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Is there a classical spin contribution to the tunnel effect?

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Abstract

The crossing of a potential barrier by a classical nonrelativistic spinning particle is analyzed. Numerical simulations show that, because of the spin structure related to the zitterbewegung, crossing is possible for kinetic energies below the top of the potential barrier. Experiments to check the spin dependence of this effect and a modification of the Schrödinger–Pauli equation to include an electric dipole term, are suggested. © 1998 Published by Elsevier Science B.V.

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1. Introduction

Let us consider the following simple experiment. We accelerate from rest a particle of mass m and electric charge e with an acceleration potential V_a . This particle is sent into some electrostatic potential barrier of top $V_0 \geq V_a$. From the quantum mechanical point of view there is a nonvanishing probability of crossing this barrier. In non-relativistic quantum mechanics the wave function of the particle satisfies either Schrödinger's equation in the spinless case, or the Schrödinger–Pauli equation if $s = 1/2$ or a higher spin equation, depending of the value of its spin. But, because there is no magnetic field in the experiment there are no spin-magnetic terms in the above equations and therefore each component of the wave function satisfies the same spinless Schrödinger equation. This means that the probability of crossing of this experiment is spin independent.

From the classical point of view if the particle is spinless, it simply never crosses the barrier. But it does under some conditions if the particle has a classical spin structure related to the zitterbewegung, as we shall show below.

To produce the corresponding classical analysis we need first a classical model of a spinning particle. In Refs. [1,2] a classical elementary particle is defined as a Lagrangian system whose *kinematical space* is a *homogeneous space* of the kinematical group G . The kinematical space is the manifold spanned by the initial (or final) variables that are held fixed as end points of the corresponding variational principle.

To describe a spinning particle we have to consider larger kinematical spaces than the four-dimensional space-time manifold that describes point particles. The largest homogeneous space of a kinematical group is the group itself. For the Galilei and Poincaré groups, the largest homogeneous space is a ten-dimensional manifold whose variables have the same dimensions as the corresponding group parameters. With this manifold we describe a spinning particle in terms of ten

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kinematical variables $(t, \mathbf{r}, \mathbf{u}, \alpha)$, that are identified with the time, position, velocity and orientation of the particle. Since the Lagrangian depends also on the derivatives of these variables, it will depend on the acceleration and angular velocity. It is because the dependence of the Lagrangian on the angular velocity and acceleration that the particle has a spin structure.

One of the salient features of a general spinning particle, when the Lagrangian depends on the acceleration, is the existence of the zitterbewegung. The center of charge moves around the center of mass with an isotropic harmonic motion, and because of this motion a classical charged spinning particle has a dipole structure and can cross a potential barrier as will be shown in next section.

In the relativistic case, a possible description is shown in [2,3] of the electron in such a way that the center of charge of the electron moves at the speed of light in a circle of radius $R = \hbar/2mc$, contained in a plane orthogonal to the spin. Thus, the frequency of this internal motion is $\omega = 2mc^2/\hbar$. They are the ones suggested by Dirac in the analysis for the electron (see Ref. [4], p. 263. The same values for these parameters R and ω will also be used in the nonrelativistic example.

2. Classical crossing of a potential barrier

To illustrate the spin structure and dynamics we will consider in the following a non-relativistic model that shares most of the features of the relativistic electron described in [3], but has a simpler mathematical structure.

Let us consider a particle whose kinematical space is $X = \mathcal{G}/SO(3)$, so that the kinematical variables are $x \equiv (t, \mathbf{r}, \mathbf{u})$, with $\mathbf{u} = d\mathbf{r}/dt$, and are interpreted as the time, position and velocity of the particle respectively. Translation invariance implies that the Lagrangian must be independent of t and \mathbf{r} , and since it must depend on the next order derivatives of the kinematical variables it should finally be a function of $\mathbf{u} = d\mathbf{r}/dt$ and $\dot{\mathbf{u}} = d^2\mathbf{r}/dt^2$. Rotation invariance leads to the conclusion that L must be a function of \mathbf{u}^2 , $\dot{\mathbf{u}}^2$ and $\mathbf{u} \cdot \dot{\mathbf{u}}$, but because this last term is a total time derivative it may be omitted. We therefore assume that our elementary system is described by the following free Lagrangian,

$$L = \frac{m}{2} \left(\frac{d\mathbf{r}}{dt} \right)^2 - \frac{m}{2\omega^2} \left(\frac{d^2\mathbf{r}}{dt^2} \right)^2, \quad (1)$$

where m is the mass and the parameter ω , represents the zitterbewegung frequency. In the case of internal circular motion with constant velocity v and radius R , it is related to the spin by $\omega = mv^2/S$, and in the case of the electron [3] it is $mc^2/S = 2mc^2/\hbar$. If $S = 0$ or $\omega \rightarrow \infty$, the last term in (1) cancels out and we recover the spinless point particle Lagrangian.

