Relativistic coupling of internal and centre of mass dynamics in classical and simple bound quantum mechanical systems

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Abstract

Although special relativity and quantum mechanics revolutionised physics in the early 20th century, the consequences of combining these two theories are still being explored a hundred years later, usually using the formidable theoretical machinery of quantum field theory. However, a formalism accessible to undergraduates has been recently developed which shows how the centre of mass and internal dynamics of classical and quantum systems is relativistically coupled with interesting consequences. Here we explore some of the implications of this coupling, first classically, where we find that the dynamics of the system is time dilated when moving relative to another inertial frame. We then apply the dynamics to a quantum 2-level atom bound in a one-dimensional infinite potential well, and show that the coupling produces collapses and revivals in quantum interference. This example provides an illustration of how the combination of special relativity and quantum mechanics can be studied in situations familiar to most undergraduates.

Keywords: relativity, quantum mechanics, centre of mass, entanglement

(Some figures may appear in colour only in the online journal)
1. Introduction

Einstein’s discovery that a body’s rest energy $E_{\text{rest}}$ is related to its inertial mass $m$ by

$$E_{\text{rest}} = mc^2, \tag{1}$$

where $c$ is the speed of light, is arguably among the most famous in physics. While most treatments of relativistic mechanics deal with particles, Einstein is clear in his original paper that equation (1) is meant to be applied to any body, and speculates that the formula can be tested by searching for mass changes in materials with variable internal energy content such as radium salts [1]. As a consequence, for a system with internal dynamics, one should expect that the internal motions would affect the centre of mass motion through its effect on the system’s inertial mass. A container of gas at room temperature has a larger mass than the same gas at a lower temperature since the warmer gas has greater internal energy from the increased average kinetic energy of the gas molecules. Yet, one does not find much discussion in textbooks of how equation (1) might modify the dynamics of a system as compared to a particle. Presumably this is because the effects are tiny in most practical situations and the energy is a constant of motion.

When a bright undergraduate attempts to raise similar questions in the quantum realm, an interesting problem arises. In the usual time-dependent Schrödinger wave equation for the wave function $\Psi(\vec{r}, t)$ of a free particle encountered in quantum mechanics courses,

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t), \tag{2}$$

the particle’s mass $m$ is a parameter. If one considers the system to be an atom, then the centre of mass motion of the atom would be described by equation (2), but now what should we use for the mass? If we take Einstein seriously, then the mass should include the internal energy of the atom, but a quantum atom might not have a definite energy if it is in a superposition of internal energy states. If the Universe obeyed Galilean relativity, then Bargmann’s theorem forbids a quantum system from existing in a superposition of mass states [2–5], which would be inconsistent with Einstein. Of course, as Einstein showed, our universe does not obey Galilean relativity, but obeys special relativity (if we exclude gravity as we do here). Even in the non-relativistic limit, features of the non-Galilean nature of the Universe remain and void Bargmann’s argument [5]. Yet, there still remains the problem of how to describe quantum mechanically the motion of the centre of mass of a system in a superposition of internal energy states.

One might think that quantum field theory would be needed to address this problem, but recently several authors have developed a natural approach for incorporating the internal dynamics of a system into the dynamics of the system’s centre of mass by essentially making the mass of the system a dynamical variable [6–13]. They have shown that in the quantum realm, this idea leads to special and general relativistic entanglement between a system’s internal and external dynamics, producing a loss of coherence in quantum twin paradox interference experiments [6] and Universal decoherence from gravitational time dilation [9]. (However, see [14] for a criticism of the latter effect and [15, 16] for alternative interpretations.) The general principle at work is that a quantum system with internal dynamics (a ‘quantum clock’) can be produced in a superposition of states that experience different proper times, leading to novel interference effects.

In this paper, we will examine this work with a simple derivation of the Hamiltonian motivated by Einstein’s mass–energy relation equation (1) which incorporates the internal and centre of mass motions of the systems while explaining the limitations of the formalism.
A more formal derivation using Lagrangian mechanics is relegated to the appendix. Before applying the formalism to quantum mechanical systems, we first test it out classically, applying Hamilton’s equations to the new Hamiltonian and showing that they lead to time-dilated dynamics. We then extend the formalism to the quantum realm where we apply it to a 2-level atom trapped in an infinite potential well, a system involving topics familiar to any undergraduate who has taken quantum mechanics. This simple system illustrates the consequences of the relativistic entanglement of internal and centre of mass dynamics at a level appropriate for an upper-level undergraduate quantum mechanics course.

2. System Hamiltonian

In this section, we provide a simple derivation of the formalism developed in [6–13] for a small isolated system of interacting particles that are non-relativistic relative to their centre of mass frame. In the appendix a more formal derivation is given of the system Hamiltonian using Lagrangian mechanics.

