Including nuclear degrees of freedom in a lattice Hamiltonian

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Abstract.

Motivated by many observations of anomalies in condensed matter systems, we consider a new fundamental Hamiltonian in which condensed matter and nuclear systems are described initially on the same footing. Since it may be possible that the lattice will respond to the mass change associated with a excited nuclear state, we adopt a relativistic description throughout based on a many-particle Dirac formalism. This approach has not been used in the past, perhaps due to the difficulty in separating the center of mass and relative degrees of freedom of the nuclear system, or perhaps due to an absence of applications for such a model. We recently found a way to separate the center of mass and relative contributions to the Hamiltonian for the many-particle Dirac model, which leads to somewhat different expressions for the kinematic mass, Newton mass, and deBroglie mass of the many-particle Dirac composite. It is not clear at this time whether such a difference is reflected in experiment. This separation allows us to reduce the condensed matter and nuclear Hamiltonian into a more manageable form. In the resulting model, there appears a new term in which nuclear transitions are coupled to lattice vibrations.

1. Introduction

From a condensed matter viewpoint, a solid is made of of nuclei and electrons, where the nuclei can for the most part be treated as point particles [1]. In cases where a more sophisticated description is needed, the basic description is augmented with nuclear spin, magnetic moments, and electric quadrupole moments [2]. Essentially the only place that excited states show up is in Mössbauer studies where they are required in order to describe the absorption or emission of a gamma [3]. The picture that results is both wonderfully simple and very rich; simple, in that the Born-Oppenheimer separation allows us to reduce the problem to electronic bands and phonon modes; and rich, as the models that result describe a wide range of basic, subtle, and occasionally unexpected physical phenomena. This basic approach to condensed matter physics has been sufficiently successful over the years that it would require some rather dramatic new experimental result before we might be motivated to revise it in any significant way.

In recent years there have been claims of experimental results which at a fundamental level seem not to be consistent with this basic viewpoint of condensed matter physics. In the Fleischmann-Pons excess heat effect [4, 5], a great deal of energy is generated which is thought to have a nuclear origin (since there are no commensurate chemical byproducts, and since ^{4}He is observed as a possible product in amounts proportional to the energy produced [6, 7, 8]), without commensurate energetic nuclear products [9]. In these experiments it almost seems as if the solid is taking up an MeV quantum; if so, then this constitutes an effect which seems very hard to understand within our current condensed matter framework. Given that such an effect seems impossible to contemplate within modern condensed matter physics (and also within modern nuclear physics), a natural reaction has been to go with the existing picture (supported by a very large body of experimental results and a consistent and mature theory), and to reject the Fleischmann-Pons experiment as simply being in error [10].

During the past two decades and more this de facto solution has been adopted generally, and it has worked surprisingly well. Science has advanced substantially; there are now even more experimental and theoretical results which support the modern condensed matter viewpoint; and those who pursue anomalies such as the Fleischmann-Pons experiment are isolated from science and ignored [11].

Meanwhile, another experimental result has been put forth which challenges our modern view of condensed matter physics. Karabut has studied a variety of anomalies in high-current density glow discharge experiments, and in the course of the work noticed that collimated x-ray emission occurred in powerful bursts normal to metal coin-shaped samples that served as cathodes [12, 13, 14, 15]. Although anomalous emission effects are seen when the discharge is on, the powerful bursts of collimated x-rays are observed on the order of a millisecond after the discharge is turned off. A current spike occurs when the discharge is shut off, which we might imagine causes vibrations in the sample. It seems as if the vibrational energy is being communicated somehow to produce in-phase electronic or nuclear excitation at x-ray energies, which then produces collimated x-ray emission through a phased array emission effect. We note that a related effect involving the collimated emission of gamma-rays in beamlets was reported earlier by Gozzi [16]. Needless to say, such an effect has no place in modern condensed matter physics.

In experiments performed by the Piantelli group, hydrogen is absorbed in nickel samples at elevated temperature, resulting in a thermal effect (consistent with energy generation) [17],[18], low-level nuclear effects (gamma and neutron emission [19],[20]), and the appearance of new elements [21]. This latter effect (appearance of new elements) in these experiments is not a low-level effect. Once again, such effects are not predicted in modern condensed matter physics.

These experimental results, and many others, have motivated us to explore new models that might be relevant. A major issue that we have been interested in is the possibility of coherent energy exchange between quantum systems with mismatched characteristic energies, which we considered to be the biggest theoretical problem associated with the anomalies. Coherent energy exchange between mismatched quantum systems occurs in high harmonic generation [22], so we know that it is possible in principle. However, there seems to be no analog to Corkum's mechanism [23],[24] present in the condensed matter system. A lesser version of the effect is known within the multiphoton regime of the spin-boson model, which is used to model basic linear interactions of two-level systems with an oscillator [25],[26],[27]. We found that if the two-level system is augmented with loss, the coherent energy exchange rate is increased dramatically. This is due to the fact that destructive interference limits the rate at which coherent energy exchange occurs in the spin-boson model, so augmenting the model with a mechanism that removes this destructive interference would be expected to improve coherent energy exchange rates [28],[29],[30],[31].