Vector \mathbf{r} represents the charge position, as can be seen by considering the interaction of the system with an external electromagnetic field. The interaction Lagrangian is

$$L_I = -eV(t, \mathbf{r}) + e\mathbf{A}(t, \mathbf{r}) \cdot \mathbf{u}. \quad (2)$$

From the total Lagrangian $L + L_I$ we get the dynamical equations

$$\frac{1}{\omega^2} \frac{d^4\mathbf{r}}{dt^4} + \frac{d^2\mathbf{r}}{dt^2} = \frac{e}{m} [\mathbf{E}(t, \mathbf{r}) + \mathbf{u} \times \mathbf{B}(t, \mathbf{r})], \quad (3)$$

where the electric \mathbf{E} and magnetic field \mathbf{B} , are constructed from the potentials in the usual way. The center of mass and spin are defined in Refs. [2,3] as

$$\mathbf{q} = \mathbf{r} + \frac{1}{\omega^2} \frac{d^2\mathbf{r}}{dt^2}, \quad \mathbf{S} = \frac{m}{\omega^2} \frac{d^2\mathbf{r}}{dt^2} \times \frac{d(\mathbf{r} - \mathbf{q})}{dt}, \quad (4)$$

where it is shown that the dependence on the acceleration gives rise to the spin and to the separation between \mathbf{r} and \mathbf{q} . The dynamical equations can thus be separated into the following equations,

$$m \frac{d^2\mathbf{q}}{dt^2} = e [\mathbf{E}(t, \mathbf{r}) + \mathbf{u} \times \mathbf{B}(t, \mathbf{r})], \quad (5)$$

$$\frac{d^2\mathbf{r}}{dt^2} + \omega^2(\mathbf{r} - \mathbf{q}) = 0, \quad (6)$$

where the center of mass \mathbf{q} satisfies Newton's equation under the action of the total external Lorentz force, while point \mathbf{r} evolves in an isotropic harmonic motion of angular frequency ω around the center of mass \mathbf{q} . This zitterbewegung is independent of the external interaction and according to (4) this motion is orthogonal to the spin. The external force and fields are evaluated at \mathbf{r} and it is the velocity of point \mathbf{r} that enters into the expression of the Lorentz force. As a consequence, the vector \mathbf{r} clearly represents the charge position.

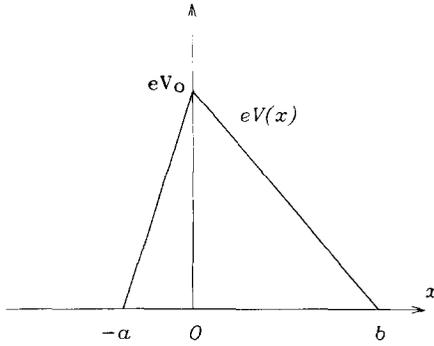


Fig. 1. Potential barrier to be crossed by spinning particles.

We now turn to the analysis of the barrier crossing by particles governed by the dynamical equations (5) and (6). Discontinuous potential barriers produce infinite forces that cannot be handled numerically. We consider instead, continuous potentials of the form depicted in Fig. 1, for which the quantum solution is known. V_0 represents the top of the potential.

In a static electric field, the total energy $H = P^2/2m + eV(\mathbf{r}) - H_0$, is conserved. Here

$$H_0 = \frac{m\omega^2}{2}(\mathbf{r} - \mathbf{q})^2 + \frac{m}{2} \left(\frac{d(\mathbf{r} - \mathbf{q})}{dt} \right)^2 \quad (7)$$

is the internal energy of the isotropic harmonic motion. For a spinless particle $\mathbf{q} = \mathbf{r}$ and this internal energy vanishes: $H_0 = 0$. A spinless particle with mechanical linear momentum \mathbf{P} , can never cross the barrier if $P^2/2m < eV_0$, but in the case of a spinning particle of the same mass and charge, the internal energy H_0 can compensate the extra potential energy in such a manner that the crossing becomes possible.

Let us assume for simplicity that the spin is pointing up or down in the z direction and the charge motion takes place in the XOY plane. Let q_x, q_y and $q_z = 0$, be the coordinates of the center of mass and x, y and $z = 0$, the position of the charge. To perform the numerical analysis we shall define the following dimensionless variables,

$$\hat{q}_x = q_x/R, \quad \hat{q}_y = q_y/R, \quad \hat{x} = x/R, \\ \hat{y} = y/R, \quad \hat{a} = a/R, \quad \hat{b} = b/R,$$

where we take for the average separation between the center of mass and center of charge the value $R = \hbar/2mc$, and for m the electron mass. The dimension-