We begin with the relativistic Hamiltonian describing a free point particle of mass $m$ with momentum $\vec{P}$ [17]:

$$ H_{\text{particle}} = \sqrt{m^2c^4 + P^2c^2}. \quad (3) $$

Let us now replace the particle with a very small compact system such as an atom or molecule of mass $M$. Relative to the system’s centre of mass, the total momentum of the system vanishes, so the total energy of the system $E_{\text{rest}} = Mc^2$ in this frame (the rest energy) is an invariant quantity:

$$ E_{\text{rest}} = \left(c \sum_{\mu = 0}^{3} \eta_{\mu\nu} P^\mu_{\text{tot}} P^\nu_{\text{tot}} \right)^{1/2} = \sqrt{E^2_{\text{tot}} - P^2_{\text{tot}}c^2}. \quad (4) $$

Here $P^\mu_{\text{tot}} = (E_{\text{tot}}/c, \vec{P}_{\text{tot}})$ is the total four-momentum of the system, and $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ is the flat spacetime metric tensor. Thus, the total energy relative to an arbitrary inertial frame can be written as

$$ E = \sqrt{E^2_{\text{rest}} + P^2c^2}, \quad (5) $$

where from now on we will write $\vec{P}_{\text{tot}} = \vec{P}$.

We now make the ansatz that the total Hamiltonian of the system can be obtained from equation (5) by making the replacement

$$ E_{\text{rest}} = Mc^2 \rightarrow M_0c^2 + H_{\text{int}}, \quad (6) $$

where $M_0$ is a constant, and $H_{\text{int}}$ is the system’s Hamiltonian relative to the centre of mass frame, which, by definition, is written in terms of only the internal coordinates. Then $M_0c^2$ represents the non-dynamical part of the rest energy (e.g., the sum of the rest energies of the constituent particles). In order for the concept of centre of mass to make sense here, we assume that there exists a frame in which all of the system particles are non-relativistic so that a centre of mass frame can be defined [20]. (See [16] for more discussion of the issue of centre of mass in this context.) This requires that we assume

$$ \frac{H_{\text{int}}}{M_0c^2} \ll 1, \quad (7) $$

for all subsequent calculations, and that we retain only first order terms in $H_{\text{int}}/M_0c^2$. With these assumptions, the total Hamiltonian of the freely propagating system becomes
where $\vec{P}$ is the total momentum, and $q_j$ and $p_j$ are the generalised coordinates and momenta relative to the centre of mass.

If the system is under the influence of a time-independent external potential $U_{\text{ext}}(\vec{R})$ which is sufficiently uniform over the size of the system $\ell$ that

$$\frac{\ell |\nabla U_{\text{ext}}(\vec{R})|}{|U_{\text{ext}}(\vec{R})|} \ll 1,$$

where $\vec{R}$ is the position of the centre of mass, the effect of $U_{\text{ext}}(\vec{R})$ should depend only on $\vec{R}$ and be independent of the internal state of the system. Assuming this condition, we write the Hamiltonian of the system in the presence of this external interaction as

$$H(\vec{R}, \vec{P}, q_j, p_j) = H_0 + U_{\text{ext}}(\vec{R})$$

$$= \sqrt{M_0^2 c^4 + P^2 c^2} + U_{\text{ext}}(\vec{R}) + \frac{M_0 c^2 H_{\text{int}}(q_j, p_j)}{\sqrt{M_0^2 c^4 + P^2 c^2}},$$

(10)

The first two terms on the right side of equation (10) represent the special relativistic Hamiltonian of a point particle of mass $M_0$ and momentum $P$ in an external potential $U_{\text{ext}}(\vec{R})$ [17]. The third term on the right side of equation (10) contains both centre of mass and internal coordinates, and represents the relativistic coupling of the centre of mass and internal dynamics. Note that we have taken a conventional approach to incorporating a potential into the problem, which explicitly breaks Lorentz invariance without affecting the mass of the system. One can find alternative approaches, where the potential produces a position-dependent mass (e.g., [18]), but these go beyond the scope of this paper. In addition, if the external potential varies significantly over the size of the system, additional coupling terms will arise [19], but these non-relativistic couplings are not of interest here.

For the rest of the paper, we will explore the consequences of equation (10) that arise from the third term which couples the centre of mass motion with its internal dynamics.

### 3. Classical dynamics

We begin our investigation of the Hamiltonian given by equation (10) by first applying classically Hamilton’s equations to the centre of mass momentum and position coordinates. The momentum equation for the $i$th component gives

$$\frac{dP_i}{dt} = -\frac{\partial H}{\partial X_i} = -\frac{\partial U_{\text{ext}}}{\partial X_i}$$

(11)

or

$$\frac{d\vec{P}}{dt} = -\nabla U_{\text{ext}}(\vec{R}),$$

(12)

which is the usual result from Newton’s 2nd law when an external force acts on the system. Similarly, the equation for the system’s centre of mass velocity component $V_i = \dot{X}_i \equiv dX_i/dt$, where $X_i$ is the $i$th component of the system’s centre of mass position, is
which gives for the expression for the centre of mass velocity
\[
\vec{v} = \frac{\vec{p}_c}{\sqrt{M_0^2c^4 + p^2c^2}} \left(1 - \frac{M_0 c^2 H_{\text{int}}}{M_0^2 c^4 + p^2c^2}\right)
\]  
(14)

Equation (14) is exactly what one would expect from the usual point particle formula,
\[
\vec{V}_{\text{point}} = \frac{\vec{p}_c}{E} = \frac{\vec{p}_c}{\sqrt{M^2c^4 + p^2c^2}}.
\]
(15)
after making the replacement equation (6) and retaining only the leading order term in \(H_{\text{int}}/M_0c^2\).