Coherent energy exchange in these models works best when the coupling between the two-level transition (representing electronic and nuclear transitions) and oscillator (representing a vibrational mode) is strong. We studied a further generalization of the lossy spin-boson model in which two transitions are coupled to an oscillator, where one is strongly-coupled and one is weakly-coupled [32]. We found that the strongly coupled system could assist coherent energy exchange for the weakly coupled system. The model that resulted appeared to us to be very closely related to excess heat production in the Fleischmann-Pons experiment, assuming that the mechanism involved $D_2/^4He$ transitions that were weakly coupled to a phonon mode (weakly coupled due to the Coulomb repulsion between the deuterons), and that a strongly-coupled transition were also present. The big problem in this kind of model ends up being the identification of the strongly-coupled transition. Finding an appropriate strongly-coupled transition with sufficiently strong coupling to do the job seems problematic within the approach [33].

After analyzing many candidate transitions, we came to the conclusion that there were no physical transitions which could serve as the strongly-coupled two-level transition within the model. We were optimistic in our writing about the possibility that systems described by three-level systems (or N-level systems) would be able to do the job. After putting in a great deal of work on analyzing the strongly-coupled three-level system, it seemed once again that the coupling was simply not strong enough to make a connection with experiment. This conclusion was supported by spectral data from Karabut [34], which seemed to be qualitatively consistent with the approach and models, but which would require much stronger coupling to explain.

All of this has led us to the conclusion that we are going to need a new kind of model in order to account for the experimental results. To obtain coupling sufficiently strong to be consistent with the Karabut experiment, we require very strong interactions that are on the general order of what would occur in a nuclear configuration mixing calculation. Yet there is no reason to expect that nuclear configuration interactions can couple to a phonon mode. In our earlier efforts to describe such an effect, we concluded that the internal nuclear degrees of freedom associated with configuration mixing separated cleanly from the vibrational degrees of freedom. For many years there has seemed to be no viable solution within the general approach, which has been very discouraging.

The intuitive picture that has emerged over the past few years of thinking about the problem is that the different excited states of the nucleus have different masses, and under appropriate conditions it may be possible for the nucleus to notice the mass differences of the different configurations. This could provide the physical basis for phonon exchange in association with configuration mixing. To describe such an effect, we need to develop a description of the associated coupling, which seems not to be available in the literature. One approach is to begin with a relativistic model for the nucleons, and then reduce it in some way to obtain a low momentum approximation in which the associated mass effects are retained.

The issues under discussion fit within the generic heading of relativistic quantum mechanics, which before 1950 would likely have implied the two-body Dirac equation as a starting place. However, the need for a manifestly covariant relativistic quantum theory more generally led to the development of modern quantum field theory, which could in principle be used for problems of interest to us. Field theory is much more complicated than relativistic quantum mechanics, so we would prefer a simpler model derived from relativistic quantum mechanics if possible. In this day and age, there are many relativistic quantum models that have been derived from field theory (such as the Bethe-Salpeter equation, as well as others [35]).

We started with the two-body Dirac model, and found that it was possible to define a kinematic mass in terms of exact solutions to the time-independent problem [36]. The approach that was used allowed for a simple way to separate center of mass and relative mass terms in the Hamiltonian. This is interesting in view of the discussion above, as it allows us to contemplate the construction of new lattice models in which the different masses of the nuclear excited states comes in naturally. We provide a brief review of the approach presented in [36] in the next section, and then generalize it in the following section to a finite basis state model for a nucleus. The resulting model can then be used directly to develop a new Hamiltonian for nuclei in a lattice that includes the coupling consistent with a many-particle Dirac formulation.

Interestingly, the model that results seems to include a relativistic effect which provides a direct coupling between the lattice motion and excitations in the nucleus. The resulting model appears to be much more closely connected with our earlier models than we had expected, which provides the motivation to explore the model further in the future.

2. Modified deBroglie relation for a Dirac composite eigenstate

We begin with a description of the nucleus in terms of Dirac particles within the context of a many-particle Dirac Hamiltonian

$$\hat{H} = \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j M_j c^2 + \sum_{j<k} V_{jk}(\mathbf{r}_k - \mathbf{r}_j) \tag{1}$$

Protons and neutrons are composite particles with internal quark structure, and one might criticize the use of a Dirac point-particle description for composites in this case; however, for our purposes it seems the simplest place to start. The Dirac $\boldsymbol{\alpha}$ and β matrices are

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{2}$$

The interaction between two nucleons appears here as $V_{jk}(\mathbf{r}_k - \mathbf{r}_j)$; we assume that this includes strong force and electromagnetic interactions. We assume the Φ is an exact solution to the time-independent equation

$$\hbar\omega\Phi = \left[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j M_j c^2 + \sum_{j<k} V_{jk}(\mathbf{r}_k - \mathbf{r}_j)\right]\Phi \tag{3}$$

2.1. Center of mass and relative coordinates

The classical center of mass coordinate satisfy

$$M\mathbf{R} = \sum_j m_j \mathbf{r}_j \tag{4}$$

with

$$M = \sum_j m_j \tag{5}$$

The relative position coordinates are

$$\boldsymbol{\xi}_j = \mathbf{r}_j - \mathbf{R} \tag{6}$$

The total classical momentum is

$$\mathbf{P} = \sum_j \mathbf{p}_j \tag{7}$$

and the relative momenta are

$$\boldsymbol{\pi}_j = \mathbf{p}_j - \frac{m_j}{M}\mathbf{P} \tag{8}$$

One of the relative position operators is redundant, since the sum of all relative position operators is zero; similarly one of the relative momentum operators is redundant.

