Kinematic mass of a composite in the many-particle Dirac model

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Abstract.

We are interested in the energy-momentum relation for a moving composite in relativistic quantum mechanics in many-particle Dirac models. For a manifestly covariant model one can apply the Lorentz transform to go from the rest frame to a moving frame to establish an energy-momentum relation of the form $\sqrt{(M^*c^2)^2 + c^2|P|^2}$ where $M^*$ is the kinematic mass. However, the many-particle Dirac model is not manifestly covariant, and some other approach is required. We have found a simple approach that allows for a separation of relative and center of mass contributions to the energy. We are able to define the associated kinematic energy and determine the energy-momentum relation. Our result can be expressed as a modified deBroglie relation of the form

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

where the kinematic mass $M^*$ will depend on the total momentum $P$ for a general noncovariant potential. The prefactor that occurs we associate with a time dilation effect, the existence of which has been discussed previously in the literature.

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1. Introduction

The many-particle Dirac model describes relativistic quantum mechanics of particles with spin 1/2. It is widely used for relativistic atomic, molecular, and nuclear structure calculations. For relativistic kinematics, other relativistic quantum mechanical models derived from quantum field theory are much more widely used since they have been constructed to be manifestly covariant. Although the many-particle Dirac model is useful for static problems, it is not used very often for kinematic calculations involving many-particle composites away from the rest frame.

A potential advantage of the many-electron Dirac model is that it is much simpler than quantum field theory, the Bethe-Salpeter equation, and other modern relativistic models; we would like to be able to use it systematically to a wider class of problems than just static structure calculations. At issue is how the energy scales with the center of mass momentum, since the many-particle Dirac model is not manifestly covariant. In this regard, consider the discussion given recently by Marsch [1], in which the two-body Dirac-Coulomb problem is solved in the rest frame; in the case of a hydrogen atom in motion the energy is given as

\[ E(P) = \sqrt{E_0^2 + c^2|P|^2} \]

where \( E_0 \) is the rest frame energy. This is what we would expect in the case of a manifestly covariant theory [2]; however, the two-body Dirac-Coulomb model is not manifestly covariant, and it is not clear that we should expect this to come out as a result of a calculation done with the two-body Dirac-Coulomb model. A relativistic model need not exhibit a covariant energy based on the kinematic center of mass energy, as demonstrated by Artru [3]. This point has been emphasized recently by Javenin [4].

In a theory that is manifestly covariant one can take advantage of the Lorentz transform to establish how the energy of a composite varies with the total momentum. In a relativistic quantum model that is not manifestly covariant, we would not expect a Lorentz boost of a wavefunction in the rest frame to be consistent with a moving wavefunction in that model. Consequently, in general we must use some other approach to determine the relation between the energy for a composite at rest and in motion.

This problem is closely related to the separation of the center of mass and relative degrees of freedom in relativistic quantum mechanics. We would expect that in a consistent scheme in which relative and center of mass degrees of freedom are separated, the center of mass problem should be that of a free particle in the absence of an external
potential. Probably we would be concerned if this were not the case in a particular relativistic quantum model.

There is a substantial literature on two-body equations (and also for more complicated systems) in relativistic quantum mechanics as well as quantum field theory, as discussed in [5], [6], [7], [8], and [4].

Our interest in the problem is motivated by issues rather different than those that have been of concern to previous authors. We have recently been interested in the impact of configuration mixing, or of an excited state superposition, of a composite on the center of mass dynamics. The basic issue here is that if the different internal states have different energies, then they have different masses, which should impact the ratio of momentum and velocity in the nonrelativistic regime. To study such problems we would like to use the many-particle Dirac model as a foundation if possible (since it is simpler than field theory, and simpler than manifestly covariant models derived from field theory), since we require a relativistic model to describe the different masses associated with different excited states. A model that is approximately correct at low center of mass momentum is sufficient for us, which means we do not require the model to be precise in the limit that the composite approaches the speed of light. Finally, we do not require a manifestly covariant theory, but instead we would like an understandable energy-momentum relation that has the correct (or at least understandable) scaling at low center of mass momentum.

We found a very simple approach that allows for a separation of the center of mass and relative contributions to the eigenvalue in the many-particle Dirac model. The resulting relation between eigenvalue and energy was unexpected (at least by us). A part of the relation can clearly be associated with an energy-momentum relation of the form of Equation (1), which allows for a consistent definition of the kinematic mass. There is in addition a prefactor, which may have physical significance within the theory, in the context of a modified deBroglie relation.
2. Two-body Dirac model

Although our approach is general, it is simplest to focus on the two-body version of the problem here. The associated relative problem has been of interest since the early days of quantum mechanics [9], [10], and the associated time-independent relative equation is sometimes called the Kemmer-Fermi-Yang equation [11], [12].