Applying Hamilton’s equations to the internal coordinates, we find
\[
\frac{dq_i}{dr} = \frac{\partial H}{\partial p_i} = \frac{M_0 c^2}{\sqrt{M_0^2 c^4 + p^2c^2}} \frac{\partial H_{\text{int}}}{\partial q_i},
\]
(16)
\[
\frac{dp_i}{dr} = -\frac{\partial H}{\partial q_i} = -\frac{M_0 c^2}{\sqrt{M_0^2 c^4 + p^2c^2}} \frac{\partial H_{\text{int}}}{\partial q_i}.
\]
(17)

Since
\[
\sqrt{1 - V^2/c^2} = \frac{M_0 c^2}{\sqrt{M_0^2 c^4 + p^2c^2}} + O\left(\frac{H_{\text{int}}}{M_0c^2}\right).
\]
(18)
equations (16) and (17) are the time-dilated Hamilton’s equations viewed in the co-moving frame:
\[
\frac{dq_i}{d\tau} = \frac{\partial H_{\text{int}}}{\partial p_i},
\]
(19)
\[
\frac{dp_i}{d\tau} = -\frac{\partial H_{\text{int}}}{\partial q_i},
\]
(20)
where \(d\tau\) is the proper time interval
\[
d\tau = dt\sqrt{1 - V^2/c^2}.
\]
(21)
Therefore, the Hamiltonian given by equation (10) leads to physically intuitive and reasonable results for classical systems. It also provides a more general underpinning for dynamical approaches of obtaining time dilation through the analysis of the physical mechanisms of clocks as done by Jefimenko [21]. Let us now turn our attention to the dynamics of a quantum system governed by equation (10).

### 4. Quantum dynamics

In this section, we will quantise the Hamiltonian equation (10). Previous authors have obtained this Hamiltonian and used it to examine the quantum interference of essentially freely propagating systems in gravitational fields [6–13]. Here we will show that similar quantum interference arises in the simplest bound system encountered by undergraduate
students: a 2-level atom in a one-dimensional infinite potential well. Not only is this system simple, it also can be solved exactly. For novel behaviour to be observed, the system will then be prepared in a superposition of both internal and centre of mass states. Using the density operator formalism to trace over the internal states, the centre of mass position probability density is obtained, revealing a collapse and revival of the centre of mass position interference due to the relativistic coupling.

4.1. Hamiltonian operator

In our analysis of the classical system, we assumed that one can find a frame in which the system is non-relativistic with a well-defined centre of mass. We then placed essentially no restrictions on the motion of this centre of mass. In this paper, we wish to investigate the quantum aspects of our problem without having to deal with the significant complications of particle creation, which requires a treatment using quantum field theory. Therefore, we will now assume $P^2/M_0^2 c^2 \ll 1$ and include only the leading order special relativistic terms of our Hamiltonian equation (10), which now becomes

$$H(\vec{R}, \vec{P}, q, p) \approx M_0 c^2 + \frac{p^2}{2M_0} - \frac{p^4}{8M_0^3 c^2} + U_{\text{ext}}(\vec{R}) + H_{\text{int}}(q, p) \left(1 - \frac{p^2}{2M_0^2 c^2}\right).$$

(22)

So far our treatment has been classical and three-dimensional. For the rest of this paper, we will focus our attention on one-dimensional quantum mechanical systems, where we replace the centre of mass canonical coordinates $X$ and $P_X$ with their corresponding quantum mechanical operators $\hat{X}$ and $\hat{P}_X$, while making similar substitutions with the internal coordinates. This leads to the quantum mechanical Hamiltonian describing a small quantum system bound to a potential,

$$\hat{H} \approx M_0 c^2 + \frac{\hat{P}_X^2}{2M_0} - \frac{\hat{P}_X^4}{8M_0^3 c^2} + U_{\text{ext}}(\hat{X}) + \hat{H}_{\text{int}}(\hat{q}, \hat{p}) \left(1 - \frac{\hat{P}_X^2}{2M_0^2 c^2}\right).$$

(23)

To account for ground state energies, the constant $M_0$ is defined so that the energy of the internal system vanishes when it is in its ground state.