2.2. Kinematic mass

The eigenvalue can be expressed in terms of relative and center of mass matrix elements according to

$$\begin{aligned}\hbar\omega &= \left\langle \Phi \middle| \left(\sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \right) \cdot c\hat{\mathbf{P}} \middle| \Phi \right\rangle \\ &\quad + \left\langle \Phi \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \middle| \Phi \right\rangle \end{aligned} \tag{9}$$

where Φ is an exact solution to the eigenvalue equation [Equation (3)]. We can add and subtract mass terms to obtain

$$\begin{aligned}\hbar\omega &= \left\langle \Phi \middle| \left(\sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \right) \cdot c\hat{\mathbf{P}} + \left(\sum_j \frac{m_j}{M} \beta_j \right) M^* c^2 \middle| \Phi \right\rangle \\ &\quad + \left\langle \Phi \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) - \left(\sum_j \frac{m_j}{M} \beta_j \right) M^* c^2 \middle| \Phi \right\rangle \end{aligned} \tag{10}$$

If we define the kinematic mass M^* according to

$$M^* c^2 = \frac{\left\langle \Phi \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \middle| \Phi \right\rangle}{\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle} \tag{11}$$

2.3. Eigenvalue relation for a single configuration

With this definition of the kinematic mass the eigenvalue simplifies to

$$\hbar\omega = \left\langle \Phi \middle| \left(\sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \right) \cdot c\hat{\mathbf{P}} + \left(\sum_j \frac{m_j}{M} \beta_j \right) M^* c^2 \middle| \Phi \right\rangle \tag{12}$$

We can rotate to obtain

$$\hbar\omega = \left\langle \Phi' \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi' \right\rangle \sqrt{(M^* c^2)^2 + c^2 |\mathbf{P}|^2} \tag{13}$$

where we used

$$\Phi' \sim e^{i\mathbf{P}\cdot\mathbf{R}/\hbar} \tag{14}$$

These are the basic results that we reported in [36]. We interpret Equation (13) as a modified deBroglie relation, in which $\hbar\omega$ is now related to the relativistic energy $\sqrt{(M^* c^2)^2 + c^2 |\mathbf{P}|^2}$ with a proportionality factor that is associated with a time dilation effect [37],[38].

2.4. Composite masses

We see that the composite has a kinematic mass M^*, which will in general depend on $\mathbf{P}$ since the Dirac Hamiltonian in general is not covariant. For our purposes we will assume a constant kinematic mass in the vicinity of the rest frame (which means that a covariant model is not strictly required for interactions with the lattice).

The nonrelativistic kinetic energy term that results from an expansion of the square root is

$$\hat{H} \;\rightarrow\; \left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle \frac{|\mathbf{P}|^2}{2M^*} \tag{15}$$

The equivalent classical model derived using Ehrenfest's theorem will be

$$\frac{d}{dt}\langle \mathbf{R} \rangle \;=\; \frac{\langle \hat{\mathbf{P}} \rangle}{M_N} \qquad\qquad \frac{d}{dt}\langle \hat{\mathbf{P}} \rangle \;=\; 0 \tag{16}$$

where M_N is the Newton mass

$$M_N \;=\; \frac{M^*}{\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle} \tag{17}$$

assuming rest frame wavefunctions for the evaluation of the time dilation factor.

We might also consider the relation for a composite in the rest frame

$$\hbar\omega \;=\; \left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle M^* c^2 \;=\; M_{dB} c^2 \tag{18}$$

to define the deBroglie mass (which we have denoted by M_{dB}).

2.5. Need for experimental clarification

Although the appearance of these three different masses is clear in the many-particle Dirac model, it is not at all clear yet that nature respects the distinction in experiment. One could imagine a set of high precision experiments in which one works with composite bodies that can be either in the ground state or and excited state.

The relative deBrgolie mass could be accessed spectroscopically

$$\begin{aligned}
\hbar(\omega_2 - \omega_1) \;&=\; \left[\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle M^* c^2 \right]_2 - \left[\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle M^* c^2 \right]_1 \\
&=\; \left(M_{dB} c^2 \right)_2 - \left(M_{dB} c^2 \right)_1
\end{aligned} \tag{19}$$

once again assume a rest frame estimate for the time dilation factor.

Information about the Newton mass could be developed from velocity measurements at constant momentum

$$
\begin{aligned}
\mathbf{v}_2 - \mathbf{v}_1 &= \mathbf{P} \left[\frac{\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle}{M^*} \right]_2 - \mathbf{P} \left[\frac{\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle}{M^*} \right]_1 \\
&= \mathbf{P} \left[\left(\frac{1}{M_N} \right)_2 - \left(\frac{1}{M_N} \right)_1 \right]
\end{aligned}
\tag{20}
$$

or from other suitable low energy experiments.

Information about the relative kinematic mass could be obtained in principle from time of flight measurements in the relativistic regime

$$
\mathbf{v}_j \Delta t_j = \left[\left\langle \Phi' \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi' \right\rangle \frac{c^2 \mathbf{P} \Delta t}{\sqrt{(M^* c^2)^2 + c^2 |\mathbf{P}|^2}} \right]_j \tag{21}
$$

where measurements at different momentum values can be used to determine the kinematic mass.

In general these measurements are likely to be nontrivial since we expect the mass factor to be close to unity for atomic systems

$$
\left\langle \Phi \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi \right\rangle \approx 1 \tag{22}
$$

This situation may be different for mesons and nucleons in a many-particle Dirac model [39],[40], since the bare quark masses are low and the equivalent potential is very strong.

