this exponential explosion of coupling terms. However, this would not be expected to be true in general.

Consider the case of an excitation transfer effect mediated by phonon exchange in a lattice, where second-order coupling terms results in the excitation at one site to be coupled to identical nuclei at a great many other sites. In this case a description of the problem without the additional rotation seems most straightforward. Working with a rotated version of the problem to model excitation transfer is of course possible (since a rotation implements a basis change but otherwise does not change the model), but in this case the unrotated version of the problem would be preferred.

12.4. Connection with spin-boson type models

From these arguments we see that the separability of the free space problem with no interaction between composites does not immediately translate into a guaranteed separability when nuclei are in a lattice. The simple rotation that works cleanly for the free space problem now generates and explosion of terms in the lattice version of the problem. While there are cases where the resulting separated model will be a good approximation for the physical system, there is no reason to believe that this is true universally.

The lattice problem with nuclei interacting through effective forces is much more complicated, and the only way to develop reliable predictions is to work with models for the coupled lattice nucleus problem. In the highly idealized case where the nuclear system is abstracted by equivalent two-level systems, and the multi-mode lattice vibrations are replaced by a single oscillator, then what remains is a spin–boson model [243]. And it is well known that a variety of dynamical effects involving many two-level systems occur in the spin-boson model. We have argued that when the lossy spin-boson model is augmented with loss that efficient coherent energy exchange is possible in the multi-phonon regime [243–248].

13. Relativistic Models for Composites

In the past few sections we have covered some of the more important models and issues that relate to the use of composites for condensed matter nuclear science. What remains are topics which might help to complete our review of models for composites, and which may point to future directions for composite model development for applications.

For example, it would be nice to have a simple few-level Poincaré invariant model that we might adapt for us in the context of a lattice model. In this case we might be able to address concerns about how the coupling with vibrational degrees of freedom work, starting from models easier to understand. Alternatively, it would be nice to have a covariant version of the many-particle Dirac model with interactions, since there might be concerns about the coupling provided by the noncovariant many-particle Dirac model used in the sections above.

These and other issues provide motivation for us to consider other composite models which have been discussed in the literature which might provide a different starting place for constructing new models in the future. For example, there are models which can be viewed as essentially covariant N-level systems; there are a variety of covariant or Poincaré invariant models for composites, as well as other models that are approximately Poincaré invariant. In this section our goal is to provide a survey of some of the alternate approaches.

13.1. Elementary particle models with different spin states

In Section 4 we discussed the Rarita–Schwinger model [49] for a spin 3/2 particle; as was discussed this model includes constraints which eliminate two spin 1/2 states with the same mass. If these constraints were not imposed, then we would be left with the underlying relativistically invariant model which describes a particle with three different available sets of states, all with the same mass. One could imagine making use of this model as a kind of Poincaré invariant equivalent N-level model to in which transitions and relativistically invariant kinematics could be studied.

The Rarita–Schwinger model is not unique in this regard. There are several relativistic wave equations in the literature that include two or more spin configurations, as discussed in [249,250].

13.2. Elementary particle models with different mass states

We also considered in Section 4 the Dirac–Fierz–Pauli model [46,47] for a spin 3/2 particle, which once again involves constraints in order to remove a spin 1/2 state with a different mass. Were we to discard the constraint, the resulting elementary particle model could describe a composite with a spin 1/2 and spin 3/2 states of different masses. This is interesting, as it potentially provides us with a relatively simple Poincaré invariant model with nondegenerate states; however, we would prefer a to work with a model in which we could arbitrarily specify the state energies. Other models with two states are discussed in [251–256].

13.3. Infinite-component wave equations

In an early paper on relativistic wave equations, Majorana proposed possible generalizations of the Dirac equation based on wave functions with an infinite number of components [257] (see also [258,259]). In this study $\boldsymbol{\alpha}$ and β matrices were constructed using relatively simple raising and lowering operators, which allowed for both the construction, and also for the determination of the mass spectrum and associated spins. While the goal was to develop a wave equation without negative energy states applicable to elementary particles with arbitrary spin, this construction pointed the way to a new class of relativistic models for composites in which the internal degrees of freedom are treated algebraically. There have been many studies of this approach, and proposals for specific (solvable) Majorana wave equation constructions [260–270].

Perhaps the most important application of these models is for the construction of infinite component wave equations for baryons; the resulting mass spectrum could be fitted to the observed bayron masses, which allows for the estimation of form factors, magnetic moments, and other observables [271–281].

This approach was also used to construct relativistic equations for the hydrogen atom as a composite, where the center of mass motion is relativistic (and has the correct relativistic dispersion relation), and where the internal dynamics are approximately that of the nonrelativistic hydrogen atom [263,282–292]. In the construction of [288] and subsequent papers, the energy is given by

$$E_{\rm n}(\mathbf{P}) = \sqrt{(M_{\rm n}c^2)^2 + c^2|\mathbf{P}|^2} \tag{216}$$

for the positive energy solutions, where the mass spectrum in general is

$$M_{\rm n}^2 = m_{\rm p}^2 + m_{\rm e}^2 \pm 2m_{\rm p}m_{\rm e}\sqrt{1-\frac{\alpha^2}{n^2}} \tag{217}$$

and the positive energy mass solutions approximately match those of the nonrelativistic hydrogen atom in the sense

$$M_{\rm n} \ \rightarrow \ m_{\rm p} + m_{\rm e} - \frac{\mu\alpha^2}{2n^2} + \cdots \tag{218}$$

Infinite component wave equations have been constructed for rotators [293,294] as well as for other systems [295,296].

13.4. Poincaré invariant and approximately invariant approaches

We recall the discussion given in [224] in which a two-body Hamiltonian of the form

$$\hat{H} = \sqrt{(\hat{M}c^2)^2 + c^2|\hat{\mathbf{P}}|^2} \tag{219}$$

was considered in connection with Poincaré invariance, with the mass operator $\hat{M}$ a function of internal degrees of freedom. One can imagine a many-particle generalization of this with

$$\hat{M}c^2 = Nmc^2 + \sum_j \frac{|\hat{\boldsymbol{\pi}}_j|^2}{2m} + \sum_{j<k} \hat{V}_{jk} \tag{220}$$

with spin-dependent (and also isospin-dependent) potentials in connection with a many-particle wave function built up from two-component single particle wave functions. There seem only to be a few papers that make use of this approach [297,298].

One can find models that are approximately Poincaré invariant based on Hamiltonians of the form [194,232,299–301]

$$\hat{H} = \sum_j \sqrt{(mc^2)^2 + c^2|\hat{\mathbf{p}}|^2} + \sum_{j<k} \hat{V}_{jk}. \tag{221}$$

13.5. Covariant many-time models

A many-time covariant generalization of the many-particle Dirac equation was proposed by Barut in [302]. A simplified version of the covariant two-body equation can be written in the form

$$\begin{aligned}&\left(i\hbar\frac{\partial}{\partial t_1}-\boldsymbol{\alpha}_1\cdot c\hat{\mathbf{p}}_1-\beta_1 mc^2+i\hbar\frac{\partial}{\partial t_2}-\boldsymbol{\alpha}_2\cdot c\hat{\mathbf{p}}_2-\beta_2 mc^2\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)\\&=\hat{V}\left(\sqrt{|\mathbf{r}_2-\mathbf{r}_1|^2+c^2(t_2-t_1)^2}\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2).\end{aligned}\tag{222}$$

In the two-body case there is a simplification in connection with the different times, which allows for the construction of solutions; good results are obtained [304–306].

Much earlier a qualitatively different approach was proposed by Tomonaga [307]. A simplified version of this approach for the two-body problem can be written as

$$\begin{aligned}&\left(i\hbar\frac{\partial}{\partial t_1}-\boldsymbol{\alpha}_1\cdot c\hat{\mathbf{p}}_1-\beta_1 mc^2\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)=\hat{V}\left(\sqrt{|\mathbf{r}_2-\mathbf{r}_1|^2+c^2(t_2-t_1)^2}\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)\\&\left(i\hbar\frac{\partial}{\partial t_2}-\boldsymbol{\alpha}_2\cdot c\hat{\mathbf{p}}_2-\beta_2 mc^2\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)=\hat{V}\left(\sqrt{|\mathbf{r}_2-\mathbf{r}_1|^2+c^2(t_2-t_1)^2}\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2).\end{aligned}\tag{223}$$

Some of the technical issues associated with this approach were discussed in subsequent papers [308–310]. The use of a many times approach was discussed by Dirac in (1932) [311]. See [312] for a retrospective of these ideas in connection with the development of quantum electrodynamics.