We note in passing that all of these results could have been obtained by starting with the single particle Hamiltonian

$$\hat{H} = M c^2 + \frac{\hat{P}_s^2}{2M} - \frac{\hat{P}_s^4}{8M^3 c^2} + U_{\text{ext}}(\hat{X})$$

(24)

and replacing the particle mass $M$ with the mass operator $\hat{M}$ defined by [8]

$$\hat{M} \equiv M_0 + \frac{\hat{H}_{\text{int}}}{c^2}$$

(25)

and keeping only first order terms in $\hat{H}_{\text{int}}/M_0 c^2$. In essence, this takes Einstein’s famous formula equation (1) seriously in the quantum realm where systems can be in superpositions of energy states, which also means they should be in superpositions of mass eigenstates. Arguments have been made against mass superpositions [2–5], but they are based on Galilean
relativity rather than the non-relativistic limit of special relativity [10]. Finally, one can similarly deal with unstable quantum particles by replacing $M$ in equation (24) with a complex mass [22, 23]

$$M = M_0 - \frac{i\hbar \Gamma_0}{2},$$

(26)

where $\Gamma_0$ is the decay rate of the particle in its rest frame, and keeping only leading order terms in $\hbar \Gamma_0/M_0 c^2$. In both cases, the system with an internal Hamiltonian $\hat{H}_{\text{int}}$ and the unstable particle with width $\Gamma_0$, the quantum system has indefinite mass.

In practice, one frequently considers problems where the non-relativistic centre of mass and internal dynamics are known, and the remaining portions are small in comparison. To use perturbation theory in this case, it is helpful to separate the Hamiltonian equation (23) into two parts,

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

(27)

Here the unperturbed Hamiltonian,

$$\hat{H}_0 = \frac{\hat{p}_x^2}{2M_0} + U_{\text{ext}}(\hat{X}) + M_0 c^2 + \hat{H}_{\text{int}},$$

(28)

can also be written as the sum of two parts:

$$\hat{H}_0 = \hat{H}_{0,\text{cm}} + \hat{H}_{0,\text{int}},$$

(29)

where the centre of mass portion,

$$\hat{H}_{0,\text{cm}} = \frac{\hat{p}_x^2}{2M_0} + U_{\text{ext}}(\hat{X})$$

(30)

is the usual non-relativistic quantum Hamiltonian for a particle in an external potential, and

$$\hat{H}_{0,\text{int}} = M_0 c^2 + \hat{H}_{\text{int}},$$

(31)

is the usual internal Hamiltonian relative to the centre of mass (including rest energies of the component particles). The small perturbation is given by

$$\hat{H}_1 = -\frac{\hat{p}_x^4}{8M_0^3 c^2} - \frac{\hat{p}_x^2 \hat{H}_{\text{int}}}{2M_0^2 c^2},$$

(32)

where the first term leads to small corrections to the centre of mass motion, while the second term will couple the centre of mass and internal dynamics.

4.2. System: 2-level atom in infinite potential well

So far our system has been left unspecified. Let us now focus our attention on the simplest possible system that will exhibit the desired features: a 2-level atom. The eigenvalue equation for $\hat{H}_{0,\text{int}}$ will be
\[ \hat{H}_{0,\text{int}}|n\rangle = E_n^{\text{int}}|n\rangle, \]  
where \( n = 0, 1, E_0^{\text{int}} = 0 \) is the ground state energy, and \( E_1^{\text{int}} \) is the energy of the excited state.

The simplest bound system is a particle in a one-dimensional infinite potential well of length \( L \) given by

\[ U_{\text{ext}}(X) = U_{\text{well}}(X) = \begin{cases} 0, & \text{if } 0 < X < L, \\ \infty, & \text{otherwise}. \end{cases} \]

In this case, the eigenvalue equation of the unperturbed centre of mass motion Hamiltonian equation (30) is [24]

\[ \hat{H}_{0,\text{cm}}|N\rangle = E_N^{\text{up}}|N\rangle, \]  
where

\[ E_N^{\text{up}} = \frac{(N + 1)^2\pi^2\hbar^2}{2m_0L^2}, \quad N = 0, 1, 2, \ldots \]

and the energy wave functions are

\[ \psi_N^{\text{up}}(X) = \langle X|N\rangle = \begin{cases} \frac{2}{L} \sin \left( \frac{(N + 1)\pi x}{L} \right), & \text{if } 0 < X < L, \\ 0, & \text{otherwise.} \end{cases} \]

(We have chosen the unconventional notation of numbering the ground state \( N = 0 \) instead of \( N = 1 \) so that both the centre of mass and internal Hamiltonian ground states in this paper will be labelled with \( N = n = 0 \).) Combining the results of equations (33) and (35), the total unperturbed eigenvalue equation is

\[ \hat{H}_0|N, n\rangle = E_{Nn}^{\text{up}}|N, n\rangle, \]  
where the energy of the unperturbed system is

\[ E_{Nn}^{\text{up}} = E_N^{\text{up}} + E_n^{\text{int}} = \frac{(N + 1)^2\pi^2\hbar^2}{2m_0L^2} + E_n^{\text{int}}. \]