3. Finite basis state model

We would like to expand our description to include a finite set of states, and in the process we would like a formulation in which the state mass impacts the kinematics. We begin by assuming a finite basis state model of the form

$$\Psi \;=\; \sum_j c_j \Phi_j \tag{23}$$

We make use of the variational method to obtain the matrix equation

$$\hbar\omega \mathbf{c} \;=\; \mathbf{H}\cdot\mathbf{c} \tag{24}$$

where the matrix $\mathbf{H}$ has individual matrix elements given by

$$H_{kl} \;=\; \langle \Phi_k | \hat{H} | \Phi_l \rangle \tag{25}$$

3.1. Diagonal matrix elements and kinematic masses

To arrange for dynamics with the kinematic mass matched to the state, we focus first on the diagonal matrix elements and write

$$H_{kk} \;=\; \langle \Phi_k | \hat{H}_{\mathbf{R}} | \Phi_k \rangle + \langle \Phi_k | \hat{H}_{\mathbf{r}} | \Phi_k \rangle \tag{26}$$

where the center of mass and relative parts are

$$\langle \Phi_k | \hat{H}_{\mathbf{R}} | \Phi_k \rangle \;=\; \left\langle \Phi_i \middle| \left(\sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \right) \cdot c\hat{\mathbf{P}} + \left(\sum_j \frac{m_j}{M} \beta_j \right) M_k^* c^2 \middle| \Phi_k \right\rangle \tag{27}$$

$$\langle \Phi_k | \hat{H}_{\mathbf{r}} | \Phi_k \rangle \;=\; \left\langle \Phi_k \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) - \left(\sum_j \frac{m_j}{M} \beta_j \right) \middle| \Phi_k \right\rangle \tag{28}$$

If we require the relative contribution to vanish, then the state-dependent kinematic mass M_k^* is consistent with

$$M_k^* c^2 \;=\; \frac{\left\langle \Phi_k \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \middle| \Phi_k \right\rangle}{\left\langle \Phi_k \middle| \sum_j \frac{m_j}{M} \beta_j M_k^* c^2 \middle| \Phi_k \right\rangle} \tag{29}$$

3.2. Off-diagonal matrix elements

The off-diagonal matrix elements may be written as

$$
\begin{aligned}
H_{kl} &= \left\langle \Phi_k \middle| \sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} \middle| \Phi_l \right\rangle \\
&\quad + \left\langle \Phi_k \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \middle| \Phi_l \right\rangle \qquad (30)
\end{aligned}
$$

where the first term is associated with the center of mass, and the second term is associated with the relative problem.

3.3. Finite basis eigenvalue relations

The finite basis eigenvalue relations for a composite in free space can be written in the form

$$
\hbar\omega_0 c_k = \left[\left\langle \Phi'_k \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi'_k \right\rangle \sqrt{(M_k^* c^2)^2 + c^2 |\mathbf{P}|^2} \right] c_k + \sum_{l \neq k} H_{kl} c_l \qquad (31)
$$

It will be convenient to write the off-diagonal matrix element in this case as

$$
H_{kl} = \overline{\boldsymbol{\alpha}}_{kl} \cdot (c\mathbf{P}) + V_{kl} \qquad (32)
$$

where V_{kl} is the coupling matrix element from the relative part of the problem

$$
V_{kl} = \left\langle \Phi_k \middle| \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \middle| \Phi_l \right\rangle \qquad (33)
$$

and where the vectors $\overline{\boldsymbol{\alpha}}_{kl}$ are defined by

$$
\overline{\boldsymbol{\alpha}}_{kl} = \left\langle \Phi_k \middle| \sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \middle| \Phi_l \right\rangle \qquad (34)
$$

We consider in the Appendix the nonrelativistic reduction of a representative $\overline{\boldsymbol{\alpha}}_{kl} \cdot c\hat{\mathbf{P}}$ matrix element.

3.4. Rest frame eigenvalue equations

The eigenvalue equations above are unfamiliar and moderately complicated. It is useful to consider them in the rest frame; in this case, we obtain

$$
\hbar\omega_0 c_k = \left[\left\langle \Phi_k \middle| \sum_j \frac{m_j}{M} \beta_j \middle| \Phi_k \right\rangle M_k^* c^2 \right] c_k + \sum_{l \neq k} V_{kl} c_l \qquad (35)
$$

It seems useful to extend the definition of the deBroglie mass to this case, and write

$$\left(M_{dB}c^2\right)_k \;=\; \left\langle \Phi_k \middle| \sum_j \frac{m_j}{M}\beta_j \middle| \Phi_k \right\rangle M_k^* c^2 \tag{36}$$

This allows us to write

$$\hbar\omega \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} (M_{dB}c^2)_1 & V_{12} & V_{13} & \cdots \\ V_{21} & (M_{dB}c^2)_2 & V_{23} & \cdots \\ V_{31} & V_{32} & (M_{dB}c^2)_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \tag{37}$$

It will be convenient to think of this as the basic unperturbed problem

$$\hbar\omega\mathbf{c} \;=\; \mathbf{H}_0 \cdot \mathbf{c} \tag{38}$$

3.5. Low-momentum eigenvalue relations

We can expand the square root terms to lowest order to obtain an eigenvalue equation relevant to the low-momentum case; we write

$$\hbar\omega_0 c_k \;=\; \left\langle \Phi_k \middle| \sum_j \frac{m_j}{M}\beta_j \middle| \Phi_k \right\rangle \left[M_k^* c^2 + \frac{|\mathbf{P}|^2}{2M_k^*} + \cdots \right] c_k + \sum_{l \neq k} \left[\overline{\boldsymbol{\alpha}}_{kl} \cdot (c\mathbf{P}) + V_{kl} \right] c_l \tag{39}$$

where we have approximated

$$\left\langle \Phi_k' \middle| \sum_j \frac{m_j}{M}\beta_j \middle| \Phi_k' \right\rangle \;\to\; \left\langle \Phi_k \middle| \sum_j \frac{m_j}{M}\beta_j \middle| \Phi_k \right\rangle \tag{40}$$