2.1. Hamiltonian

The two-body Dirac Hamiltonian is

\[ \hat{H} = \alpha_1 \cdot c\hat{p}_1 + \alpha_2 \cdot c\hat{p}_2 + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r_2 - r_1) \]  \hspace{1cm} (2)

The \( \alpha \) and \( \beta \) matrices are

\[ \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \]  \hspace{1cm} (3)

where the \( \sigma \) matrices are Pauli matrices. Only relative forces are included in this model; the center of mass problem here is that of a composite particle in free space.

2.2. Classical center of mass and relative variables

We define the classical center of mass and relative variables according to

\[ M \mathbf{R} = m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2 \]  \hspace{1cm} (4)
\[ \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \]  \hspace{1cm} (5)
\[ \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \]  \hspace{1cm} (6)
\[ \frac{\mathbf{p}}{\mu} = \frac{\mathbf{p}_2}{m_2} - \frac{\mathbf{p}_1}{m_1} \]  \hspace{1cm} (7)

The total mass \( M \) is

\[ M = m_1 + m_2 \]  \hspace{1cm} (8)

and the relative mass \( \mu \) satisfies

\[ \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \]  \hspace{1cm} (9)

The classical position and momentum vectors are then

\[ \mathbf{r}_1 = \mathbf{R} - \frac{m_2}{M} \mathbf{r} \quad \mathbf{r}_2 = \mathbf{R} + \frac{m_1}{M} \mathbf{r} \]  \hspace{1cm} (10)
\[ \mathbf{p}_1 = \frac{\mu}{m_2} \mathbf{P} - \mathbf{p} \quad \mathbf{p}_2 = \frac{\mu}{m_1} \mathbf{P} + \mathbf{p} \]  \hspace{1cm} (11)
2.3. Hamiltonian in terms of center of mass and relative variables

The Hamiltonian can be written in terms of the quantum momentum and relative position operators as

\[
\hat{H} = \alpha_1 \cdot \left( \frac{\mu}{m_2} \hat{P} - \hat{p} \right) + \alpha_2 \cdot \left( \frac{\mu}{m_1} \hat{P} + \hat{p} \right) + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) \tag{12}
\]

This can be recast as

\[
\hat{H} = \left( \frac{m_1}{M} \alpha_1 + \frac{m_2}{M} \alpha_2 \right) \cdot \hat{cP} + (\alpha_2 - \alpha_1) \cdot \hat{cP} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) \tag{13}
\]

This is consistent with Barut and Stroebel [13].

2.4. Time-dependent problem and eigenvalue equation

The time-dependent two-body Dirac equation is

\[
i\hbar \frac{\partial}{\partial t} \Psi(r_1, r_2, t) = \hat{H} \Psi(r_1, r_2, t) \tag{14}\]

We assume a stationary state solution of the form

\[
\Psi(r_1, r_2, t) = e^{-i\omega t} \Phi(r_1, r_2) \tag{15}\]

where \( \Phi(r_1, r_2) \) satisfies the eigenvalue equation

\[
\hbar \omega \Phi(r_1, r_2) = \hat{H} \Phi(r_1, r_2) \tag{16}\]
3. Center of mass and relative contributions to the eigenvalue

In the nonrelativistic problem, we are able to split the Hamiltonian cleanly into center of mass and relative pieces. Although there is no equivalent separation in relativistic quantum mechanics, it appears to be possible to develop a simple separation of the associated Hamiltonians (as we discuss in this section).

We note that Barut and coworkers have discussed the separation of relative and center of mass degrees of freedom for this problem [13], [14], [15]. Of the relevant papers in the literature, our approach is most closely related to the ideas in these papers; however, our conclusions are quite different.