We are fortunate that for this system that the unperturbed Hamiltonian and the perturbation commute, \([\hat{H}_0, \hat{H}_1] = 0\), so that the eigenstates of \( \hat{H}_0 \) are also eigenstates of \( \hat{H}_1 \), and thus, of the Hamiltonian \( \hat{H} \):

\[ |E_{Nn}\rangle = |N, n\rangle. \]

The energy contribution from \( \hat{H}_1 \) is then

\[ E_{Nn}^{1} = \langle N, n|\hat{H}_1|N, n\rangle \]

\[ = - \langle N, n|\left( \frac{\hat{P}_x^4}{8M_0^2c^2} + \frac{\hat{P}_x^2\hat{H}_\text{int}}{2M_0^2c^2} \right)|N, n\rangle \]

\[ = - \left[ \frac{1}{8M_0^2c^2} \langle N|\hat{P}_x^4|N\rangle + \frac{E_n^{\text{int}}}{2M_0^2c^2} \langle N|\hat{P}_x^2|N\rangle \right]. \]
Using the infinite potential well wave functions given by equation (37),

\[ \langle N | \hat{P}_x^2 | N \rangle = -\hbar^2 \int_0^L dX \, |\psi_{N}^{\text{IP}}(X)|^2 \frac{d^2 \psi_{N}^{\text{IP}}(X)}{dX^2} \]

\[ = -\hbar^2 \left[ -\frac{\pi^2 (N+1)^2}{L^2} \right] \times \frac{2}{L} \int_0^L dX \, \sin^2 \left( \frac{(N+1)\pi X}{L} \right) \]

\[ = \frac{(N+1)^2 \pi^2 \hbar^2}{L^2} = 2M_0 E_N^{\text{IP}} \]

(42)

and

\[ \langle N | \hat{P}_y^2 | N \rangle = \hbar^4 \int_0^L dX \, |\psi_{N}^{\text{IP}}(X)|^2 \frac{d^4 \psi_{N}^{\text{IP}}(X)}{dX^4} \]

\[ = \frac{(N+1)^4 \pi^4 \hbar^4}{L^4} = 4M_0^2 (E_N^{\text{IP}})^2. \]

Substituting these results into equation (41) gives

\[ E_{Nn}^l = -\frac{(E_N^{\text{IP}})^2}{2M_0 c^2} - \frac{E_N^{\text{IP}} E_n^{\text{int}}}{M_0 c^2}, \]

(44)

so the total energy of the system is

\[ E_{Nn} = E_N^{\text{IP}} + E_n^{\text{int}} - \frac{(E_N^{\text{IP}})^2}{2M_0 c^2} - \frac{E_N^{\text{IP}} E_n^{\text{int}}}{M_0 c^2}. \]

(45)

For a particle in an infinite potential well, \( E_N^{\text{IP}} \) is just the kinetic energy, so the first two terms on the right side of equation (45) are the usual non-relativistic kinetic and internal energies, while the third term is the leading order relativistic correction to the kinetic energy. The fourth term on the right side of equation (45) is the contribution to the kinetic energy due to the system’s internal energy.

We now have everything needed to investigate the dynamics of this system.

4.3. Dynamics

The quintessential quantum phenomenon is interference, which arises when a quantum system exists in a coherent superposition of states, which is analogous to the coherent superposition of wave amplitudes that gives rise to classical wave interference \([25, 26]\). Coherence is preserved as long as there is no way of determining which state the system is in. If information about which state the system is in can be transferred to another system (i.e., the states of the two systems become entangled), coherence is lost and interference disappears.

In order to observe interference in the centre of mass motion of our atom in the infinite potential well, the system needs to be placed into a superposition of centre of mass energy states. Furthermore, to investigate the effects of the system having an indefinite mass, the atom should also be in a superposition of internal energy states. Therefore, we will assume the system begins at \( t = 0 \) in state that is a tensor product of superpositions of centre of mass and internal states,
\[
|\Psi(0)\rangle = \left[ \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \right]_{\text{cm}} \otimes \left[ \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \right]_{\text{int}} \\
= \frac{1}{2} (|0, 0\rangle + |0, 1\rangle + |1, 0\rangle + |1, 1\rangle). \tag{46}
\]

That is, this initial state is not entangled so knowing the internal state provides no information about the centre of mass state, and vice versa. Then for \( t > 0 \), the state vector for the system can be written down by including exponential factors \( e^{-iE_{\text{tot}}t/\hbar} \) since \( |N, n\rangle \) is an eigenstate of the total Hamiltonian:

\[
|\Psi(t)\rangle = \frac{1}{2} \sum_{N=0}^{1} \sum_{n=0}^{1} e^{-iE_{\text{tot}}t/\hbar} |N, n\rangle \\
= \frac{1}{2} \left( e^{-iE_{\text{tot}}t/\hbar} |0, 0\rangle + e^{-iE_{\text{tot}}t/\hbar} |0, 1\rangle \right. \\
+ \left. e^{-iE_{\text{tot}}t/\hbar} |1, 0\rangle + e^{-iE_{\text{tot}}t/\hbar} |1, 1\rangle \right). \tag{47}
\]