It seems useful here to extend the definition of the Newton mass to individual basis states

$$(M_N c^2)_k \;=\; \frac{M_k^* c^2}{\left\langle \Phi_k \middle| \sum_j \frac{m_j}{M}\beta_j \middle| \Phi_k \right\rangle} \tag{41}$$

We can write the eigenvalue equations that result as

$$\hbar\omega_0 c_k \;=\; \left[\left(M_{dB}c^2\right)_k + \frac{|\mathbf{P}|^2}{2(M_N)_k} \right] c_k + \sum_{l \neq k} \left[V_{kl} + \overline{\boldsymbol{\alpha}}_{kl} \cdot \mathbf{P} \right] c_l \tag{42}$$

In matrix notation, this might be written as

$$\hbar\omega\mathbf{c} \;=\; \left[\mathbf{H}_0 + \mathbf{M}_N^{-1} \frac{|\mathbf{P}|^2}{2} + \mathbf{a} \cdot (c\mathbf{P}) \right] \cdot \mathbf{c} \tag{43}$$

where

$$\mathbf{M}_N^{-1} \;=\; \begin{pmatrix} (M_N)_1^{-1} & 0 & 0 & \cdots \\ 0 & (M_N)_2^{-1} & 0 & \cdots \\ 0 & 0 & (M_N)_3^{-1} & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \tag{44}$$

and where

$$\mathbf{a} = \begin{pmatrix} 0 & \overline{\boldsymbol{\alpha}}_{12} & \overline{\boldsymbol{\alpha}}_{13} & \cdots \\ \overline{\boldsymbol{\alpha}}_{21} & 0 & \overline{\boldsymbol{\alpha}}_{23} & \cdots \\ \overline{\boldsymbol{\alpha}}_{31} & \overline{\boldsymbol{\alpha}}_{32} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \tag{45}$$

4. A Hamiltonian for nuclei in a lattice

There has been discussion over the years as to develop a suitable formalism that would be capable of systematically addressing the anomalies of interest in condensed matter nuclear science. It was proposed in [41] that one begin with a fundamental Hamiltonian based on nucleons and electrons, and then reduce the model for applications by first building up nuclei from nucleons, then solving for electronic degrees of freedom in a Born-Oppenheimer picture, and finally focusing on the vibrational problem. We imagine a similar approach here, only instead of starting with a nonrelativistic fundamental Hamiltonian we use a relativistic one.

The separation of center of mass and relative degrees of freedom is straightforward in the nonrelativistic version of the problem, which is why we focused on it in [41]. But we see in the discussion above that it is possible to separate the center of mass and relative Hamiltonians for a many-particle Dirac model, even in the context of a finite basis approximation. This separation allows us to extend the earlier program systematically to a relativistic formulation (including now a new relativistic coupling between the nuclear motion and internal nuclear degrees of freedom) based on an underlying many-particle Dirac model.

4.1. Hamiltonian for electrons and nucleons

We begin with a formal model based on many-particle Dirac Hamiltonians for the electrons and nucleons

$$\begin{aligned}\hat{H} \ = \ & \Big[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j M_j c^2 + \sum_{j<k} V_{jk}^{nn}(\mathbf{r}_k - \mathbf{r}_j) \Big]_{nucleons} \\ & + \Big[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j m_e c^2 + \sum_{j<k} V_{jk}^{ee}(\mathbf{r}_k - \mathbf{r}_j) \Big]_{electrons} + \sum_{j,k} V_{jk}^{en}(\mathbf{r}_k - \mathbf{r}_j) \end{aligned} \tag{46}$$

In the first term in brackets we find a relativistic nucleon Hamiltonian including mass, velocity, and potential terms (including strong force interactions as well as electromagnetic interactions). Nuclear models of this kind can be found in the literature [42],[43]. In the second term in brackets we find a relativistic electron Hamiltonian also including mass, velocity and potential terms (in this case electromagnetic interactions). Although there is no reason to believe that a relativistic description for the electrons is required for the problems of interest, somehow it seems appropriate to maintain the same level of description in the fundamental Hamiltonian. Finally, the last term includes electron-nucleon potential terms, which are electromagnetic here. A further augmentation of the model to include weak interaction physics is possible, but we will not pursue it here.

4.2. Reduction of the nucleon Hamiltonian

The developments presented in the previous sections allows for a systematic reduction for the nucleon Hamiltonian in the form

$$\begin{aligned} & \left[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j M_j c^2 + \sum_{j<k} V_{jk}^{nn}(\mathbf{r}_k - \mathbf{r}_j) \right]_{nucleons} \\ \rightarrow & \sum_l \left[\mathbf{M}_{dB} c^2 + \frac{|\hat{\mathbf{P}}|^2}{2\mathbf{M}_N} + \mathbf{a} \cdot (c\hat{\mathbf{P}}) \right]_l \end{aligned} \tag{47}$$

where the sum over nucleons is now replaced with a sum over nuclei, and where the different matrices associated with the nuclear finite basis expansion are selected to be appropriate for the nucleus indexed by l.