3.1. Eigenvalue equation and expectation values

Consider now the time-independent two-body Dirac equation

\[
\hbar \omega \Phi = \left[ \left( \frac{m_1}{M} \alpha_1 + \frac{m_2}{M} \alpha_2 \right) \cdot c \hat{P} + (\alpha_2 - \alpha_1) \cdot c \hat{p} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) \right] \Phi
\] (17)

Suppose now that \( \Phi \) is an exact solution. If so, then the eigenvalue may be expressed in terms of expectation values according to

\[
\hbar \omega = \langle \Phi \left| \left( \frac{m_1}{M} \alpha_1 + \frac{m_2}{M} \alpha_2 \right) \cdot c \hat{P} \right| \Phi \rangle + \langle \Phi \left| (\alpha_2 - \alpha_1) \cdot c \hat{p} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) \right| \Phi \rangle
\] (18)

3.2. Kinematic mass

Suppose that we now add and subtract kinematic mass terms to the expectation values; this allows us to write

\[
\hbar \omega = \langle \Phi \left| \left( \frac{m_1}{M} \alpha_1 + \frac{m_2}{M} \alpha_2 \right) \cdot c \hat{P} + \left( \frac{\mu}{m_2} \beta_1 + \frac{m_2}{M} \beta_2 \right) M^* c^2 \right| \Phi \rangle + \langle \Phi \left| (\alpha_2 - \alpha_1) \cdot c \hat{p} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) - \left( \frac{\mu}{m_2} \beta_1 + \frac{m_2}{M} \beta_2 \right) M^* c^2 \right| \Phi \rangle
\] (19)

If we assume that the contribution of the kinematic mass to the energy appears only through the first term, then the second term must vanish.
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\[ \left\langle \Phi \left| (\alpha_2 - \alpha_1) \cdot \hat{c} \hat{p} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) - \left( \frac{m_1}{M} \beta_1 + \frac{m_2}{M} \beta_2 \right) M^* c^2 \right| \Phi \right\rangle = 0 \]  

(20)

This allows us to define the kinematic mass from the ratio

\[ M^* c^2 = \frac{\left\langle \Phi \left| (\alpha_2 - \alpha_1) \cdot \hat{c} \hat{p} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(r) \right| \Phi \right\rangle}{\left\langle \Phi \left| \frac{m_1}{M} \beta_1 + \frac{m_2}{M} \beta_2 \right| \Phi \right\rangle} \]  

(21)

Note that it is possible that the kinematic mass defined in this way will have different values for different choices of the center of mass momentum, since the two-body Dirac model with arbitrary \( V(r) \) is not manifestly covariant.

3.3. Eigenvalue and energy

With the kinematic mass defined in this way, the eigenvalue then simplifies to

\[ \hbar \omega = \left\langle \Phi \left| \left( \frac{m_1}{M} \alpha_1 + \frac{m_2}{M} \alpha_2 \right) \cdot \hat{c} \hat{P} + \left( \frac{m_1}{M} \beta_1 + \frac{m_2}{M} \beta_2 \right) M^* c^2 \right| \Phi \right\rangle \]  

(22)

We can rotate to obtain

\[ \hbar \omega = \left\langle \Phi \left| \left( \frac{m_1}{M} \beta_1 + \frac{m_2}{M} \beta_2 \right) \sqrt{(M^* c^2)^2 + c^2 |\hat{P}|^2} \right| \Phi' \right\rangle \]  

(23)

If we assume that \( \Phi' \) has a plane-wave dependence on the center of mass coordinate

\[ \Phi' \sim e^{i \hat{P} \cdot \hat{R} / \hbar} \]  

(24)

then we may simplify to

\[ \hbar \omega = \left\langle \Phi \left| \frac{m_1}{M} \beta_1 + \frac{m_2}{M} \beta_2 \right| \Phi' \right\rangle \sqrt{(M^* c^2)^2 + c^2 |\hat{P}|^2} \]  

(25)

We recall that the relativistic energy for a moving composite is

\[ E(P) = \sqrt{(M^* c^2)^2 + c^2 |P|^2} \]  

(26)

with a fixed kinematic mass. We see that the eigenvalue \( \hbar \omega \) is proportional to the energy-momentum relation, but a prefactor is evident. We may write

\[ \hbar \omega(P) = \left\langle \Phi'(P) \left| \frac{m_1}{M} \beta_1 + \frac{m_2}{M} \beta_2 \right| \Phi'(P) \right\rangle \sqrt{(M^*(P) c^2)^2 + c^2 |P|^2} \]  

(27)
3.4. Rest frame kinematic mass

Bound state computations are usually performed in the rest frame, which suggests that the kinematic mass in the rest frame (where probably the potential model will be most relevant) should be estimated first by solving

$$\hbar \omega \Phi = \left[ (\alpha_2 - \alpha_1) \cdot \mathbf{c} \mathbf{p} + \beta_1 m_1 c^2 + \beta_2 m_2 c^2 + V(\mathbf{r}) \right] \Phi$$

and then evaluating

$$M^* c^2 = \frac{\langle \Phi \left| \sum \frac{m_j}{M} \beta_j \right| \Phi \rangle}{\langle \Phi \left| \sum \frac{m_j}{M} \beta_j \right| \Phi \rangle} \left| \mathbf{P} = 0 \right|$$