13.6. Bethe–Salpeter approach

An important covariant two-body model was proposed by Bethe and Salpeter in connection with the development of field theory and quantum electrodynamics [313]. Although not usually written in this way, for the purposes of the discussion in this section we could write a many-time version of it in the form

$$\begin{aligned}&\left(i\hbar\frac{\partial}{\partial t_1}-\boldsymbol{\alpha}_1\cdot c\hat{\mathbf{p}}_1-\beta_1 mc^2\right)\left(i\hbar\frac{\partial}{\partial t_2}-\boldsymbol{\alpha}_2\cdot c\hat{\mathbf{p}}_2-\beta_2 mc^2\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)\\&=\hat{V}\left(\sqrt{|\mathbf{r}_2-\mathbf{r}_1|^2+c^2(t_2-t_1)^2}\right)\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2).\end{aligned}\tag{224}$$

Most people work instead with a single-time version. This model has been widely used for two-body bound state problems; for the hydrogen atom [314–317]; for the deuteron [318–322]; for the two-quark system [323–326]; and for the three-quark system [327–329]. There has appeared some discussion of general N-body Bethe–Salpeter models [330,331].

13.7. Proper time models

An alternate approach to the problem was proposed by Stueckelberg [332,333], who proposed making use of a proper time to develop a new kind of relativistic quantum mechanics. Interest in this approach in recent times has been stimulated by Horwitz and Piron [335]; in the following years there has accumulated a substantial body of work on this kind of model [336–345]. A review appears in [343].

A covariant two-body model based on an internal nonrelativistic potential problem can be written in the form

$$i\hbar\frac{\partial}{\partial\tau}\Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2,\tau) = \left[\frac{|\hat{\mathbf{p}}_1|^2+\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t_1^2}}{2M}+\frac{|\hat{\mathbf{p}}_2|^2+\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t_2^2}}{2M}+\hat{V}\left(\sqrt{|\mathbf{r}_2-\mathbf{r}_1|^2+c^2(t_2-t_1)^2}\right)\right] \times \Psi(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2,\tau). \tag{225}$$

One can see that the spacetime position and time variables are treated on the same footing naturally in this kind of model. This approach has been used for detailed calculations for two-body problems with a radial potential with good results [341,344–347]. The general approach is readily adapted to internal relativistic models.

It has been proposed by Davidson that variable rest mass effects in this kind of approach might account for anomalies in condensed matter nuclear science [348,349].

13.8. Approximate separation in the many-particle Dirac model

We have considered yet another approach which involves approximate separation in the many-particle Dirac model [350]. We begin by writing the model in terms of center of mass and relative coordinates according to

$$\hat{H} = \frac{1}{N}\sum_j \boldsymbol{\alpha}_j\cdot c\hat{\mathbf{P}} + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j\cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk}(\boldsymbol{\xi}_j-\boldsymbol{\xi}_k). \tag{226}$$

As we have remarked above, the center of mass and relative mass parts of the model share the same mass operators. We can rewrite this model as

$$\begin{aligned}\hat{H} =& \frac{1}{N}\sum_j \boldsymbol{\alpha}_j\cdot c\hat{\mathbf{P}} + \sum_j \beta_j m^* c^2 \\ &+ \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j\cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk}(\boldsymbol{\xi}_j-\boldsymbol{\xi}_k) - \sum_j \beta_j m^* c^2,\end{aligned} \tag{227}$$

where in the first line we have what amounts to a Bargmann–Wigner type of model for noninteracting spin 1/2 particles with a modified mass; in the second line we see a version of the relative Hamiltonian with a counter term.

We consider now the time-independent Schrödinger equation

$$E\Psi = \hat{H}\Psi. \tag{228}$$

An approximate product solution for the time-independent Schrödinger equation is proposed according to

$$\Psi = X(\{\boldsymbol{\xi}\})Y(\mathbf{R}), \tag{229}$$

where Ψ is a 4^N component wave function, where X is a 4^N component rest frame wave function, and where Y is a $4^N \times 4^N$ matrix. The Schrödinger equation for the product is

$$EXY = \left[\frac{1}{N} \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} + \sum_j \beta_j m^* c^2 \right] XY$$
$$+ \left[\sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) - \sum_j \beta_j m^* c^2 \right] XY. \tag{230}$$

We can arrange for approximate separability by requiring X to satisfy a (nonstandard) eigenvalue equation of the form

$$m^* c^2 \sum_j \beta_j X(\{\boldsymbol{\xi}\}) = \left[\sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] X(\{\boldsymbol{\xi}\}). \tag{231}$$

We normally work with rest frame eigenfunctions that satisfy

$$E\psi(\{\boldsymbol{\xi}\}) = \left[\sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) \right] \psi(\{\boldsymbol{\xi}\}), \tag{232}$$

hence the presence of a mass operator in connection with the eigenvalue makes the eigenvalue equation above in this case be nonstandard. However, within this approximation we achieve a measure of separation, and the resulting center of mass equation is

$$EXY = \left[\frac{1}{N} \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} + \sum_j \beta_j m^* c^2 \right] XY. \tag{233}$$

In essence the center of mass problem is modeled using a Bargmann–Wigner Hamiltonian based on the mass eigenvalue. We would expect the energy eigenvalue for the rest frame problem to give a better approximation to the mass energy than the mass eigenvalue, so it would of course be possible as an additional approximation to choose m^* to be consistent with the rest frame energy eigenvalue. Solving for the large matrix Y is not so easy in this case; however, the bigger issue here is the connection between the realistic many-particle Dirac model for the relative problem and the covariant Bargmann–Wigner model for the center of mass dynamics. We are not aware of literature on this kind of approximation outside of the proposal of [350].

14. Finite basis Approximation

The last issue that we have to consider is the finite basis approximation. In a realistic composite model for a multi-nucleon nucleus there are an infinite number of internal states, which is inconvenient for use in a lattice model that involves many nuclei. In this case it is convenient to make use of a finite basis approximation. Such models have been discussed previously for this application [157].

14.1. Matrix elements for a multi-particle Dirac model

In the case of a multi-particle Dirac model we start with a Hamiltonian of the form

$$\begin{aligned}\hat{H} =& \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) + \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\left[\hat{\boldsymbol{\pi}}_j - q_j\mathbf{A}(\mathbf{R}+\boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R})\right] \\ &+ \sum_{j<k}\hat{V}_{jk}(\boldsymbol{\xi}_j - \boldsymbol{\xi}_k) + Q\Phi + \sum_j\left[q_j\Phi(\mathbf{R}+\boldsymbol{\xi}_j) - \frac{Q}{N}\Phi(\mathbf{R})\right].\end{aligned} \tag{234}$$

It is convenient to work with basis states defined in terms of rest frame states that satisfy

$$E_n\phi_n = M_nc^2\phi_n = \left[\sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j\cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k}\hat{V}_{jk}(\boldsymbol{\xi}_j-\boldsymbol{\xi}_k)\right]\phi_n. \tag{235}$$

Matrix elements of the Hamiltonian in this basis can be written as

$$\begin{aligned}\langle\phi_n|\hat{H}|\phi_{n'}\rangle =& M_nc^2\delta_{n,n'} + \left\langle \phi_n \left| \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \right| \phi_{n'}\right\rangle \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) + Q\Phi\delta_{n,n'} \\ &+ \left\langle \phi_n \left| \sum_j \left[q_j\Phi(\mathbf{R}+\boldsymbol{\xi}_j) - \frac{Q}{N}\Phi(\mathbf{R})\right]\right| \phi_m \right\rangle \\ &- \left\langle \phi_n \left| \sum_j \boldsymbol{\alpha}_j \cdot c\left[q_j\mathbf{A}(\mathbf{R}-\boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R})\right]\right| \phi_{n'} \right\rangle.\end{aligned} \tag{236}$$

14.2. Finite basis model

Approximate solutions to the time-dependent problem can be constructed keeping only a finite number of basis states; we can write

$$\Psi(\{\boldsymbol{\xi}\},\mathbf{R},t) = \sum_n \Psi_n(\mathbf{R},t)\phi_n(\{\boldsymbol{\xi}\}). \tag{237}$$

We can use this to construct an approximate solution to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\{\boldsymbol{\xi}\},\mathbf{R},t) = \hat{H}\Psi(\{\boldsymbol{\xi}\},\mathbf{R},t). \tag{238}$$

Within the finite basis approximation individual channel wave functions satisfy

$$i\hbar\frac{\partial}{\partial t}\Psi_n(\mathbf{R},t) = \sum_{n'}\langle\phi_n|\hat{H}|\phi_{n'}\rangle\Psi_{n'}(\mathbf{R},t). \tag{239}$$