The system’s density operator is then

\[
\hat{\rho}(t) = |\Psi(t)\rangle \langle \Psi(t)| = \frac{1}{4} \sum_{N,N'=0}^{1} \sum_{n,n'=0}^{1} e^{-i(E_{N'\text{ent}}-E_{N'\text{cm}})t/\hbar} |N, n\rangle \langle N', n'|. \tag{48}
\]

Let us now focus our attention on the centre of mass motion of the system. Tracing equation (48) over the internal energy states gives the reduced density operator of the centre of mass motion, which has matrix elements

\[
\langle K|\hat{\rho}_{\text{cm}}(t)|K'\rangle = \frac{1}{4} \left( \delta_{K,K'} \sum_{k=0}^{1} \langle K, k|\hat{\rho}(t)|K', k\rangle, \\
\right.
\]

\[
= \frac{1}{4} \sum_{N,N'=0}^{1} \sum_{n,n'=0}^{1} \sum_{k=0}^{1} c^{-i(E_{N'\text{ent}}-E_{N'\text{cm}})t/\hbar} \\
\times \langle K, k|N, n\rangle \langle N', n'|K', k\rangle \\
= \frac{1}{4} \left[ e^{-i(E_{\text{cm}}-E_{\text{ent}})t/\hbar} + e^{-i(E_{\text{cm}}-E_{\text{ent}})t/\hbar} \right]. \tag{49}
\]

The diagonal matrix elements of \( \hat{\rho}_{\text{cm}}(t) \) are constant,

\[
\langle 0|\hat{\rho}_{\text{cm}}(t)|0\rangle = \langle 1|\hat{\rho}_{\text{cm}}(t)|1\rangle = \frac{1}{2}, \tag{50}
\]

so there is always a 50% probability of the centre mass energy being in either of the lowest two energy states. The interference in the centre of mass motion arises from the off-diagonal elements:

\[
\langle 0|\hat{\rho}_{\text{cm}}(t)|1\rangle = \langle 1|\hat{\rho}_{\text{cm}}(t)|0\rangle^* \\
= \frac{1}{4} \left[ e^{-i(E_{\text{cm}}-E_{\text{int}})t/\hbar} + e^{-i(E_{\text{int}}-E_{\text{cm}})t/\hbar} \right] \\
= \frac{1}{2} e^{i\Omega_{\text{ent}}t} \cos(\Omega_{\text{cm}}t). \tag{51}
\]

We see that two natural frequencies, \( \Omega_{\text{cm}} \) and \( \Omega_{\text{ent}} \), arise. First, there is the frequency of the centre of mass motion \( \Omega_{\text{cm}} \) that depends primarily on the energy difference of the two centre of mass energy states,
This result has a nice intuitive interpretation. This frequency would arise for a particle in a superposition of the first two infinite square well energy states if it had a mass

\[ M = M_0 + \frac{\langle \hat{H}_{\text{int}} \rangle}{c^2}, \]

where

\[ \langle \hat{H}_{\text{int}} \rangle = \frac{1}{2}(E_0^{\text{int}} + E_1^{\text{int}}) \]

is the average internal energy. The second natural frequency \( \Omega_{\text{ent}} \) which appears in equation (51) arises purely from the coupling term of the Hamiltonian and depends on the product of the differences in centre of mass and internal energy levels:

\[ \Omega_{\text{ent}} \equiv \frac{|E_{11} + E_{10} - E_{01} - E_{00}|}{2\hbar} \]

\[ = \frac{1}{2\hbar M_0 c^2} (E_1^{\text{IP}} - E_0^{\text{IP}})(E_0^{\text{int}} + E_1^{\text{int}}) \]

\[ = \frac{(E_1^{\text{IP}} - E_0^{\text{IP}})}{\hbar} \left[ 1 - \frac{E_0^{\text{int}} + E_1^{\text{int}}}{2M_0 c^2} \right] - \frac{1}{2\hbar M_0 c^2} [(E_1^{\text{IP}})^2 - (E_0^{\text{IP}})^2]. \]  

(52)

We will see that this frequency is associated with the collapse and revival of the interference due to the entanglement of the centre of mass and internal motions. This effect will not occur if the centre of mass and/or the internal systems are in energy eigenstates.