less time $\alpha = \omega t$ is just the phase of the internal motion, where we take for $\omega = 2mc^2/\hbar$. The dynamical equations (5) and (6) become

$$\frac{d^2 \hat{q}_x}{d\alpha^2} = A(\hat{x}), \quad \frac{d^2 \hat{q}_y}{d\alpha^2} = 0, \\ \frac{d^2 \hat{x}}{d\alpha^2} + \hat{x} - \hat{q}_x = 0, \quad \frac{d^2 \hat{y}}{d\alpha^2} + \hat{y} - \hat{q}_y = 0,$$

where $A(\hat{x})$ is given by

$$A(\hat{x}) = -eV_0/\hat{a}m\omega^2 R^2, \quad \text{for } \hat{x} \in (-\hat{a}, 0), \\ = eV_0/\hat{b}m\omega^2 R^2, \quad \text{for } \hat{x} \in (0, \hat{b}), \\ = 0, \quad \text{otherwise.}$$

For $V_0 = 1$ V, the dimensionless parameter $eV_0/m\omega^2 R^2 = 1.9569 \times 10^{-6}$. If we choose as initial conditions for the center of mass $\hat{q}_y(0) = 0$ and $d\hat{q}_y(0)/d\alpha = 0$, then the center of mass is moving along the OX axis, and the problem reduces to the analysis of the evolution of \hat{q}_x and \hat{x} . We will suppress the carets from now on. The dynamical equations to be solved numerically are then

$$\frac{d^2 q}{d\alpha^2} = A(x), \quad \frac{d^2 x}{d\alpha^2} + x - q = 0. \quad (8)$$

Numerical integration is performed by means of the computer package *ODE Workbench* [5]. All codes have adaptive step size control and we check that smaller tolerances do not change the results.

Crossing is appreciable if one of the sides of the barrier is of the order of R . With $a = b = 1$, $V_0 = 10^2$ V and for the initial kinetic energy $K = m\dot{q}(0)^2/2eV_0 = 0.41$, below the top of the potential, we obtain the numerical result depicted in Fig. 2 where the variation of the kinetic energy of the particle $K(q)$ is shown against the center of mass position during the crossing.

The particle always crosses the barrier for kinetic energies above this value. In Fig. 3 we show the results for $a = 1$ and $b = 10$, $K = 0.91$ and a potential of $V_0 = 10^3$ V. If the initial kinetic energy is below 0.4 and 0.9 in the previous two cases, respectively, the particle never crosses the barrier. It must be remarked that because of (5), the kinetic energy starts decreasing when the charge \mathbf{r} penetrates into the potential, even before the center of mass \mathbf{q} reaches that region. This produces a variation of the kinetic energy when the center of mass is in the interval $(-a - R, b + R)$. The

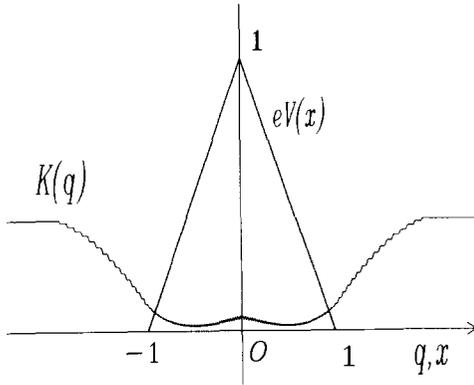


Fig. 2. Evolution of the kinetic energy during the crossing of the barrier with $a = b = 1$, initial energy $K = 0.41$ and extraction potential $V_0 = 100$ V.

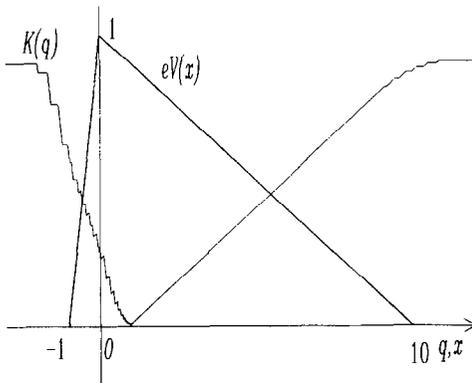


Fig. 3. Evolution of the kinetic energy during the crossing of the barrier with $a = 1, b = 10$, initial energy $K = 0.91$ and extraction potential $V_0 = 1000$ V.

ladder aspect of the variation of the kinetic energy is produced when the charge leaves the field region and therefore the center of mass has a uniform motion.

If in both examples the parameter a is varied from 1 to 0.05, making the left slope higher, there is no appreciable change in the crossing energy. In consequence, we compute the minimum crossing energy for different b values, $K_c(b)$, keeping $a = 1$. This function $K_c(b)$, which will be used in the next section, is independent of the value of the potential V_0 because the problem is dimensionless.