This we can expand out in the form

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\Psi_n(\mathbf{R},t) =& M_n c^2 \Psi_n(\mathbf{R},t) + \sum_{n'} \left\langle \phi_m \left| \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \right| \phi_n \right\rangle \cdot c(\hat{\mathbf{P}} - Q\mathbf{A})\Psi_{n'}(\mathbf{R},t) + Q\Phi\Psi_n(\mathbf{R},t) \\
&+ \sum_{n'} \left\langle \phi_n \left| \sum_j \left[q_j \Phi(\mathbf{R}+\boldsymbol{\xi}_j) - \frac{Q}{N}\Phi(\mathbf{R}) \right] \right| \phi_{n'} \right\rangle \Psi_{n'}(\mathbf{R},t) \\
&- \sum_{n'} \left\langle \phi_n \left| \sum_j \boldsymbol{\alpha}_j \cdot c \left[q_j \mathbf{A}(\mathbf{R}-\boldsymbol{\xi}_j) + \frac{Q}{N}\mathbf{A}(\mathbf{R}) \right] \right| \phi_{n'} \right\rangle \Psi_{n'}(\mathbf{R},t).
\end{aligned} \tag{240}
$$

In terms of vectors and matrices this can be recast as

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\boldsymbol{\Psi}(\mathbf{R},t) =& \left[\mathbf{M}c^2 + \mathbf{a}\cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) + q\Phi \right] \boldsymbol{\Psi}(\mathbf{R},t) \\
&- \mathbf{d}\cdot\mathbf{E}_L \boldsymbol{\Psi}(\mathbf{R},t) - \mathbf{j}\cdot\mathbf{A}\boldsymbol{\Psi}(\mathbf{R},t) + \cdots
\end{aligned} \tag{241}
$$

The vector wave function $\boldsymbol{\Psi}(\mathbf{R},t)$ here contains the channel wave functions $\Psi_n(\mathbf{R},t)$, and the matrices are constructed from the different parts of the Hamiltonian matrix elements; for example

$$
\mathbf{a}_{nn'} = \left\langle \phi_m \left| \frac{1}{N}\sum_j \boldsymbol{\alpha}_j \right| \phi_n \right\rangle . \tag{242}
$$

Only the lowest-order dipole interactions between the external field and the internal states have been kept explicitly in the matrix and vector version of the Schrödinger equation.

We have made use of this approach in earlier work on anomalies in condensed matter nuclear science [157].

14.3. Partial Foldy–Wouthuysen transformed model

In the future, we will likely make use of a finite basis approximation in connection with the partial Foldy–Wouthuysen transformation. We were able to make use of a partial F–W transformation in Section 10 to develop a model in which the center of mass degrees of freedom are described in a nonrelativistic type of approximation, and the internal states are treated relativistically. We can write the transformed Hamiltonian as

$$
\begin{aligned}
\hat{H}' =& \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M} + Q\Phi - \frac{\hbar Q}{2M}\frac{1}{N}\sum_j \boldsymbol{\Sigma}_j \cdot \mathbf{B} - \frac{\hbar^2 Q}{8M^2c^2}\nabla\cdot\mathbf{E} \\
&+ \frac{\hbar Q}{8M^2c^2}\sum_j \boldsymbol{\Sigma}_j \cdot \left[(\hat{\mathbf{P}} - Q\mathbf{A}) \times \mathbf{E} - \mathbf{E} \times (\hat{\mathbf{P}} - Q\mathbf{A})\right] \\
&+ \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk} \\
&+ \sum_j \left[q_j \Phi(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\Phi(\mathbf{R})\right] - \sum_j \boldsymbol{\alpha}_j \cdot c \left[q_j \mathbf{A}(\mathbf{R} + \boldsymbol{\xi}_j) - \frac{Q}{N}\mathbf{A}(\mathbf{R})\right] \\
&+ \frac{1}{M}\sum_j \beta_j \hat{\boldsymbol{\pi}}_j \cdot (\hat{\mathbf{P}} - Q\mathbf{A}) + \frac{1}{2Mc}\sum_{j<k}\left[(\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k), \hat{V}_{kl}\right] \cdot (\hat{\mathbf{P}} - Q\mathbf{A}) \\
&\frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M}\left(\frac{1}{N}\sum_j(\beta_j - \mathbf{I}_j)\right) - \frac{\hbar Q}{2M}\frac{1}{N}\sum_j(\beta_j - \mathbf{I}_j)\boldsymbol{\Sigma}_j \cdot \mathbf{B} + \cdots
\end{aligned} \tag{243}
$$

We can make use of a similar finite basis approximation to write

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\boldsymbol{\Psi}(\mathbf{R},t) =& \mathbf{M}c^2\boldsymbol{\Psi}(\mathbf{R},t) + \left(\frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M} + Q\Phi - \frac{Q}{NM}\mathbf{S}\cdot\mathbf{B} - \frac{\hbar^2 Q}{8M^2c^2}\nabla\cdot\mathbf{E}\right)\boldsymbol{\Psi}(\mathbf{R},t) \\
&+ \frac{Q}{4M^2c^2}\mathbf{S}\cdot\left[(\hat{\mathbf{P}} - Q\mathbf{A}) \times \mathbf{E} - \mathbf{E} \times (\hat{\mathbf{P}} - Q\mathbf{A})\right]\boldsymbol{\Psi}(\mathbf{R},t) - \mathbf{d}\cdot\mathbf{E}\boldsymbol{\Psi}(\mathbf{R},t) - \mathbf{j}\cdot\mathbf{A}\boldsymbol{\Psi}(\mathbf{R},t) \\
&+ \mathbf{a}\cdot c(\hat{\mathbf{P}} - Q\mathbf{A})\boldsymbol{\Psi}(\mathbf{R},t) + \cdots
\end{aligned} \tag{244}
$$

Only a subset of the terms appearing in the rotated Hamiltonian appear explicitly in this matrix and vector version of the finite basis approximation. In this case elements of the $\mathbf{a}$ matrix are

$$
\mathbf{a}_{n,n'} = \left\langle \phi_n \left| \frac{1}{Mc}\sum_j \beta_j \hat{\boldsymbol{\pi}}_j + \frac{1}{2Mc}\sum_{j<k}\left[\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k, \hat{V}_{jk}\right] \right| \phi_{n'} \right\rangle. \tag{245}
$$

15. Composites in Field Theory

A reviewer has argued that the most reliable physical models available at this time are field theories (see [351,352]), such as quantum electrodynamics and quantum chromodynamics, and that our discussion should be extended to include some discussion of composites in field theory. The standard model includes QED, QCD and more; it provides the most accurate and comprehensive theory for particles and interactions through the strong, electromagnetic and weak interactions. A field theory to describe gravitational interactions runs into technical difficulties associated with mass two gravitons, for which there is no consistent renormalization scheme. There are many efforts ongoing at present to develop new models based on a generalization of field theory (which models particles as points) to string theory (in which particles are modeled as strings) and M-theory (in which particles are modeled as higher-dimensional objects).

By construction the field theories within the standard model are Poincaré invariant, and are physically and mathematically acceptable relativistic models. The models have been applied to describe composite particles, with great success. A systematic review of models for composites in field theory by itself would be book length; consequently here we will be satisfied with only the briefest outline of some of the issues and problems that have been studied.

15.1. Field theory and many-particle Dirac models

The many-particle Dirac model for electrons is widely used, but is not a correct relativistic theory; while QED is a correct relativistic theory which is less widely used for applications, in part because it is more complicated. It is possible to begin with QED and to derive a many-particle Dirac model, which in a sense references a relativistic quantum mechanical model to its equivalent in field theory. This notion underlies the early studies of Brown and Ravenhall [111] and of Salpeter [353] (see also [176,354]). Subsequently more systematic efforts were made to provide a foundation for many-particle Dirac models in [112–114].

15.2. Field theory and relativistic corrections

Wide use is made of nonrelativistic quantum mechanical models that contain relativistic corrections. Early on corrections were developed from the many-particle Dirac model; however, it has been recognized that a better starting place is from field theory. One widely cited paper where this is done is Douglas and Kroll [355]; see [356] for a discussion of an application of the approach in quantum chemistry.

Earlier in this paper we have made use of the Foldy–Wouthuysen transformation of many-particle Dirac models to obtain nonrelativistic models with relativistic corrections. However, there is no reason that the transformation cannot be applied in the case of QED; this was pursued in [357]. In [358] QED and the standard model is considered in the Foldy–Wouthuysen representation; and in [359] a nonrelativistic version of QED is discussed.

15.3. QED corrections in atomic systems

It is possible to develop good estimates for wave functions and energies based on quantum mechanical models for atomic systems; however, these models do not include a wide variety of higher-order corrections that are present in field theoretical models based on QED. In this case it is possible to isolate corrections that are due to QED and analyze them in detail. These include self-energy corrections, two-photon exchange corrections, and a wide variety of other higher-order effects. Atomic systems are composites in the sense under discussion in this paper, and the QED corrections are small compared to the binding energies since electromagnetic interactions are relatively weak.