As a demonstration of the effects of the two frequencies, let us look at the centre of mass probability density, which is given by

\[ P_{\text{cm}}(X, t) = \text{Tr}[\hat{\rho}_{\text{cm}}(t)X\langle X \rangle] \]

\[ = \sum_{K,K'=0} \langle K|\hat{\rho}_{\text{cm}}(t)|K'\rangle \langle K'|X\rangle \langle X|K \rangle \]

\[ = \sum_{K,K'=0} \langle K|\hat{\rho}_{\text{cm}}(t)|K'\rangle \psi_{K'}^{\text{IP}}(X)\psi_K^{\text{IP}}(X) \]

\[ = \frac{1}{2}|\psi_0^{\text{IP}}(X)|^2 + \frac{1}{2}|\psi_1^{\text{IP}}(X)|^2 \]

\[ + \frac{1}{2} \cos(\Omega_{\text{ent}} t) \langle \psi_0^{\text{IP}}(X)|\psi_1^{\text{IP}}(X) e^{i\Omega_{\text{cm}} t} \rangle \]

\[ + \langle \psi_0^{\text{IP}}(X)|\psi_1^{\text{IP}}(X) e^{-i\Omega_{\text{cm}} t} \rangle. \]  

(56)
Since the centre of mass wave functions are real, this simplifies to

\[
\mathcal{P}_{\text{cm}}(X, t) = \frac{1}{2} \left[ |\psi_0|^2(X) + |\psi_1|^2(X) \right]
\]

\[
+ 2\psi_0^\dagger(X)\psi_1^\dagger(X) \cos(\Omega_{\text{ent}} t) \cos(\Omega_{\text{cm}} t). \tag{57}
\]

Equation (57) has a form analogous to the probability density seen in the usual double-slit experiment [25] where, in that case, the wave functions represent the amplitudes of passing through the slits, except the interference term here depends on time instead of spatial position.

At \( t = 0 \), \( \cos(\Omega_{\text{ent}} t) = 1 \) so the centre of mass probability density oscillates with frequency \( \Omega_{\text{cm}} \) in the same manner as a particle with no internal degrees of freedom. As noted earlier, we’ve chosen to start the system completely unentangled so the centre of mass is described by a pure state wave function, and the internal state contains no information about the centre of mass motion. However, as time passes, \( \cos(\Omega_{\text{ent}} t) \) decreases as the centre of mass and internal states become entangled through the relativistic coupling. Conceptually, because all of the centre of mass energy in the infinite square well is kinetic, the particle in the higher energy \( N = 1 \) centre of mass state is travelling faster than if was in the ground \( N = 0 \) state, so the time dilation of the internal dynamics will differ. By observing how much the internal clock has slowed, one could tell which centre of mass state the system is in. This is how information about the centre of mass state becomes encoded in the internal state of the atom. Eventually, when \( t = \pi/2\Omega_{\text{ent}} \), the internal state has become completely entangled with the centre of mass state, shutting off the interference. The oscillation in the probability density \( \mathcal{P}_{\text{cm}}(X, t) \) slows to a stop. At this instant, the information about the centre of mass motion is completely encoded into the internal state. The probability density is simply the equally weighted sum of the probability densities of being in the centre of mass states \( N = 0 \) and \( N = 1 \), which is analogous to the double-slit interference when one knows through which slit the particle passes. Then, as time continues to advance, the system gradually loses its entanglement and interference is restored. In figure 1, we have plotted \( \mathcal{P}_{\text{cm}}(X, t) \) for \( t = 0 \) (when the system is unentangled and exhibits maximum interference) and \( t = \pi/2\Omega_{\text{ent}} \) (when the system is fully entangled and there is no interference). This oscillating interference due to \( \cos(\Omega_{\text{ent}} t) \) for the bound atom is analogous the oscillating visibility in quantum interferometry.
from an atom experiencing different general relativistic proper times while traversing an interferometer [6].

5. Discussion

Most treatments of Einstein’s formula equation (1) relating the inertial mass of a system to its rest energy consider the system to be a particle, while nearly all systems one encounters in reality possess internal degrees of freedom. In quantum mechanics, systems may have indefinite internal energy if they are unstable or are in an internal state that is a superposition of energy eigenstates. In textbook treatments, it is not obvious how to incorporate such an indefinite mass into the Schrödinger wave equation even though equation (1) implies that it should be possible.

In this paper, we explored the classical and quantum consequences of a new approach which takes Einstein seriously and incorporates the internal degrees of freedom for systems which have a well-defined centre of mass [6–13]. We presented both a simple and, in the appendix, a more formal derivation of the Hamiltonian equation (10) which leads to the relativistic coupling of the internal and centre of mass dynamics, and showed that for classical systems, this produces the expected time dilation of the dynamics of a system when viewed from another inertial frame.

When we quantised the formalism for nearly non-relativistic systems, we found that the resulting Hamiltonian operator equation (23) includes a term which couples the centre of mass and internal dynamics. This will lead to a change of dynamics and, using a 2-level atom bound in a one-dimensional infinite potential well, we saw that it can produce an oscillation in the entanglement between the centre of mass and internal motions, significantly altering the quantum interference compared to the situation of an analogous system with no internal degrees of freedom.

We hope that this paper will help address questions that might arise from a curious student who wishes to go beyond typical textbook discussions of relativistic particles and thinks about systems with internal dynamics. The formalism developed recently [6–13] provides a natural approach consistent with Einstein’s famous equation which leads to physically sensible classical dynamics and novel interference effects in the quantum realm. It provides an elegant way of studying the motion of a quantum system with indefinite mass due to being in an internal state that is a superposition of energy eigenstates. While we only considered applications involving special relativity in order to provide the simplest treatment, the formalism has been shown to apply more broadly to general relativistic systems. Finally, the formalism is accessible to undergraduates, giving them an opportunity to explore fundamental issues in relativity and quantum mechanics that may soon be studied in the laboratory.