The excited state energies in the rest frame appear as the eigenvalues of the deBroglie mass term $\mathbf{M}_{dB}c^2$. The lowest-order contribution to the kinetic energy of the nucleus as a composite Dirac particle is included in $\frac{|\hat{\mathbf{P}}|^2}{2\mathbf{M}_N}$, which allows for the energy of a basis state to impact the kinetic energy appropriately. Finally, there is a new term $\mathbf{a} \cdot (c\hat{\mathbf{P}})$ that describes a relativistic effect in which the nucleus center of mass momentum (which will subsequently be part of the lattice vibrations) is coupled to transitions between the different basis states. The summation over l here indicates a sum over the different nuclei in the lattice, so that there will be separate deBroglie mass matrices, Newton mass matrices, and lattice coupling terms for each nuclei. The condensed matter Hamiltonian that results is

$$\begin{aligned} \hat{H} \;=\; & \left[\sum_l \left[\mathbf{M}_{dB} c^2 + \frac{|\hat{\mathbf{P}}|^2}{2\mathbf{M}_N} + \mathbf{a} \cdot (c\hat{\mathbf{P}}) \right]_l \right]_{nuclei} \\ & + \left[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j m_e c^2 + \sum_{j<k} V_{jk}^{ee}(\mathbf{r}_k - \mathbf{r}_j) \right]_{electrons} + \sum_{j,k} V_{jk}^{en}(\mathbf{r}_k - \mathbf{r}_j) \end{aligned} \tag{48}$$

4.3. Born-Oppenheimer approximation

With nucleons replaced by nuclei, the resulting model is very similar to the standard condensed matter model, and we can similarly make use of the Born-Oppenheimer approximation to obtain a potential model for the nuclei

$$\hat{H} = \sum_l \left[\mathbf{M}_{dB} c^2 + \frac{|\hat{\mathbf{P}}|^2}{2\mathbf{M}_N} + \mathbf{a} \cdot (c\hat{\mathbf{P}}) \right]_l + \sum_{j<k} V_{jk}^{NN}(\mathbf{R}_k - \mathbf{R}_j) \tag{49}$$

This Hamiltonian is made up of individual mass, kinetic energy, and lattice coupling terms for each nucleus individually, and augmented now with effective potential interactions (electromagnetic plus electronic) between the nuclei. This model provides a generalization of the usual lattice Hamiltonian to include nuclear mass effects and lattice coupling with the nuclei.

4.4. Reduction to a standard lattice Hamiltonian

In the event that the effects associated with nuclear excitation are weak, then the new terms in the model can be dispensed with; if we we assume

$$\mathbf{a}_l \to 0 \tag{50}$$

then we recover a model that is essentially the standard condensed matter lattice Hamiltonian:

$$\hat{H} = \sum_l \left[\mathbf{M}_{dB} c^2 + \frac{|\hat{\mathbf{P}}|^2}{2\mathbf{M}_N} \right]_l + \sum_{j<k} V_{jk}^{NN}(\mathbf{R}_k - \mathbf{R}_j) \tag{51}$$

In this approximation there is no direct coupling between the nuclear excited states and lattice vibrations. If the nuclei are in ground states, we could replace the mass matrices by the mass eigenvalues, which completes the reduction:

$$\hat{H} = \sum_l \left[M_{dB} c^2 + \frac{|\hat{\mathbf{P}}|^2}{2M_N} \right]_l + \sum_{j<k} V_{jk}^{NN}(\mathbf{R}_k - \mathbf{R}_j) \tag{52}$$

5. Discussion and conclusions

This study was motivated by our interest in deriving a lattice Hamiltonian from a relativistic starting Hamiltonian in which we could study the effect of the different configuration masses on the lattice dynamics, with the goal of developing a systematic description of the anomalies associated with condensed matter nuclear science. The derivation of such a Hamiltonian from the many-particle Dirac model in particular is in general problematic due to difficulties in the separation of relative and center of mass degrees of freedom for the relativistic problem. We recently obtained a weaker result which allows for the separation of center of mass and relative contributions to the many-particle Dirac Hamiltonian. Even though this does not allow for a general separation of the degrees of freedom equivalent to that of the nonrelativistic problem, it is sufficient to allow us to develop a new kind of lattice model that includes the mass effects we set out to model.

In the process, we obtained a number of interesting results. We found that in the many-particle Dirac model the eigenvalue $\hbar\omega$ is not equal to $\sqrt{(M^*c^2)^2 + c^2|\mathbf{P}|^2}$ as we had expected, but that a proportionality factor appears which we associate with a time dilation effect. This proportionality factor means that in a kinematic model for composite center of mass dynamics, there will be a difference between the energy eigenvalue $\hbar\omega$ and the kinematic mass energy M^*c^2 in the rest frame. Also it implies that the Newton mass associated with the classical dynamics in the nonrelativistic limit will not match the kinematic mass in this model. All of this was unexpected, and motivates us to ask whether this is consistent with experiment (in which case the many-particle Dirac model was holding back yet more surprises), or not (in which case we would have good reason not to trust the model for composite kinematics).

We also found a new term that appears to provide a coupling between the center of mass momentum $\hat{\mathbf{P}}$ and transitions in the nuclear finite basis states. The origin of this effect is that the nuclear states of the composite nucleus transform under a boost in the many-particle Dirac model, which implies a mixing with other states. In the case of constant $\mathbf{P}$ the eigenvalue problem is seeking to create a version of the boosted wavefunction out of the rest frame states. However, with the composite momentum is dynamical (as occurs in a lattice), the model tries to develop boosted wavefunctions for a composite momentum that keeps changing magnitude and direction, which requires in this picture a dynamical admixture of different rest frame states.