3.5. Extension to many particles

This approach can be extended to the case of many Dirac particles, as discussed in the Appendix. The eigenvalue in this case is of the form

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

where the kinematic mass is

$$M^* c^2 = \frac{\langle \Phi \left| \sum \frac{m_j}{M} \beta_j \right| \Phi \rangle}{\langle \Phi \left| \sum \frac{m_j}{M} \beta_j \right| \Phi \rangle}$$
4. Associated deBroglie relation

From the discussion above, we have found that the many-particle Dirac equation leads us to a deBroglie relation of the form

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

In light of the energy-momentum relation from the Lorentz transform

$$E(\mathbf{P}) = \sqrt{(M^* c^2)^2 + c^2 |\mathbf{P}|^2}$$

we might view this result as consistent with a modified deBroglie relation

$$\hbar \omega = \langle \Phi' \mid \sum_j \frac{m_j}{M} \beta_j \mid \Phi' \rangle E$$  \hspace{1cm} (32)

It might be asked why such a prefactor should occur? After some thought, it seems that we might associate it with a time-dilation effect associated with the potential in the case of a bound composite. There is precedent for such an effect in the literature (see [16, 17]).
5. Discussion and conclusion

This study was motivated by our interest in problems where the internal energy of a composite impacts the kinematics and dynamics at low center of mass momentum. The many-particle Dirac model is perhaps the simplest relativistic quantum mechanical model that might be relevant, but it has not been used much in the literature for problems outside of the rest frame. Since the many-particle Dirac model in general is not manifestly covariant, we are not able to use a Lorentz transformation to understand how the energy scales with momentum.

We found a simple approach which allows us to separate the center of mass and relative contributions to the eigenvalue. The resulting eigenvalue relation in general can be written in the form

\[
\hbar \omega(P) = \langle \Phi' \sum_j \frac{m_j}{M^*} \beta_j \Phi' \rangle \sqrt{[M^*(P)c^2]^2 + c^2 |P|^2}
\]

where we have identified \( M^* \) as a kinematic mass (which we would expect to be independent of \( P \) in a covariant many-particle Dirac model).

If we view the eigenvalue relation as a modified deBroglie relation

\[
\hbar \omega = \langle \Phi' \sum_j \frac{m_j}{M} \beta_j \Phi' \rangle E
\]

then the question to be faced concerns the interpretation of the prefactor. It seems that we might best associate this with a time dilation effect, consistent with recent literature predicting such an effect.
Appendix A. Kinematic mass in the many-particle Dirac model

The arguments given in the main text for the two-body problem can be extended to more Dirac particles directly, as we discuss below.

Appendix A.1. Classical center of mass and relative coordinates

We begin by defining the classical center of mass coordinate through

$$ \mathbf{M} \mathbf{R} = \sum_j m_j \mathbf{r}_j $$ \hspace{1cm} (A.1)

where

$$ M = \sum_j m_j $$ \hspace{1cm} (A.2)

Relative coordinates can be defined according to

$$ \xi_j = \mathbf{r}_j - \mathbf{R} $$ \hspace{1cm} (A.3)

If there are \( N \) particles, then we may define \( N \) relative coordinates, but one of them is redundant because

$$ \sum_j \xi_j = 0 $$ \hspace{1cm} (A.4)

Appendix A.2. Classical momentum coordinates

The total classical momentum is the sum of the individual particle momenta

$$ \mathbf{P} = \sum_j \mathbf{p}_j $$ \hspace{1cm} (A.5)

The relative momenta are defined according to

$$ \pi_j = \mathbf{p}_j - \frac{m_j}{M} \mathbf{P} $$ \hspace{1cm} (A.6)

Once again there are more relative momenta than required, since

$$ \sum_j \pi_j = \sum_j \mathbf{p}_n - \frac{\mathbf{P}}{M} \sum_j m_j = 0 $$ \hspace{1cm} (A.7)
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Appendix A.3. Many-particle Dirac Hamiltonian

