Dirac Equation and Quantum Relativistic Effects in a Single Trapped Ion

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We present a method of simulating the Dirac equation in 3+1 dimensions for a free spin-1/2 particle in a single trapped ion. The Dirac bispinor is represented by four ionic internal states, and position and momentum of the Dirac particle are associated with the respective ionic variables. We show also how to simulate the simplified 1+1 case, requiring the manipulation of only two internal levels and one motional degree of freedom. Moreover, we study relevant quantum-relativistic effects, like the Zitterbewegung and Klein’s paradox, the transition from massless to massive fermions, and the relativistic and nonrelativistic limits, via the tuning of controllable experimental parameters.

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The search for a fully relativistic Schrödinger equation gave rise to the Klein-Gordon and Dirac equations. P. A. M. Dirac looked for a Lorentz-covariant wave equation that is linear in spatial and time derivatives, expecting that the interpretation of the square wave function as a probability density holds. As a result, he obtained a fully covariant wave equation for a spin-1/2 massive particle, which incorporated \emph{ab initio} the spin degree of freedom. It is known that the Dirac formalism describes accurately the spectrum of the hydrogen atom and that it plays a central role in quantum field theory, where creation and annihilation of particles are allowed. How-
ternal level excitation accompanies an excitation in the considered motional degree of freedom, and vice versa.

All these interactions could be applied simultaneously and addressed to different pairs of internal levels coupled to different CM modes. For example, it is possible to adjust field phases to implement a simultaneous blue and red sideband excitation scheme to form the Hamiltonian $H_{2E}^{z} = i\hbar\eta_{z}\sigma_{x}(a_{c}^\dagger - a_{x}) = 2\eta_{z}\Delta_{z}\sigma_{y}\sigma_{x}p_{z}$, with $i(a_{c}^\dagger - a_{x})/2 = \Delta_{z}p_{z}/\hbar$. Here, $\Delta_{z} := \sqrt{\hbar/2M\nu_{c}}$ is the spread in position along the $z$-axis of the zero-point wavefunction and $p_{z}$ the corresponding dimensioned momentum operator. The physics of $H_{2E}^{z}$ cannot be described anymore by Rabi oscillations. In turn, it yields a conditional displacement in the motion depending on the internal state, producing the so-called Schrödinger cat states [9, 10]. By further manipulation of laser field directions and phases, we can also implement $H_{2D}^{x} = 2\eta_{x}\Delta_{x}\sigma_{y}p_{y}$ and $H_{2D}^{z} = 2\eta_{z}\Delta_{z}\sigma_{y}p_{z}$. This kind of interactions has already been produced in the lab, under resonant [11] and dispersive conditions [12].

We define the wave vector associated with the four ionic internal levels as

$$|\Psi\rangle := \Psi_{a}|a\rangle + \Psi_{b}|b\rangle + \Psi_{c}|c\rangle + \Psi_{d}|d\rangle = \left(\begin{array}{l}
\Psi_{a} \\
\Psi_{b} \\
\Psi_{c} \\
\Psi_{d}
\end{array}\right).$$  (1)

We may apply simultaneously different laser pulses, with proper directions and phases, $\eta \equiv \eta_{x} = \eta_{y} = \eta_{z}$, $\Delta \equiv \Delta_{x} = \Delta_{y} = \Delta_{z}$, $\Omega \equiv \Omega_{x} = \Omega_{y} = \Omega_{z}$, $\Omega \equiv \Omega_{x} = \Omega_{y} = \Omega_{z}$, to compose the following Hamiltonian acting on $|\Psi\rangle$,

$$H_{D} = 2\eta\Delta\tilde{\Omega}(\sigma_{x}^{ad} + \sigma_{y}^{bc})p_{x} + 2\eta\Delta\tilde{\Omega}(\sigma_{y}^{ad} - \sigma_{y}^{bc})p_{y} + 2\eta\Delta\tilde{\Omega}(\sigma_{x}^{ac} - \sigma_{x}^{bd})p_{z} + \hbar\Omega(\sigma_{y}^{ac} + \sigma_{y}^{bd}).$$  (2)