In the end, we obtain a Hamiltonian that describes lattice dynamics and nuclear excitation that is derived consistently from an underlying relativistic Hamiltonian (the many-particle Dirac model). This model appears to be very closely related to models for two-level systems coupled to an oscillator that we have investigated over the years [28],[29], [30],[31] in connection with the excess heat effect in the Fleischmann-Pons experiment.

Appendix A. Nonrelativistic limit for the transition operator

Transitions in this model are described by the off-diagonal matrix element

$$\overline{\boldsymbol{\alpha}}_{fi} \cdot c\hat{\mathbf{P}} \;=\; \left\langle \Phi_f \middle| \sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} \middle| \Phi_i \right\rangle \tag{A.1}$$

We are interested in developing a nonrelativistic approximation for this operator which may be useful for understanding the coupling.

Expansion of the wavefunction

We assume that the solution to the relative problem can be expanded in the form

$$\Phi \;=\; \Phi_{+++\cdots} + \Phi_{-++\cdots} + \Phi_{+-+\cdots} + \Phi_{++-\cdots} + \cdots \tag{A.2}$$

where the first term involves large component channels for all nucleons, where the second involves a small component channel for the first particle, and so forth.

Channel equations

For the first term, the relative eigenvalue problem in the rest frame results in

$$\begin{aligned}\left[E - Mc^2 - \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j)\right]\Phi_{+++\cdots} \;=\;& \boldsymbol{\sigma}_1 \cdot (c\hat{\boldsymbol{\pi}}_1)\Phi_{-++\cdots} + \boldsymbol{\sigma}_2 \cdot (c\hat{\boldsymbol{\pi}}_2)\Phi_{+-+\cdots} \\ & + \boldsymbol{\sigma}_3 \cdot (c\hat{\boldsymbol{\pi}}_3)\Phi_{++-\cdots} + \cdots \end{aligned} \tag{A.3}$$

For the second term we have

$$\begin{aligned}\left[E - Mc^2 + 2m_1c^2 - \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j)\right]\Phi_{-++\cdots} \;=\;& \boldsymbol{\sigma}_1 \cdot (c\hat{\boldsymbol{\pi}}_1)\Phi_{+++\cdots} + \boldsymbol{\sigma}_2 \cdot (c\hat{\boldsymbol{\pi}}_2)\Phi_{--+\cdots} \\ & + \boldsymbol{\sigma}_3 \cdot (c\hat{\boldsymbol{\pi}}_3)\Phi_{-+-\cdots} + \cdots \end{aligned} \tag{A.4}$$

from which we approximate the channel wavefunction as

$$\Phi_{-++\cdots} \;=\; \left[E - Mc^2 + 2m_1c^2 - \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j)\right]^{-1} (\boldsymbol{\sigma}_1 \cdot c\hat{\boldsymbol{\pi}}_1)\Phi_{+++\cdots} \tag{A.5}$$

Approximate transition matrix element

To proceed we expand the transition matrix element in terms of the different pieces

$$\left\langle \Phi_f \middle| \sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} \middle| \Phi_i \right\rangle = \frac{m_1}{M} \Big[\left\langle \Phi_f(+++\cdots) \middle| (\boldsymbol{\sigma}_1 \cdot c\hat{\mathbf{P}}) \middle| \Phi_i(-++\cdots) \right\rangle$$
$$+ \left\langle \Phi_f(-++\cdots) \middle| (\boldsymbol{\sigma}_1 \cdot c\hat{\mathbf{P}}) \middle| \Phi_i(+++\cdots) \right\rangle \Big] + \cdots \tag{A.6}$$

We expect the large component to dominate, so we keep terms with a single small component and approximate according to

$$\left\langle \Phi_f \middle| \sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}} \middle| \Phi_i \right\rangle =$$
$$\frac{m_1}{M} \Big[\left\langle \Phi_f(+++\cdots) \middle| (\boldsymbol{\sigma}_1 \cdot c\hat{\mathbf{P}}) \Big[E - Mc^2 + 2m_1c^2 - \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \Big]^{-1} (\boldsymbol{\sigma}_1 \cdot c\hat{\boldsymbol{\pi}}_1) \middle| \Phi_i(+++\cdots) \right\rangle$$
$$+ \left\langle \Phi_f(+++\cdots) \middle| (\boldsymbol{\sigma}_1 \cdot c\hat{\boldsymbol{\pi}}_1) \Big[E - Mc^2 + 2m_1c^2 - \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \Big]^{-1} (\boldsymbol{\sigma}_1 \cdot c\hat{\mathbf{P}}) \middle| \Phi_i(+++\cdots) \right\rangle \Big]$$
$$+ \cdots \tag{A.7}$$

Taylor series expansion

A Taylor series expansion yields

$$\Big[E - Mc^2 + 2m_1c^2 - \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \Big]^{-1} = \frac{1}{2m_1c^2} \Big[1 + \frac{E - Mc^2}{2m_1c^2} - \frac{1}{2m_1c^2} \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) \Big]^{-1}$$
$$= \frac{1}{2m_1c^2} \Big[1 - \frac{E - Mc^2}{2m_1c^2} + \frac{1}{2m_1c^2} \sum_{j<k} V_{jk}(\boldsymbol{\xi}_k - \boldsymbol{\xi}_j) + \cdots \Big] \tag{A.8}$$