The literature on QED corrections is vast. For one-electron systems reviews have been given in [360–364]; and in the case of few-electron systems calculations have been discussed and reviewed in [365–372]. In recent years QED corrections are being calculated systematically for multi-electron atoms and ions [373–375].

In general the agreement between theory and experiment is good. The high accuracy of QED as a physical theory is evident in the determination of the electron anomalous magnetic moment, where the agreement between theory and experiment is impressive (for example, differences appear in the 10th digit in [376]).

However, in recent years the Lamb shift of muonic hydrogen was measured, and found to be in disagreement with theory [377],[378]. This has resulted in consternation, and a revisiting of theoretical models to see whether an understanding of the effect might be found (see e.g. [379]). This discrepancy currently remains unexplained [380].

15.4. Effective field theory for nuclei

The strong force coupling between nucleons in nuclei is very much stronger than the electromagnetic interaction in atoms, so that field theoretical corrections are much more important. For example, the inclusion of two-photon exchange in atomic hydrogen gives only a minor correction, while the inclusion of two-boson exchange effects is needed to have a reasonably accurate nucleon–nucleon potential for structure or scattering calculations. There are many papers in which three-boson exchange effects are included; and even higher-order models have been considered [45].

Consequently, field theory is much more important in nuclear physics. We have previous commented on Bethe–Salpeter treatments for the deuteron [318–322]; the approach has also been used for the three-nucleon problem [381,382]. In the case of nuclear physics an effective field theory (quantum hadrodynamics) is used, one which relies on nucleons and boson exchange; effective Lagrangians are found in [383–385]. Many-nucleon nuclei as composite particles in some cases are treated analogously to atomic systems, based on self-consistent field calculations but with interactions between nucleons based on the exchange of more than one boson [386,387], and self-energy and other corrections modeled [388,389].

15.5. Quantum field theory for quarks and gluons

In the 1960s there emerged a quantum field theory (quantum chromodynamics) for quarks and gluons, which make up mesons and nucleons as well as a host of other particles. The initial applications of the model were to high-energy scattering problems, where calculations could be done with modest effort and be compared with experiment. The application of QCD to bound state problems came later due to technical difficulties in the calculations. For example, quarks are tightly bound in nucleons, but the interaction due to single gluon exchange is modest in comparison. The headache comes about when quarks become somewhat separated; in this case the fields associated with the color charge are very strong and polarize the vacuum, the more so the larger the separation. Vacuum polarization produces additional quarks and gluons, leading to a much more complicated physical system than occurs for electrons in atoms, or for nucleons in nuclei. A quark and anti-quark pair has zero net color charge, and so can be bound as a meson. Three quarks of the three different colors (red, green, blue) can combine to make a color singlet, which has no net color charge, and so can be bound as a baryon.

Given this situation, quantum mechanical models have been studied (with some success) in which empirical potentials are used to model single gluon exchange and confinement [390,391]. However, it would be much better if one could work with QCD directly in order to model few-quark composites. In recent years a large amount of effort has gone into lattice QCD calculations, in which very time consuming Monte Carlo calculations are done on a set of discrete points, from which masses, expectation values, and hadron properties can be determined. The results for masses are perhaps most easily understood here; by now there have been lattice QCD calculations of hadron masses [392–394] with increasingly good agreement between values extrapolated from the calculations and experimental values. For example, a calculated value of the nucleon mass of 929 MeV is reported in [394] which compares well with the average of the proton and neutron mass which is 938.9 MeV. The mass difference between the neutron and proton is calculated in [395] to be 1.51 MeV, which is comparable to the experimental value 1.293 MeV.

16. Summary and Conclusions

Even though the notion of a quantum composite is in a sense foundational to atomic, molecular, nuclear and particle physics, there has not to our knowledge appeared previously a review.

Elementary particle models are widely used to model composite particles; most notably in the case of protons and neutrons, where the Dirac phenomenology is widely used. For spin 3/2 composite particles the Rarita–Schwinger model is also widely used; and Bargmann–Wigner models have been applied successfully to describe mesons and baryons.

Our interest in this concerns the use of composite models for nuclei in the lattice in connection with modeling anomalies in condensed matter nuclear science. In this case the clean separation between the center of mass and relative degrees of freedom that occurs in the nonrelativistic problem leads to very weak coupling, probably too weak to lead to the kinds of anomalies (excess heat, low-level nuclear radiation, elemental anomalies, collimated X-ray emission) that have been reported. This motivated us to seek a much stronger coupling in the relativistic version of the problem.

We found some years ago that a much stronger coupling appears in the many-particle Dirac model based on a Pauli reduction involving the elimination of the negative energy sectors, and we subsequently have based our modeling on this interaction. Estimates for the rate of excess heat production in the Fleischmann–Pons experiment based on this interaction appears to be consistent with experiment, under conditions where the weak coupling of the $D_2/^4He$ transitions limit the reaction rate. Attempts to connect theory with experiment without this much stronger coupling seems hopeless based on models that we have worked with so far.

However, this approach generally has been very strongly criticized in recent years, for a variety of reasons. One criticism is that due to Poincaré invariance, the center of mass and relative problems separate, so that there is no coupling between the center of mass and internal degrees of freedom. Another criticism is a more generic one that argues for the impossibility of any exchange between phonons, which are delocalized, and internal nuclear degrees of freedom, which are highly localized. Yet other criticisms have been put forth concerning the impossibility of coherent energy exchange with massive up-conversion and down-conversion. It has even been suggested that the up-conversion of many vibrational quanta is impossible because the system entropy is decreased. The local consensus among colleagues at MIT seems to be that since it is impossible for there to be any anomalies in the first place, all experimental reports of anomalies are simply wrong; and consequently any models that suggest they might have been possible should not have been considered in the first place.

Given the quantity and intensity of the criticism, there is no possibility of any response that would be considered to be satisfactory; hence there is little motivation to try. There are nonetheless a number of specific issues that have been to us of intrinsic interest and that have been clarified to some degree in the discussion above.

One of the most significant results from our perspective come in the form of the composite models that have been developed systematically in Sections 6-10. The nonrelativistic composite is simplest, and from our perspective important; but it does not appear much in the literature. The relativistic composite based on the many-particle Dirac model is also relatively simple, and also fundamental; however, the literature does not contain much discussion of it either. Composites resulting from the Foldy–Wouthuysen approximation appear to have been most widely considered, and a major motivation for this appears to have come from issues associated with the Gerasimov–Drell–Hearn sum rule [396,397].

The partial Foldy–Wouthuysen transformation described in Section 10 is new, and results in composite models where the center of mass is nonrelativistic and the internal degrees of freedom are relativistic; which from our perspective is very interesting. In the future we will focus on this kind of model for the basis of our models for anomalies in condensed matter nuclear science; since it is much easier to include in a model with lattice vibrations; since the coupling of the center of mass to internal degrees of freedom is simpler; and since we are able to rotate out terms involving the commutator with the potential for reasonably general potential models in free space.

Criticisms of our model which pertain to Poincaré invariance have in our view been the most serious to date, since if there is no sizeable interaction between the center of mass motion and the internal degrees of freedom, then it will be nearly impossible to develop a model that can connect with experiment along the lines we have pursued. The absence of such a coupling in free space as a result of Poincaré invariance is a very strong argument, and has been the source of much concern. The arguments resolving this issue are probably more subtle than one would wish, and rely on the fact that the many-particle Dirac model is approximately Poincaré invariant. Because of this, it is possible to construct a rotation that eliminates the strongest part of the interaction between the center of mass and relative degrees of freedom in free space. However, there is no guarantee that the generalization of this same rotation always works in the lattice case to produce the clean free space separation. In our work this was recognized long ago, and we have relied instead on the diagonalization of the many-nucleus problem when they are interacting (and participating in the vibrations of a highly excited phonon mode). These arguments appear in Sections 11 and 12.

In essence, the free space problem differs from the condensed matter problem since this rotation that eliminates the coupling between center of mass and internal degrees of freedom always works in free space, but conditions can be found for the lattice case where it gives rise to unexpected new effects.

There are other approaches to modeling composites discussed in Section 13, some of which involve models that are covariant or Poincaré invariant, and for which there is the potential of using to model nuclei as composites in a lattice in the future. Relativistic composite models are also interesting intrinsically and have applications in other fields. A brief discussion of more sophisticated composite models in field theory is given in Section 15.