We rewrite Eq. (2) in the suitable matrix form

$$H_{D} = \left(\begin{array}{cc}
2\eta\Delta\tilde{\Omega}(\tilde{\sigma} \cdot \tilde{p}) - i\hbar\Omega & 0 \\
0 & 2\eta\Delta\tilde{\Omega}(\tilde{\sigma} \cdot \tilde{p}) + i\hbar\Omega
\end{array}\right).$$  (3)

where each entry represents a $2 \times 2$ matrix. The associated Schrödinger equation, $i\hbar\partial\psi/\partial t = H_{D}|\psi\rangle$, forms the same dynamics as the Dirac equation in 3+1 dimensions for a free spin-1/2 particle, where $|\Psi\rangle$ represents the four-component Dirac bispinor. This is easily seen if we express the Dirac equation

$$i\hbar\frac{\partial \psi}{\partial t} = H_{D}\psi = (\sigma \cdot \tilde{p} + \beta mc^{2})\psi$$  (4)

in its “supersymmetric” representation [1]

$$H_{D} = \left(\begin{array}{cc}
0 & c(\tilde{\sigma} \cdot \tilde{p}) - i\hbar mc^{2} \\
c(\tilde{\sigma} \cdot \tilde{p}) + i\hbar mc^{2} & 0
\end{array}\right).$$  (5)

Here, the $4 \times 4$ matrix $\tilde{\sigma} := (\sigma_{x}, \sigma_{y}, \sigma_{z})$ is off-diag$(\tilde{\sigma}, \tilde{\sigma})$ is the velocity operator, $\beta :=$ off-diag$(-i\mathbb{1}_{2}, i\mathbb{1}_{2})$, and

$$c := 2\eta\Delta\tilde{\Omega}, \ hmc^{2} := \hbar\Omega,$$  (6)

are the speed of light and the electron rest energy, respectively. The notorious analogy between Eqs. (4) and (5) shows that the quantum relativistic evolution of a spin-1/2 particle can be fully reproduced in a tabletop ion-trap experiment, allowing the study of otherwise unaccessible physical regimes and effects, as shown below.

In the Dirac formalism, the spin-1/2 degree of freedom is incorporated ab initio. Moreover, the Dirac bispinor in Eq. (1) is built by components associated with positive and negative energies, $E_{\pm} = \pm\sqrt{\mathbf{p}^{2}c^{2} + m^{2}c^{4}}$. This description is the source of diverse controversial predictions, as the Zitterbewegung and the Klein’s paradox.

The Zitterbewegung is a known quantum-relativistic effect consisting of a helicoidal motion of a free Dirac particle, a natural consequence of the non-commutativity of its velocity operator components, $c_{\alpha i}$, with $i = x, y, z$. It can be proved straightforwardly [1] that the time evolution of the position operator $\tilde{\mathbf{r}} = (x, y, z)$ in the Heisenberg picture, following $d\tilde{\mathbf{r}}/dt = [\tilde{\mathbf{r}}, H_{D}]/\hbar$, reads

$$\tilde{\mathbf{r}}(t) = \tilde{\mathbf{r}}(0) + \frac{4\eta^{2}\Delta^{2}\tilde{\Omega}^{2}\mathbf{p}}{H_{D}}t$$

$$+ \left(\alpha - \frac{2\eta\Delta\tilde{\Omega}^{2}}{H_{D}}\right)i\hbar\eta\Delta\tilde{\Omega} \left(e^{2i\hbar\tilde{H}_{D}t/\hbar} - 1\right).$$  (7)

Here, the first two terms on the r.h.s. account for the classical kinematics of a free particle, while the last oscillating term is responsible for a transversal “quivering” motion. If we consider a bipartite state with a peaked momentum around $p_{0}$, $|\Psi_{0}\rangle = |a\rangle \otimes \exp(-(p - p_{0})^{2}/2\sigma_{p}^{2})$, the Zitterbewegung frequency associated with the measurable quantity $\langle \tilde{\mathbf{r}}(t) \rangle$ can be estimated as

$$\omega_{ZB} \approx 2|\tilde{E}_{D}|/\hbar \approx 2\sqrt{4\eta^{2}\Delta^{2}\tilde{\Omega}^{2}p_{0}^{2}/\hbar^{2} + \Omega^{2}}$$

$$\approx 2\sqrt{N\eta^{2}\tilde{\Omega}^{2} + \Omega^{2}},$$  (8)

where $\tilde{E}_{D} \equiv \langle H_{D} \rangle$ and $N \equiv \langle a^\dagger a \rangle$ are the average energy and phonon number, respectively. Similarly, we can estimate from Eq. (7) the Zitterbewegung amplitude associated with $\langle \tilde{\mathbf{r}}(t) \rangle$ as

$$R_{ZB} = \frac{\hbar}{2mc} \left(\frac{m^{2}c^{2}}{E}\right)^{2} = \frac{\eta^{2}\Delta\tilde{\Omega}^{2}}{4\eta^{2}\tilde{\Omega}^{2}D^{2}p_{0}^{2} + \hbar^{2}\Omega^{2}},$$  (9)

and $R_{ZB} \approx \Delta$, if $\eta\Omega \sim \Omega$.