Leading-order contribution

To evaluate the leading-order term in the expansion of the transition matrix element, we require the identity

$$(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) = \mathbf{a} \cdot \mathbf{b} + i \boldsymbol{\sigma} \cdot \mathbf{a} \times \mathbf{b} \tag{A.9}$$

This allows us to write

$$
\begin{aligned}
(\boldsymbol{\sigma}\cdot c\hat{\mathbf{P}})(\boldsymbol{\sigma}\cdot c\hat{\boldsymbol{\pi}}) + (\boldsymbol{\sigma}\cdot c\hat{\boldsymbol{\pi}})(\boldsymbol{\sigma}\cdot c\hat{\mathbf{P}}) &= 2c^2\hat{\boldsymbol{\pi}}\cdot\hat{\mathbf{P}} + i\boldsymbol{\sigma}\cdot\left(\hat{\mathbf{P}}\times\hat{\boldsymbol{\pi}} + \hat{\boldsymbol{\pi}}\times\hat{\mathbf{P}}\right) \\
&= 2c^2\hat{\boldsymbol{\pi}}\cdot\hat{\mathbf{P}} \qquad \text{(A.10)}
\end{aligned}
$$

Consequently, the leading-order term vanishes

$$
\begin{aligned}
&\sum_j \frac{m_j}{M}\Bigg[\left\langle \Phi_f(+++\cdots)\middle|(\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\frac{1}{2m_jc^2}(\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\middle|\Phi_i(+++\cdots)\right\rangle \\
&\quad + \left\langle \Phi_f(+++\cdots)\middle|(\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\frac{1}{2m_jc^2}(\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\middle|\Phi_i(+++\cdots)\right\rangle\Bigg] \\
&\quad = \frac{1}{M}\Bigg[\left\langle \Phi_f(+++\cdots)\middle|\hat{\mathbf{P}}\cdot\sum_j\hat{\boldsymbol{\pi}}_j\middle|\Phi_i(+++\cdots)\right\rangle \qquad \text{(A.11)}
\end{aligned}
$$

since

$$
\sum_j \boldsymbol{\pi}_j = \sum_j \mathbf{p}_j - \frac{m_j}{M}\mathbf{P} = 0 \qquad \text{(A.12)}
$$

First next-order term

There are two next-order terms; the first of these is

$$
\begin{aligned}
&\sum_j 2\frac{m_j}{M}\left\langle \Phi_f(+++\cdots)\middle|(\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\frac{E-Mc^2}{(2m_jc^2)^2}(\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\middle|\Phi_i(+++\cdots)\right\rangle \\
&\quad = \frac{(E-Mc^2)}{2Mc^2}\left\langle \Phi_f(+++\cdots)\middle|\sum_j\frac{\hat{\boldsymbol{\pi}}_j\cdot\hat{\mathbf{P}}}{m_j}\middle|\Phi_i(+++\cdots)\right\rangle \qquad \text{(A.13)}
\end{aligned}
$$

Note that this term contains the sum $\sum_j \frac{\hat{\boldsymbol{\pi}}_j}{m_j}$ which we may rewrite as

$$
\sum_j \frac{\hat{\boldsymbol{\pi}}_j}{m_j} = \sum_j \hat{\boldsymbol{\pi}}_j\left(\frac{1}{m_j} - \frac{1}{m_{av}}\right) \qquad \text{(A.14)}
$$

since $\sum_j \hat{\boldsymbol{\pi}}_j = 0$, where m_{av} might be an appropriate average of the different masses. Since the proton mass is 938.27 MeV/c^2 and the neutron mass is 939.56 MeV/c^2, the individual nucleon masses are little different from the average nucleon mass. Consequently, we expect this term to be small.

Second next-order term

The other next-order term is

$$\sum_j \frac{m_j}{M}\Bigg[\Big\langle \Phi_f(+++\cdots)\Big|(\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\Big[\frac{1}{(2m_jc^2)^2}\sum_{k<l}V_{kl}(\boldsymbol{\xi}_l-\boldsymbol{\xi}_k)\Big](\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\Big|\Phi_i(+++\cdots)\Big\rangle$$
$$+\Big\langle \Phi_f(+++\cdots)\Big|(\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\Big[\frac{1}{(2m_jc^2)^2}\sum_{k<l}V_{kl}(\boldsymbol{\xi}_l-\boldsymbol{\xi}_k)\Big](\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\Big|\Phi_i(+++\cdots)\Big\rangle\Bigg]$$
$$=\frac{1}{2Mc^2}\Bigg[\Big\langle \Phi_f(+++\cdots)\Big|\sum_j(\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\Big[\frac{1}{2m_jc^2}\sum_{k<l}V_{kl}(\boldsymbol{\xi}_l-\boldsymbol{\xi}_k)\Big](\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\Big|\Phi_i(+++\cdots)\Big\rangle$$
$$+\Big\langle \Phi_f(+++\cdots)\Big|\sum_j(\boldsymbol{\sigma}_j\cdot c\hat{\boldsymbol{\pi}}_j)\Big[\frac{1}{2m_jc^2}\sum_{k<l}V_{kl}(\boldsymbol{\xi}_l-\boldsymbol{\xi}_k)\Big](\boldsymbol{\sigma}_j\cdot c\hat{\mathbf{P}})\Big|\Phi_i(+++\cdots)\Big\rangle\Bigg] \quad \text{(A.15)}$$

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