We have relied heavily on the finite basis approximation in connection with models for composites in our models (this does not appear to have been pursued much in other areas). In Section 14 we outline the approach, one which we have made use of previously in the case of the many-particle Dirac model. However, it seems clear that finite basis models based on the transformed Hamiltonian from the partial Foldy–Wouthuysen transformation provide a much better starting place for this kind of modeling, and in the future we expect to make use of this approach.

Appendix A. 20-component Free Space Model for Nucleons

The relevant Hamiltonian for the three noninteracting quarks of the model is

$$\hat{H} = \Big(\beta_1 + \beta_2 + \beta_3\Big) mc^2 + \left(\frac{\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2 + \boldsymbol{\alpha}_3}{3}\right) \cdot c\hat{\mathbf{P}}. \tag{A.1}$$

We would like to construct a reduced Hamiltonian appropriate for the mixed symmetry basis states of the quark system. As discussed in Section 5 this can be written symbolically as

$$\begin{aligned}\hat{H}_{nuc} =& |[3\ 2\ 1]_C\rangle |[1\ 2\ 1]_F\rangle \hat{H}_{[1\ 2\ 1]} \langle [1\ 2\ 1]_F| \langle [3\ 2\ 1]_C| \\ &+ |[3\ 2\ 1]_C\rangle |[2\ 1\ 1]_F\rangle \hat{H}_{[2\ 1\ 1]} \langle [2\ 1\ 1]_F| \langle [3\ 2\ 1]_C|.\end{aligned} \tag{A.2}$$

The [1 2 1] part of the Hamiltonian can be written

$$\hat{H}_{[1\ 2\ 1]} = \mathbf{M}c^2 + \mathbf{a} \cdot c\mathbf{P}, \tag{A.3}$$

where $\mathbf{M}$ and $\mathbf{a}$ are 20×20 matrices. We can write for $\mathbf{M}c^2$

$$\mathbf{M}c^2 = mc^2 \left(\begin{array}{cccccccc|cccccccc|cccc}
3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&-3&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&-3&0&0&0&0&0&0&0&0&0&0&0&0\\ \hline
0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0\\ \hline
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1
\end{array} \right) . \tag{A.4}$$

Written in this form, we see three sets of $[1\ 2\ 1]$ states isolated in blocks. For the $\mathbf{a}_x$ matrix we may write

$$\mathbf{a}_x = \left(\begin{array}{cccccccc|cccccccc|cccc}
0&0&0&-\alpha&0&0&0&0&1&0&-\alpha&0&0&0&0&0&0&-\beta&0&0\\
0&0&-\alpha&0&0&0&0&0&0&-\alpha&0&1&0&0&0&0&-\beta&0&0&0\\
0&-\alpha&0&0&0&-\delta&0&0&0&0&0&0&-\alpha&0&\gamma&0&0&0&0&\delta\\
-\alpha&0&0&0&-\delta&0&0&0&0&0&0&0&0&\gamma&0&-\alpha&0&0&\delta&0\\
0&0&0&-\delta&0&0&0&-\alpha&-\alpha&0&\gamma&0&0&0&0&0&0&\delta&0&0\\
0&0&-\delta&0&0&0&-\alpha&0&0&\gamma&0&-\alpha&0&0&0&0&\delta&0&0&0\\
0&0&0&0&0&-\alpha&0&0&0&0&0&0&1&0&-\alpha&0&0&0&0&-\beta\\
0&0&0&0&-\alpha&0&0&0&0&0&0&0&0&-\alpha&0&1&0&0&-\beta&0\\ \hline
1&0&0&0&-\alpha&0&0&0&0&0&0&0&0&-\alpha&0&0&0&0&-\beta&0\\
0&-\alpha&0&0&0&\gamma&0&0&0&0&0&0&-\alpha&0&-\delta&0&0&0&0&\delta\\
-\alpha&0&0&0&\gamma&0&0&0&0&0&0&0&0&-\delta&0&-\alpha&0&0&\delta&0\\
0&1&0&0&0&-\alpha&0&0&0&0&0&0&0&0&-\alpha&0&0&0&0&-\beta\\
0&0&-\alpha&0&0&0&1&0&0&-\alpha&0&0&0&0&0&0&-\beta&0&0&0\\
0&0&0&\gamma&0&0&0&-\alpha&-\alpha&0&-\delta&0&0&0&0&0&0&\delta&0&0\\
0&0&\gamma&0&0&0&-\alpha&0&0&-\delta&0&-\alpha&0&0&0&0&\delta&0&0&0\\
0&0&0&-\alpha&0&0&0&1&0&0&-\alpha&0&0&0&0&0&0&-\beta&0&0\\ \hline
0&-\beta&0&0&0&\delta&0&0&0&0&0&0&-\beta&0&\delta&0&0&0&0&\gamma\\
-\beta&0&0&0&\delta&0&0&0&0&0&0&0&0&\delta&0&-\beta&0&0&\gamma&0\\
0&0&0&\delta&0&0&0&-\beta&-\beta&0&\delta&0&0&0&0&0&0&\gamma&0&0\\
0&0&\delta&0&0&0&-\beta&0&0&\delta&0&-\beta&0&0&0&0&\gamma&0&0&0
\end{array} \right) . \tag{A.5}$$

For the $\mathbf{a}_y$ matrix we may write

$$
\mathbf{a}_y = i \left(\begin{array}{cccccccc|cccccccc|cccc}
0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 1 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 \\
0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & 0 & -1 & 0 & 0 & 0 & 0 & -\beta & 0 & 0 & 0 \\
0 & \alpha & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & 0 & -\gamma & 0 & 0 & 0 & 0 & -\delta \\
-\alpha & 0 & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & \alpha & 0 & 0 & \delta & 0 \\
0 & 0 & 0 & \delta & 0 & 0 & 0 & \alpha & -\alpha & 0 & -\gamma & 0 & 0 & 0 & 0 & 0 & 0 & -\delta & 0 & 0 \\
0 & 0 & -\delta & 0 & 0 & 0 & -\alpha & 0 & 0 & \gamma & 0 & \alpha & 0 & 0 & 0 & 0 & \delta & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \alpha & 0 & 0 & 0 & 0 & \beta \\
0 & 0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & 0 & -1 & 0 & 0 & -\beta & 0 \\
\hline
-1 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \beta & 0 \\
0 & \alpha & 0 & 0 & 0 & -\gamma & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & 0 & \delta & 0 & 0 & 0 & 0 & -\delta \\
-\alpha & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\delta & 0 & \alpha & 0 & 0 & \delta & 0 \\
0 & 1 & 0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & -\beta \\
0 & 0 & \alpha & 0 & 0 & 0 & -1 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 \\
0 & 0 & 0 & -\gamma & 0 & 0 & 0 & \alpha & -\alpha & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & -\delta & 0 & 0 \\
0 & 0 & \gamma & 0 & 0 & 0 & -\alpha & 0 & 0 & -\delta & 0 & \alpha & 0 & 0 & 0 & 0 & \delta & 0 & 0 & 0 \\
0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 1 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & -\beta & 0 & 0 \\
\hline
0 & \beta & 0 & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & -\beta & 0 & -\delta & 0 & 0 & 0 & 0 & -\gamma \\
-\beta & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta & 0 & \beta & 0 & 0 & \gamma & 0 \\
0 & 0 & 0 & -\delta & 0 & 0 & 0 & \beta & -\beta & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & -\gamma & 0 & 0 \\
0 & 0 & \delta & 0 & 0 & 0 & -\beta & 0 & 0 & \delta & 0 & \beta & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0
\end{array} \right). \tag{A.6}
$$

Finally, for the $\mathbf{a}_z$ matrix we may write

$$
\mathbf{a}_z = \left(\begin{array}{cccccccc|cccccccc|cccc}
0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & -\beta & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 \\
0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 & -\beta & 0 & 0 \\
\alpha & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 0 & -\delta & 0 \\
0 & -\alpha & 0 & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & \delta \\
0 & 0 & \delta & 0 & 0 & 0 & \alpha & 0 & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & -\delta & 0 & 0 & 0 \\
0 & 0 & 0 & -\delta & 0 & 0 & 0 & -\alpha & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & \delta & 0 & 0 \\
0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\beta & 0 & 0 & 0 & 0 & \beta & 0 \\
0 & 0 & 0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 0 & -\beta \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\beta & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\gamma & 0 & 0 & 0 & 0 & \epsilon & 0 \\
0 & \beta & 0 & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & -\epsilon \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \delta & 0 & 0 & 0 & -\beta & 0 & 0 & -\gamma & 0 & 0 & 0 & 0 & 0 & 0 & \epsilon & 0 & 0 & 0 \\
0 & 0 & 0 & -\delta & 0 & 0 & 0 & \beta & 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 & 0 & -\epsilon & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\beta & 0 & 0 & 0 & -\delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \epsilon & 0 & 0 & 0 & 0 & -\gamma & 0 \\
0 & -\beta & 0 & 0 & 0 & \delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\epsilon & 0 & 0 & 0 & 0 & \gamma \\
0 & 0 & -\delta & 0 & 0 & 0 & \beta & 0 & 0 & \epsilon & 0 & 0 & 0 & 0 & 0 & 0 & -\gamma & 0 & 0 & 0 \\
0 & 0 & 0 & \delta & 0 & 0 & 0 & -\beta & 0 & 0 & -\epsilon & 0 & 0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0
\end{array} \right). \tag{A.7}
$$

For these matrices we have used

$$
\alpha = \frac{1}{\sqrt{3}}, \quad \beta = \frac{2}{\sqrt{3}}, \quad \gamma = \frac{1}{3}, \quad \delta = \frac{2}{3}, \quad \epsilon = \frac{4}{3}. \tag{A.8}
$$

We have also constructed the [2 1 1] Hamiltonian, which in our construction is identical in form, but involves [2 1 1] basis states instead of [1 2 1] basis states. Strictly speaking this indicates that the Hamiltonian actually involves 40×40 matrices; however, since the form of the constituent 20×20 matrices are the same it should be possible to make do with a reduced 20×20 model.