Appendix. More formal derivation of system Hamiltonian

In this appendix, we review a more complete derivation of the free system Hamiltonian, equation (10), that was outlined in [9]. We begin with the action of a small system in a frame co-moving with its centre of mass,

\[ S = \int L_{\text{real}}(q, q') \, dq, \]  

(A.1)
where $L_{\text{rest}}(q_i, q'_i)$ is the system Lagrangian relative to this rest frame, $q_i$ and $q'_i$ are the generalised coordinates and velocities for the system relative to the centre of mass frame. We use primes to denote derivatives with respect to the system’s proper time $\tau$, e.g., $q'_i = dq_i/d\tau$. If the system is simply a point particle with mass $m$, $L_{\text{rest}} = -mc^2$.

If we now view the system’s motion relative to an inertial frame, then the action equation (A.1) can be written as

$$S = \int L_{\text{rest}}(q_i, q'_i, \frac{d}{d\tau}/d\tau) \, d\tau \, dt,$$

where the proper time interval $d\tau$ is related to the inertial frame time interval $dt$ by

$$d\tau = dt\sqrt{1 - V^2/c^2}$$

and dots over a quantity denote time derivatives with respect to $t$, e.g., $\dot{q}_i = dq_i/dt$. Thus, the Lagrangian for the system relative to the inertial frame is

$$L = L_{\text{rest}}(q_i, q'_i, \frac{d}{d\tau}/d\tau) \, d\tau = L_{\text{rest}}[q_i, q'_i, (q_i, V)] \sqrt{1 - V^2/c^2}.$$  

(A.4)

Using equation (A.4), we can obtain the canonical momenta associated with the internal coordinate $q_i$,

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

$$= \sum_j \frac{\partial L_{\text{rest}}}{\partial \dot{q}'_j} \frac{dq'_i}{dq'_j} \sqrt{1 - V^2/c^2}$$

$$= \frac{\partial L_{\text{rest}}}{\partial q'_i}. \quad (A.5)$$

and the centre of mass coordinate $X_i$, where $X_1 = X$, $X_2 = Y$, and $X_3 = Z$,

$$p_i = \frac{\partial L}{\partial X_i}$$

$$= \sum_j \frac{\partial L_{\text{rest}}}{\partial \dot{q}'_j} \frac{dq'_i}{dX_j} \sqrt{1 - V^2/c^2} + L_{\text{rest}} \frac{\partial}{\partial X_i} \sqrt{1 - V^2/c^2}$$

$$= \left( \sum_j \frac{\partial L_{\text{rest}}}{\partial \dot{q}'_j} \right) \dot{X}_i \frac{X_i/c^2}{\sqrt{1 - V^2/c^2}}, \quad (A.6)$$

where we have used $V^2 = \sum_{k=1}^3 \dot{X}_k^2$. Since the rest energy of the system is

$$E_{\text{rest}} = \sum_j \frac{\partial L_{\text{rest}}}{\partial \dot{q}'_j} q'_j - L_{\text{rest}}, \quad (A.7)$$

we can write the canonical momentum relative to the centre of mass velocity $\dot{V}$ as

$$\vec{p} = \frac{(E_{\text{rest}}/c^2)\dot{V}}{\sqrt{1 - V^2/c^2}}. \quad (A.8)$$

This agrees with the usual expression for a system of mass $M = E_{\text{rest}}/c^2$.

To obtain the Hamiltonian, we first begin with the constant of motion in terms of coordinates and velocities:
The Hamiltonian is obtained by replacing the coordinate velocities with their associated canonical momenta. From equation (A.8), we find
\[
\frac{1}{\sqrt{1 - V^2/c^2}} = \sqrt{\frac{E_{\text{rest}}^2 + P^2c^2}{E_{\text{rest}}}},
\]
so equation (A.9) becomes
\[
H_0 = \sqrt{E_{\text{rest}}^2 + P^2c^2},
\]
which is the expected answer for a small system with invariant rest energy $E_{\text{rest}}/c^2$. Now we write this rest energy as
\[
E_{\text{rest}} = M_0 c^2 + H_{\text{int}}(q_j, p_j),
\]
where all the dynamics of the internal system results from the internal Hamiltonian $H_{\text{int}}(q_j, p_j)$. Here we assume that relative to the centre of mass, the system is non-relativistic so $H_{\text{int}}/M_0 c^2 \ll 1$. Then expanding equation (A.11) to first order in $H_{\text{int}}/M_0 c^2$, we obtain the final result:
\[
H_0(X_i, P_i, q_j, p_j) = \sqrt{M_0^2 c^4 + P^2c^2} + \frac{M_0 c^2 H_{\text{int}}(q_j, p_j)}{\sqrt{M_0^2 c^4 + P^2c^2}}.
\]

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