The standard explanation of this erratic motion for a free Dirac particle invokes the interference between the positive- and negative-energy components of the Dirac bispinor following the dynamics in Eqs. (3) and (5). The predicted values for a real electron, $\omega_{ZB} \sim 10^{28}$Hz and $R_{ZB} \sim 10^{-30}A$, are out of experimental reach, the effect has never been observed, and its existence is even questioned by quantum field theory considerations. To simulate quantum-relativistic effects in other physical systems, like trapped ions or graphene, is not aimed at proving their existence, but at exploiting the differences and
analogies in each field. Given the flexibility of trapped-ion systems, we will have access to a wide range of tunable experimental parameters \[3\], allowing for realistic and measurable \( \omega_{ZB} \approx 0 - 10^9 \text{Hz} \) and \( R_{ZB} \approx 0 - 10^4 \text{A} \), depending on the initial vibronic states. Due to our piecewise build-up of the 3+1 Dirac Hamiltonian of Eq. (2), we can strongly reduce the experimental demands to study Dirac equations in 1+1 and 2+1 dimensions \[1, 12\].

In those cases, the Clifford algebra that characterizes the Dirac matrices is satisfied by the anticommuting Pauli matrices, \( \{\sigma,\sigma_j\} = 2\delta_{ij} \), where \( \{A, B\} := AB + BA \), given that we only need 2(3) anticommuting matrices in the 1+1(2+1) case. Accordingly, the four components of the Dirac bispinor are conveniently reduced to only two.

We focus now on the 1+1 dimensional case, which could be reached by current experiments, keeping most striking results available. After a unitary transformation around the \( x \)-axis, transforming \( \sigma_y \) into \( \sigma_z \), the 1+1 Dirac equation stemming from Eq. (2) can be cast into

\[
i\hbar \partial_t |\Psi(1)\rangle = \mathcal{H}_D^{(1)} |\Psi(1)\rangle \quad \text{with} \quad \mathcal{H}_D^{(1)} = \frac{i\hbar\Delta \tilde{\Omega} \sigma_z}{\hbar} + h\Omega \sigma_z,
\]

where the Dirac “spinor” \( |\Psi(1)\rangle = \Psi_a^{(1)} |a\rangle + \Psi_b^{(1)} |b\rangle \). Note that these two components are not associated with the spin-1/2 degree of freedom but are linear combinations of positive- and negative-energy solutions \[13\]. Our setup is now reduced to a simultaneous \( JC + AJC \) interaction, \( \sigma_x p_z \), and a Stark-shift term \( \sigma_z \) acting on two internal levels. In Eq. (10), the use of \( \sigma_z \) is for the sake of pedagogy, and returning to \( \sigma_y \) will not affect the results.

In the nonrelativistic limit, \( mc^2 \gg p_z c \), or equivalently \( \Omega \gg \hbar \Omega \), we may identify the dispersive limit in Eq. (10), and derive the squeezing-second-order Hamiltonian

\[
\mathcal{H}_{eff}^{(1)} = \frac{2\eta^2 \Delta \tilde{\Omega}}{\hbar \Omega} \sigma_x p_z^2 \equiv \sigma_z \frac{p_z^2}{2m},
\]

yielding the expected Schrödinger Hamiltonian associated with the classical kinetic energy of a free particle. In the relativistic limit, \( mc^2 \ll p_z c \), which includes \( m = 0 \), the 1+1 case reduces to \( \mathcal{H}_D^{(1)} = i\hbar \tilde{\Omega} \sigma_x (a_+^\dagger - a_-) \), which produces Schrödinger cats, as commented above \[8, 10\].

For a massless particle, we can show that \( dx/dt = [x, \mathcal{H}_D^{(1)}]/i\hbar = 2\eta \Delta \tilde{\Omega} \sigma_z \) and \( da_x/dt = [\sigma_x, \mathcal{H}_D^{(1)}]/i\hbar = 0 \). In consequence, \( \sigma_z \) is a constant of motion and the time evolution of the position operator,

\[
x(t) = x(0) + 2\eta \Delta \tilde{\Omega} \sigma_z t,
\]

is classical and does not involve Zitterbewegung. On the other hand, for a massive particle, \( da_x/dt = [\sigma_x, \mathcal{H}_D^{(1)}]/i\hbar = -2\eta \sigma_y \), \( da_y/dt \neq 0 \), and so forth. The produced set of differential equations yields a Zitterbewegung oscillatory solution similar to Eq. (7), with the evident simplification via the replacements of \( H_D \) by \( \mathcal{H}_D^{(1)} \), \( \tilde{p} \) by \( p_x \), and \( \sigma \) by \( \sigma_z \). It is noteworthy to mention that the phenomenon of mass acquisition, which could be done here in a continuous manner by raising the coupling strength \( \Omega \), is related to the spontaneous symmetry breaking mechanism of the Higgs field.