Appendix B. Implementation of the Partial F–W Transformation

Due to the relative simplicity of the single-particle Dirac equation with external field coupling it is possible to eliminate odd operators in the Hamiltonian to high order [160,190,398,399]. For the partial Foldy–Wouthuysen transformation of the center of mass part of the many-particle Dirac Hamiltonian in Section 10, the operators involved are much more complicated. Because of this our focus in this case needs to be on the development of low-order terms, of which there are many.

B.1. Even and odd operators of the F–W transformation

We are interested in evaluating to low-order the rotation of the center of mass Hamiltonian

$$\hat{H}'_{\mathbf{R}} = \mathrm{e}^{i\hat{S}}\left(\hat{H}_{\mathbf{R}} - i\hbar\frac{\partial}{\partial t}\right)\mathrm{e}^{-i\hat{S}}$$

and then subsequently rotate the other parts of the overall Hamiltonian The center of mass Hamiltonian can be written in terms of even and odd operators according to

$$\hat{H}_{\mathbf{R}} = \sum_j \beta_j mc^2 + \mathcal{E} + \sum_j \mathcal{O}_j, \tag{B.1}$$

which generalizes the Foldy–Wouthuysen approach a bit (reminiscent of [197]), where the even and odd operators satisfy

$$\beta_j \mathcal{E} = \mathcal{E}\beta_j, \tag{B.2}$$

$$\begin{aligned} \beta_j \mathcal{O}_j &= -\mathcal{O}_j \beta_j, \\ \beta_j \mathcal{O}_k &= \mathcal{O}_k \beta_j \quad (j \neq k). \end{aligned} \tag{B.3}$$

B.2. Calculation of low-order contributions to the transformation

In general we can carry out the F–W transformation using

$$\begin{aligned} \hat{H}'_{\mathbf{R}} =& \hat{H}_{\mathbf{R}} + i[\hat{S},\hat{H}_{\mathbf{R}}] - \frac{1}{2}[\hat{S},[\hat{S},\hat{H}_{\mathbf{R}}]] - \frac{i}{6}[\hat{S},[\hat{S},[\hat{S},\hat{H}_{\mathbf{R}}]]] + \frac{1}{24}[\hat{S},[\hat{S},[\hat{S},[\hat{S},\hat{H}_{\mathbf{R}}]]]] + \cdots \\ & - \hbar\frac{\partial \hat{S}}{\partial t} - \frac{i}{2}\left[\hat{S},\hbar\frac{\partial \hat{S}}{\partial t}\right] + \frac{1}{6}\left[\hat{S},\left[\hat{S},\hbar\frac{\partial \hat{S}}{\partial t}\right]\right] + \cdots \end{aligned} \tag{B.4}$$

with

$$\hat{S} = -i\frac{1}{2mc^2}\sum_j \beta_j \mathcal{O}_j. \tag{B.5}$$

By direct calculation we obtain

$$i[\hat{S}, \hat{H}_{\mathbf{R}}] = -\sum_j \mathcal{O}_j + \frac{1}{2mc^2}\sum_j \beta_j \Big[\mathcal{O}_j, \mathcal{E}\Big] + \frac{1}{mc^2}\sum_j \beta_j \mathcal{O}_j^2, \tag{B.6}$$

$$\begin{aligned}-\frac{1}{2}\Big[\hat{S}, \Big[\hat{S}, \hat{H}_{\mathbf{R}}\Big]\Big] =& -\frac{1}{2mc^2}\sum_j \beta_j \mathcal{O}_j^2 - \frac{1}{8m^2c^4}\sum_j \Big[\mathcal{O}_j, \Big[\mathcal{O}_j, \mathcal{E}\Big]\Big] \\ &+ \frac{1}{8m^2c^4}\sum_j\sum_{k\neq j}\beta_j\beta_k \Big[\mathcal{O}_j, \Big[\mathcal{O}_k, \mathcal{E}\Big]\Big] - \frac{1}{2m^2c^4}\sum_j \mathcal{O}_j^3,\end{aligned} \tag{B.7}$$

$$\begin{aligned}-\frac{i}{6}[\hat{S}, [\hat{S}, [\hat{S}, \hat{H}_{\mathbf{R}}]]] =& \frac{1}{6m^2c^4}\sum_j \mathcal{O}_j^3 + \frac{1}{48m^3c^6}\sum_j\sum_k\sum_l \Big[\beta_j\mathcal{O}_j, \Big[\beta_k\mathcal{O}_k, \beta_l\Big[\mathcal{O}_l, \mathcal{E}\Big]\Big]\Big] \\ &- \frac{1}{6m^3c^6}\sum_j \beta_j \mathcal{O}_j^4,\end{aligned} \tag{B.8}$$

$$\begin{aligned}\frac{1}{24}[\hat{S}, [\hat{S}, [\hat{S}, [\hat{S}, \hat{H}_{\mathbf{R}}]]]] =& \frac{1}{24m^3c^6}\sum_j \beta_j \mathcal{O}_j^4 \\ &+ \frac{1}{384m^3c^6}\sum_j\sum_k\sum_l\sum_m \Big[\beta_j\mathcal{O}_j, \Big[\beta_k\mathcal{O}_k, \Big[\beta_l\mathcal{O}_l, \beta_m\Big[\mathcal{O}_m, \\ &+ \frac{1}{24m^3c^6}\sum_j \mathcal{O}_j^5,\end{aligned} \tag{B.9}$$

$$-\hbar\frac{\partial \hat{S}}{\partial t} = i\frac{\hbar}{2mc^2}\sum_j \beta_j \frac{\partial \mathcal{O}_j}{\partial t}, \tag{B.10}$$

$$-\frac{i}{2}\left[\hat{S}, \hbar\frac{\partial \hat{S}}{\partial t}\right] = -i\frac{\hbar}{8m^2c^4}\sum_j \left[\mathcal{O}_j, \frac{\partial \mathcal{O}_j}{\partial t}\right] + i\frac{\hbar}{8m^2c^4}\sum_j\sum_{k\neq j}\beta_j\beta_k\left[\mathcal{O}_j, \frac{\partial \mathcal{O}_k}{\partial t}\right], \tag{B.11}$$

$$\frac{1}{6}\left[\hat{S}, \left[\hat{S}, \hbar\frac{\partial \hat{S}}{\partial t}\right]\right] = i\frac{\hbar}{48m^3c^6}\sum_j\sum_k\sum_l \left[\beta_j\mathcal{O}_j, \left[\beta_k\mathcal{O}_k, \beta_l\frac{\partial \mathcal{O}_l}{\partial t}\right]\right]. \tag{B.12}$$