The many-particle Dirac Hamiltonian is

$$\hat{H} = \sum_j \alpha_j \cdot \hat{c}\hat{p} + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\mathbf{r}_k - \mathbf{r}_j)$$  \hspace{1cm} (A.8)

where we presume that the potentials $V_{jk}$ are functions of relative coordinates. We can recast this in terms of center of mass and relative coordinates to obtain

$$\hat{H} = \sum_j \alpha_j \cdot c\left(\hat{\pi}_j + \frac{m_j}{M}\hat{P}\right) + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\xi_k - \xi_j)$$  \hspace{1cm} (A.9)

Appendix A.4. Solution and expectation values

We assume that $\Phi$ satisfies the time-independent Dirac equation

$$\hbar \omega \Phi = \hat{H} \Phi$$  \hspace{1cm} (A.10)

The eigenvalue then can be expressed in terms of the wavefunction as

$$\hbar \omega = \left\langle \Phi \left| \left( \sum_j \frac{m_j}{M} \alpha_j \right) \cdot c\hat{P} \right| \Phi \right\rangle$$

$$+ \left\langle \Phi \left| \sum_j \alpha_j \cdot c\hat{\pi}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\xi_k - \xi_j) \right| \Phi \right\rangle$$  \hspace{1cm} (A.11)

Appendix A.5. Kinematic mass

We can add kinematic mass terms and write

$$\hbar \omega = \left\langle \Phi \left| \left( \sum_j \frac{m_j}{M} \alpha_j \right) \cdot c\hat{P} + \left( \sum_j \frac{m_j}{M} \beta_j \right) M^* c^2 \right| \Phi \right\rangle$$

$$+ \left\langle \Phi \left| \sum_j \alpha_j \cdot c\hat{\pi}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\xi_k - \xi_j) - \left( \sum_j \frac{m_j}{M} \beta_j \right) M^* c^2 \right| \Phi \right\rangle$$ \hspace{1cm} (A.12)

Once again we require that the eigenvalue have no contribution from the relative problem, which occurs if we compute the kinematic mass according to

$$M^* c^2 = \frac{\left\langle \Phi \left| \sum_j \alpha_j \cdot c\hat{\pi}_j + \sum_j \beta_j m_j c^2 + \sum_{j<k} V_{jk}(\xi_k - \xi_j) \right| \Phi \right\rangle}{\left\langle \Phi \left| \sum_j \frac{m_j}{M} \beta_j \right| \Phi \right\rangle}$$  \hspace{1cm} (A.13)
Appendix A.6. Eigenvalue and energy

The eigenvalue for the many particle Dirac problem in this case is

\[ \hbar \omega = \left\langle \Phi \left| \left( \sum_j \frac{m_j}{M} \alpha_j \right) \cdot \hat{P} + \left( \sum_j \frac{m_j}{M} \beta_j \right) M^* c^2 \right| \Phi \right\rangle \]  \quad (A.14)

We can rotate to obtain

\[ \hbar \omega = \left\langle \Phi' \left| \sum_j \frac{m_j}{M} \beta_j \right| \Phi' \right\rangle \sqrt{(M^* c^2)^2 + c^2 |P|^2} \]  \quad (A.15)

assuming that

\[ \Phi' \sim e^{i\mathbf{P} \cdot \mathbf{R}/\hbar} \]  \quad (A.16)
References

[1] E Marsch 2005 Ann. Phys. (Leipzig) 14 324
[2] E Salpeter and H A Bethe 1951 Phys. Rev. 84 1232
[3] X Artru 1984 Phys. Rev. D 29 1279
[4] M Järvinen 2007 Spin and Relativistic Motion of Bound States (PhD Thesis) University of Helsinki Report Series in Physics HU-P-D142, Section 3.1
[5] B D Keister and W N Polyzou 1991 Adv. Nucl. Phys. 20 225
[6] M Malvetti and H M Pilkuhn 1994 Physics Reports 248 1
[7] F Gross 1999 Relativistic Quantum Mechanics and Field Theory John-Wiley and Sons, New York
[8] H M Pilkuhn 2003 Relativistic Quantum Mechanics 173-179
[9] N Kemmer 1937 Helv. Phys. Acta 10 48
[10] E Fermi and C N Yang 1949 Phys. Rev. 76 1739
[11] Y Koide 1982 Il Nuovo Cimento 70 A 411
[12] J A McNeil and B K Wallin 1992 Phys. Lett. B 297 223
[13] A O Barut and G L Strobel 1986 Few Body Systems 1 167
[14] A O Barut and S Komy 1985 Fortschr. Phys. 33 309
[15] A O Barut and N Unal 1985 Fortschr. Phys. 33 319
[16] J W van Holten 1991 Nucl. Phys. B 356 3
[17] J W van Holten 1992 Physica A 182 279