At this stage, it is clear that the measurement of the expectation value of the position operator, \( \langle x(t) \rangle \), as a function of the interaction time \( t \) is of importance. A recent proposal for realizing fast measurements of motional quadratures \[14\] relies on the possibility of measuring the population of an ionic internal level, \( \rho_m \), at short probe-motion interaction times \( \tau \) with high precision \[15\].

Given an initial vibronic state \( \rho(0) = |+\rangle \langle +| \otimes \rho_m \), where \( |\pm\rangle = (|a\rangle \pm e^{i\phi}|b\rangle)/\sqrt{2} \) and \( \rho_m \) describes an unknown motional density operator, we can make use of

\[
\langle Y_\phi \rangle = \frac{d}{d\tau} P_{e^\phi}(\tau) \bigg|_{\tau=0},
\]

where the generalized quadrature \( Y_\phi = (ae^{-i\phi} - a^\dagger e^{i\phi})/2i \). Then, position and momentum operators are measured when choosing \( \phi = -\pi/2 \) and \( \phi = 0 \), respectively. To apply this technique, it is required a particular initial state of the internal states, so the measurement of \( \langle x(t) \rangle \) would have to be done in two parts, one associated with each of the suitably projected states, \( |+\rangle \) and \( |-\rangle \).

We turn now to the possible simulation of Klein’s paradox. In 1929, Klein noticed \[16\] the anomalous behavior of Dirac particles in regions where a high potential energy \( V \) exists: \( H_V^{(1)} = H_D^{(1)} + V \mathbb{1}_2 \). When \( V > 2mc^2 \), negative-energy electrons (components) may swallow \( V \), acquiring positive energy and behaving as ordinary electrons, while leaving a hole in the Dirac sea. This stems from the fact that the relativistic energy related to \( H_V^{(1)} \) may be recast into \( (pc)^2 = (E_V^{(1)} - V - mc^2)(E_V^{(1)} - V - mc^2) \), which is positive when either both factors are positive or negative. In the second case, the total energy \( E_V^{(1)} < -mc^2 + V \) can be larger than \( mc^2 \), as noticed by Klein. In this case an \( e^- - e^+ \) (electron-positron) pair could be created from \( V \). The sudden raise of the constant potential \( V(|a\rangle \langle a| + |b\rangle \langle b|) \), at a certain time \( t = 0 \) after an evolution associated with \( H_D^{(1)} \), could simulate this phenomenon. We suggest to produce potential \( V \) with the required characteristics through a fast and homogeneous Stark shift in both internal levels. The natural way to detect Klein’s paradox, assuming an initial positive-energy internal state \( |a\rangle \) (\( \rho_m = 0 \)), is via measurement of nonzero population in the negative-energy component \( |b\rangle \).

Finally, in as much as massless chiral fermions in condensed matter, we could also produce a 1+1 axial anomaly \[17\] by changing Eq. (10) into \( H_D^{(1)} = c\sigma_z p_x + qE x \), where \( x \propto (a + a^\dagger) \) is a motional displacement.

The basic ingredients to implement the 1D Dirac dynamics of Eq. (10) with a single trapped ion are two independent electronic (internal) states coupled to a one-dimensional motional degree of freedom. The required
states could be composed by two ground-state hyperfine levels of an earth alkaline atomic ion, e.g. of $^{25}$Mg$^+$ by $|F = 3; m_f = -3\rangle$ and $|F = 2; m_f = -2\rangle$, $|a\rangle$ and $|b\rangle$, respectively, as depicted in Fig. 1. A constant external magnetic field will define the quantization axis and lift the degeneracy of levels being potentially useful to provide additional states (like $|c\rangle$ and $|d\rangle$ in Fig. 1) necessary for higher dimensional simulations, see Eq. [2].

At the start, the ions will be laser cooled close to the motional ground state and optically pumped into state $|a\rangle$. One red/blue sideband and one carrier transition will be driven simultaneously [11, 21] to implement the desired dynamics of Eq. (5) via two-photon stimulated Raman transitions between states $|a, n = 1\rangle$ and $|b, n = 0, 1, 2\rangle$: red sideband (dotted line), carrier (solid line), and blue sideband (dashed line).

In conclusion, we have shown how to simulate the Dirac equation in 3+1 dimensions for a free spin-1/2 particle, and quantum-relativistic effects like the Zitterbewegung and Klein’s paradox, in a single trapped ion. We have studied the 1+1 case, where experimental needs are minimal while keeping most striking predictions. We believe that these simulations open attractive avenues and a fruitful dialog between different scientific communities.

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