We can collect the results above and write

$$\begin{aligned}\hat{H}'_{\mathbf{R}} =& \sum_j \beta_j mc^2 + \mathcal{E} + \frac{1}{2mc^2}\sum_j \beta_j \Big[\mathcal{O}_j, \mathcal{E}\Big] + \frac{1}{2mc^2}\sum_j \beta_j \mathcal{O}_j^2 - \frac{1}{8m^2c^4}\sum_j \Big[\mathcal{O}_j, \Big[\mathcal{O}_j, \mathcal{E}\Big]\Big] \\ &+ \frac{1}{8m^2c^4}\sum_j\sum_{k\neq j}\beta_j\beta_k\Big[\mathcal{O}_j, \Big[\mathcal{O}_k, \mathcal{E}\Big]\Big] - \frac{1}{3m^2c^4}\sum_j \mathcal{O}_j^3 \\ &+ \frac{1}{48m^3c^6}\sum_j\sum_k\sum_l \Big[\beta_j\mathcal{O}_j, \Big[\beta_k\mathcal{O}_k, \beta_l\Big[\mathcal{O}_l, \mathcal{E}\Big]\Big]\Big] - \frac{1}{8m^3c^6}\sum_j \beta_j\mathcal{O}_j^4 \\ &+ \frac{1}{384m^3c^6}\sum_j\sum_k\sum_l\sum_m \Big[\beta_j\mathcal{O}_j, \Big[\beta_k\mathcal{O}_k, \Big[\beta_l\mathcal{O}_l, \beta_m\Big[\mathcal{O}_m, \mathcal{E}\Big]\Big]\Big]\Big] + \frac{1}{24m^3c^6}\sum_j \mathcal{O}_j^5 \\ &+ i\frac{\hbar}{2mc^2}\sum_j \beta_j\frac{\partial \mathcal{O}_j}{\partial t} - i\frac{\hbar}{8m^2c^4}\sum_j \left[\mathcal{O}_j, \frac{\partial\mathcal{O}_j}{\partial t}\right] + i\frac{\hbar}{8m^2c^4}\sum_j\sum_{k\neq j}\beta_j\beta_k\left[\mathcal{O}_j, \frac{\partial \mathcal{O}_k}{\partial t}\right] \\ &+ i\frac{\hbar}{48m^3c^6}\sum_j\sum_k\sum_l\left[\beta_j\mathcal{O}_j, \left[\beta_k\mathcal{O}_k, \beta_l\frac{\partial\mathcal{O}_l}{\partial t}\right]\right] + \cdots \end{aligned} \tag{B.13}$$

If we retain terms only up to $O(1/m^2)$ this reduces to

$$\begin{aligned}\hat{H}'_{\mathbf{R}} \to& \sum_j \beta_j mc^2 + \mathcal{E} + \frac{1}{2mc^2}\sum_j \beta_j \Big[\mathcal{O}_j, \mathcal{E}\Big] + \frac{1}{2mc^2}\sum_j \beta_j \mathcal{O}_j^2 - \frac{1}{8m^2c^4}\sum_j \Big[\mathcal{O}_j, \Big[\mathcal{O}_j, \mathcal{E}\Big]\Big] \\ &+ \frac{1}{8m^2c^4}\sum_j\sum_{k\neq j}\beta_j\beta_k\Big[\mathcal{O}_j, \Big[\mathcal{O}_k, \mathcal{E}\Big]\Big] - \frac{1}{2m^2c^4}\sum_j \mathcal{O}_j^3 + \frac{1}{6m^2c^4}\sum_j \mathcal{O}_j^3 \\ &+ i\frac{\hbar}{2mc^2}\sum_j \beta_j\frac{\partial \mathcal{O}_j}{\partial t} - i\frac{\hbar}{8m^2c^4}\sum_j \left[\mathcal{O}_j, \frac{\partial\mathcal{O}_j}{\partial t}\right] + i\frac{\hbar}{8m^2c^4}\sum_j\sum_{k\neq j}\beta_j\beta_k\left[\mathcal{O}_j, \frac{\partial \mathcal{O}_k}{\partial t}\right]. \end{aligned} \tag{B.14}$$

B.3. Evaluation of the F-W transformation

We can write for the even and odd operators

$$\mathcal{E} = Q\Phi, \tag{B.15}$$

$$\mathcal{O}_j = \frac{1}{N}\boldsymbol{\alpha}_j \cdot c(\hat{\mathbf{P}} - Q\mathbf{A}). \tag{B.16}$$

We can evaluate

$$\mathcal{O}_j^2 = \frac{c^2}{N^2}|\hat{\mathbf{P}} - Q\mathbf{A}|^2 - \frac{\hbar c^2 Q}{N^2}\boldsymbol{\Sigma}_j \cdot \mathbf{B}, \tag{B.17}$$

$$\left[\mathcal{O}_j, \mathcal{E}\right] = -i\frac{\hbar Qc}{N}\boldsymbol{\alpha}_j \cdot \nabla\Phi, \tag{B.18}$$

$$\begin{aligned}\left[\mathcal{O}_j, \left[\mathcal{O}_j, \mathcal{E}\right]\right] + i\hbar\left[\mathcal{O}_j, \frac{\partial \mathcal{O}_j}{\partial t}\right] =& \frac{\hbar^2 Qc^2}{N^2}\nabla\cdot\mathbf{E} - \frac{\hbar Qc^2}{N^2}\boldsymbol{\Sigma}_j\cdot(\hat{\mathbf{P}} - Q\mathbf{A})\times\mathbf{E} \\ &+ \frac{\hbar Qc^2}{N^2}\boldsymbol{\Sigma}_j\cdot\mathbf{E}\times(\hat{\mathbf{P}} - Q\mathbf{A}),\end{aligned} \tag{B.19}$$

$$\left[\mathcal{O}_j, \left[\mathcal{O}_k, \mathcal{E}\right]\right]_{j\neq k} = -\frac{\hbar^2 c^2 Q}{N^2}\Big((\boldsymbol{\alpha}_j\cdot\nabla)(\boldsymbol{\alpha}_k\cdot\nabla)\Phi\Big)_{j\neq k}, \tag{B.20}$$

$$\left[\mathcal{O}_j, \frac{\partial \mathcal{O}_j}{\partial t}\right] = i\frac{\hbar c^2 Q}{N^2}\nabla\cdot\frac{\partial \mathbf{A}}{\partial t} - i\frac{c^2 Q}{N^2}\left(\boldsymbol{\Sigma}_j\cdot(\hat{\mathbf{P}} - Q\mathbf{A})\times\frac{\partial \mathbf{A}}{\partial t} - \boldsymbol{\Sigma}_j\cdot\frac{\partial \mathbf{A}}{\partial t}\times(\hat{\mathbf{P}} - Q\mathbf{A})\right), \tag{B.21}$$

$$\left[\mathcal{O}_j, \frac{\partial \mathcal{O}_k}{\partial t}\right]_{j\neq k} = i\frac{\hbar c^2 Q}{N^2}\left[(\boldsymbol{\alpha}_j\cdot\nabla)\left(\boldsymbol{\alpha}_k\cdot\frac{\partial \mathbf{A}}{\partial t}\right)\right]_{j\neq k}. \tag{B.22}$$

We can make use of these results to write

$$\begin{aligned}\hat{H}'_{\mathbf{R}} =& \sum_j \beta_j mc^2 + \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M}\frac{1}{N}\sum_j \beta_j + Q\Phi - \frac{\hbar Q}{2M}\frac{1}{N}\sum_j \beta_j\boldsymbol{\Sigma}_j\cdot\mathbf{B} \\ &- \frac{\hbar^2 Q}{8M^2c^2}\sum_j \nabla\cdot\mathbf{E} + \frac{\hbar Q}{8M^2c^2}\sum_j \boldsymbol{\Sigma}_j\cdot\left[(\hat{\mathbf{P}} - Q\mathbf{A})\times\mathbf{E} - \mathbf{E}\times(\hat{\mathbf{P}} - Q\mathbf{A})\right] \\ &+ i\frac{\hbar Qc}{2Mc^2}\sum_j \beta_j\boldsymbol{\alpha}_j\cdot\mathbf{E} - \frac{\hbar^2}{8M^2c^2}\sum_j\sum_{k\neq j}\beta_j\beta_k\left[(\boldsymbol{\alpha}_j\cdot\nabla)(\boldsymbol{\alpha}_k\cdot\nabla)\Phi\right] \\ &- \frac{1}{3M^2c^2}\frac{1}{N}\sum_j\left[|\hat{\mathbf{P}} - Q\mathbf{A}|^2 - \hbar Q\boldsymbol{\Sigma}_j\cdot\mathbf{B}\right]\boldsymbol{\alpha}_j\cdot c(\hat{\mathbf{P}} - Q\mathbf{A}) \\ &- \frac{\hbar^2 Q}{8M^2c^2}\sum_j\sum_{k\neq j}\beta_j\beta_k\left[(\boldsymbol{\alpha}_j\cdot\nabla)\left(\boldsymbol{\alpha}_k\cdot\frac{\partial \mathbf{A}}{\partial t}\right)\right] + \cdots\end{aligned} \tag{B.23}$$

The terms on the last three lines all have odd pieces, so they are smaller and can be removed with further F–W rotations (the discussion in [197] is relevant here). The terms that survive to $O(1/m^2)$ are

$$\begin{aligned}\hat{H}'_{\mathbf{R}} \;\rightarrow\; & \sum_j \beta_j mc^2 + \frac{|\hat{\mathbf{P}} - Q\mathbf{A}|^2}{2M}\frac{1}{N}\sum_j \beta_j + Q\Phi - \frac{\hbar Q}{2M}\frac{1}{N}\sum_j \beta_j\boldsymbol{\Sigma}_j\cdot\mathbf{B} \\ &- \frac{\hbar^2 Q}{8M^2c^2}\sum_j \nabla\cdot\mathbf{E} + \frac{\hbar Q}{8M^2c^2}\sum_j \boldsymbol{\Sigma}_j\cdot\left[(\hat{\mathbf{P}} - Q\mathbf{A})\times\mathbf{E} - \mathbf{E}\times(\hat{\mathbf{P}} - Q\mathbf{A})\right].\end{aligned} \tag{B.24}$$

This provides the generalization of the Foldy–Wouthuysen single particle result to the center of mass degrees of freedom of the composite.

Appendix C. Reviewer Comments

The reviewer has raised a number of issues, most of which were addressed in a significant revision of the paper. However, it seems worth while to consider the remaining issues in this Appendix. One issue has to do with the focus of the paper and conclusions; another issue has to do with other approaches to the problem of anomalies in condensed matter nuclear science.

C.1. Coupling and projection operators

The reviewer wrote:

> It is argued that the many particle Foldy–Wouthuysen theory, projected onto positive energy solutions, might allow some sort of coupling between the center of mass momentum of a composite, and the internal degrees of freedom that might facilitate coupling between nuclear events and phonons or plasmons in a solid, or at least that is how I read it. But the projections onto the positive energy space of Foldy–Wouthuysen transformations are complicated, and a specific reason why they might lead to the coupling that is desired linking internal nuclear degrees of freedom to extended quasi-particles like phonons or plasmons in a solid was not given. Obviously this is an open topic for future work. The hope seems to be that a process of elimination might yield the desired result. Since just about every other source for coupling between the nuclear degrees of freedom and the solid are ruled out, only the complexity of the positive energy projection in the Foldy–Wouthuysen transformation leaves it alone as a possibility. It might be so, but explicit evidence to that effect was not given in this paper, as far as I could tell.

In response, we note that there are a number of different issues raised in this comment, which are probably worth sorting out. One issue has to do with the projection operators, which are required in a relativistic theory in order to cure Brown–Ravenhall disease (coupling to negative energy states) that occurs in the many-particle Dirac model. The majority of relativistic Dirac Hartree–Fock atomic physics calculations that have been done over the years make use of Coulomb plus Breit interactions without explicit projection operators. In this case projection is generally implemented instead through the inclusion of positive energy basis states (in a Furry picture sense), such as in a multi-state eigenvalue calculation, transition calculation or scattering calculation. In a self-consistent calculation the selection of positive energy eigenvalues for individual orbitals ends up restricting the calculation to the positive energy sector. An alternate approach is to make use of some of the "no-pair" formulations that are available, and which are used for relativistic quantum chemistry calculations; negative energy contributions, again in the Furry picture sense, are eliminated by the formalism.

Projection operators occur in the formal development of the nucleon-nucleon interaction (see e.g. [401,400]). In previous years the majority of nuclear calculations were done with nonrelativistic models so that there was no issue. In relativistic models there is a potential issue; however, it is easy to deal with as in the atomic case through a restriction of the basis states used (to positive energy states), or through the selection of positive energy orbitals in a Dirac-Fock type of calculation. In the literature there is no indication that headaches arise when the center of mass coupling is implemented [232–235].

Perhaps a good way to think about the appearance of the projection operators in a many-particle Dirac model is that they are present in order to prevent coupling to (single particle) negative energy states; but otherwise contribute relatively minor corrections (which would be important in a high precision calculation [176]).

A second issue concerns the coupling between lattice degrees of freedom and the internal degrees of freedom in a nucleus. There is no difficulty in finding external field interactions that will provide a weak coupling between vibrations and internal nuclear transitions; one can see such terms in the composite models described above. The headache is that these terms are weak. The center of mass interaction terms that we have emphasized in this work can mediate a coupling between vibrations and internal nuclear transitions, even though we have found no papers (outside of our own) which consider this possibility. In essence, this coupling is present in many-particle Dirac models, and in Poincaré invariant models more generally, and it can produce an interaction between lattice vibrations and nuclear transitions which has not been previously considered. In coherent models that we have investigated this coupling is sufficiently large to account for D_2/^{4}He transitions occurring at a rate consistent with experiment, as long as the large nuclear quantum can be down-shifted efficiently. Based on the present work we now have much greater confidence that this interaction must be present in a Poincaré invariant model, and is not a mistake or an artifact.

Finally, it is definitely the case that in our research we tried every other coupling we could think of, and the process of elimination succeeded in eliminating all interactions that we were aware of as being candidates to implement the effects we were interested in. It was not the purpose of this work to argue for, or to attempt to prove, that this interaction is responsible for the anomalies in condensed matter nuclear science. It is true as the reviewer has indicated that external field interactions are sufficiently weak such that we would not expect them to provide much coupling between the lattice and internal nuclear states; hence we would not expect them to be very important in connection with the anomalies under consideration. However, we have already spent some years working with this center of mass interaction in connection with excess heat, and in connection with collimated X-ray emission; and in both cases the center of mass interaction looks very promising (and there seem to be no alternatives). The purpose of this paper in connection with this point is to understand the center of mass interaction in the context of quantum composite models, to understand what relevant literature is available that discusses the interaction, and also to gain some understanding as to what the interaction is. In other works we have considered applications, and in future papers we will revisit calculations of the coupling matrix element as well as applications to conventional physical systems as well as to anomalies in condensed matter nuclear science.

C.2. Nonperturbative effects

The reviewer wrote:

> The author may want to look at and discuss another feature of the standard model and QED, which is the infrared divergence phenomena which was first described by the Bloch–Nordsieck model. This is a nonperturbative feature of QED. It leads to modifications to the particle propagators which have been termed infraparticles (see https://en.wikipedia.org/wiki/Infraparticle). This infra-red phenomenon could lead to the type of nonlocal features the author is looking for in interactions between the nucleus and the solid. It would be nice to add them to the discussion in this paper. These "dressed" particles of QED are not fully understood, especially not in a nonequilibrium condensed matter setting, but they involve infinite numbers of photons interacting with a charged particle, and due to the infrared divergence, they lead to a blurring of the mass of the charged particle. The propagators for the charged particle ends up no longer being a simple pole in the 4-momentum squared. This is hard to interpret in conventional quantum field theory, and so I would say this is an unresolved issue in QED. The behavior of these dressed QED particles in nonequilibrium condensed matter settings are largely unknown. Because they involve an infinite number of photons, and are consequently nonperturbative effects, they might provide the kind of nonlocal coupling between a charged particle and the extended solid that is required in LENR and that the author is seeking. Moreover, as they do not have a fixed mass, they might also provide a basis for off-mass-shell behavior as in Fock–Stueckelberg theory.

Our hope back in 1989 was to find some straightforward bit of physics which would account for the anomalies in a way that could be easily understood. For example, it was clear that we would expect a weak coupling between vibrations and internal nuclear transitions mediated by electric and magnetic fields. Since there was little question as to how lattice vibrations work, or how transitions between nuclear states work, the only issue left seemed to concern what happens when the vibrations are coupled to the transitions. It was clear early on that we might have Dicke enhancement factors showing up, which could serve to amplify the small interaction. However, the big issue then as now was whether it was possible to down-convert a large quantum into lots of small quanta, or vice versa with up-conversion. Over the years we managed to develop models which described the kind of up-conversion and down-conversion required, and we have been successful in quantifying these models under ideal conditions.

Looking back, there have been two "new" components to the models under investigation; one is the new up-conversion mechanism; and the other has been the center of mass coupling. In this study the issue of the coupling has in our view been clarified. We have solid derivations, clean formulas for the interaction, a connection with the literature, and a simple understanding of what the interaction is. What remains is to carry out calculations of the coupling matrix elements for specific transitions of interest. What we need to do is to go back to the up-conversion and down-conversion mechanism, and to see whether we might push them further theoretically, and also see whether we might connect with experiment in an unambiguous way. At present we are attempting to develop some simple experiments that would test these ideas.

I will be the first to agree with the reviewer that there are some subtle effects that emerge in quantum field theory models; that there are unresolved issues in QED; and that there are issues with "dressed" particles in QED and in condensed matter physics which can be very nonintuitive. A measure of my interest level might be the large number of books and papers collected and in many cases read. An unfortunately reality of our field has been, and continues to be, a relative lack of resources. I can see a potential solution to the puzzle (which are the anomalies) in the approach and in the models I have pursued; and if I can find a way to continue working on the approach I might just be able to clarify whether it is a solution, or whether it is yet another dead end. And if it is to be the dead end, then the suggestions of the reviewer are approaches that might be considered next.

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