3. Quantum tunnel effect

In the quantization of generalized Lagrangians [3] the wave function for this system is a squared-integrable function $\psi(t, \mathbf{r}, \mathbf{u})$, of the seven kinematical variables and the generators of the Galilei group when acting on this function have the form [3]

$$H = i\hbar \frac{\partial}{\partial t}, \quad \mathbf{P} = -i\hbar \nabla, \\ \mathbf{K} = m\mathbf{r} - t\mathbf{P} + i\hbar \nabla_u, \quad \mathbf{J} = \mathbf{r} \times \mathbf{P} + \mathbf{S}, \quad (9)$$

where ∇_u is the gradient operator with respect to the \mathbf{u} variables. These generators satisfy the commutation relations of the extended Galilei group [6], and the spin is given by $\mathbf{S} = -i\hbar \mathbf{u} \times \nabla_u$.

One Casimir operator of this extended Galilei group, is the Galilei invariant internal energy of the system, which in the presence of an external electromagnetic field and with the minimal coupling prescription is written as

$$\mathcal{E} = H - eV - \frac{1}{2m} (\mathbf{P} - e\mathbf{A})^2, \quad (10)$$

where V and \mathbf{A} are the external scalar and vector potentials, respectively.

In our system $\mathbf{A} = 0$, and V is only a function of the x variable. It turns out that because of the structure of the above operators we can find simultaneous eigenfunctions of the following observables: the Casimir operator (10), H, P_y, P_z, S^2 and S_z . The particle moves along the OX axis, with the spin pointing in the OZ direction, and we look for solutions which are eigenfunctions of the above operators in the form

$$\left(H - eV(x) - \frac{1}{2m} \mathbf{P}^2 \right) \psi = \mathcal{E} \psi, \\ H\psi = E\psi, \quad P_y\psi = 0, \quad P_z\psi = 0, \quad (11)$$

$$S^2\psi = s(s+1)\hbar^2\psi, \quad S_z\psi = \pm s\hbar\psi, \quad (12)$$

so that ψ is independent of y and z , and its time dependence is of the form $\exp(-iEt/\hbar)$. Since the spin operators have derivatives only with respect to the velocity variables, we can look for solutions with the variables separated in the form

$$\psi(t, x, \mathbf{u}) = e^{-iEt/\hbar} \phi(x) \chi(\mathbf{u}),$$

and thus

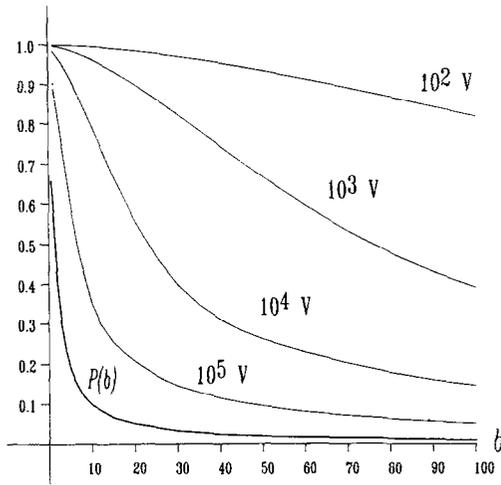


Fig. 4. Classical probability of crossing $P(b)$ and quantum tunneling for four different potentials V_0 .

$$\left(\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + E - eV(x) - \mathcal{E} \right) \phi(x) = 0, \quad (13)$$

$$S^2 \chi(\mathbf{u}) = s(s+1) \hbar^2 \chi(\mathbf{u}),$$

$$S_z \chi(\mathbf{u}) = \pm s \hbar \chi(\mathbf{u}), \quad (14)$$

where the spatial part $\phi(x)$ is uncoupled with the spin part $\chi(\mathbf{u})$, and $E - eV(x) - \mathcal{E}$ represents the kinetic energy of the system. The spatial part satisfies the one-dimensional Schrödinger equation, and the spin part is independent of the interaction, so that the probability of quantum tunneling is contained in the spatial part and does not depend of the particular value of the spin. If the particle is initially on the left hand side of the barrier, with an initial kinetic energy $E_0 = E - \mathcal{E}$, then we can determine the quantum probability for crossing for $a = 1$ and different values of the width b . For energies below the top of the barrier eV_0 we show in Fig. 4 the average probability for quantum tunneling for four different potentials: $V_0 = 10^2, 10^3, 10^4$ and 10^5 V. This average probability has been computed by assuming that on the left hand side of the barrier there is a uniform distribution of particles of energies below eV_0 .

If we consider for the classical spinning particle the same uniform distribution of particles, then the function $P(b) = 1 - K_c(b)$, where $K_c(b)$ is the dimensionless minimum kinetic energy for crossing computed before, represents the ratio of the particles that with kinetic energy below the top of the potential cross

the barrier because of the spin contribution. This function $P(b)$ is also depicted in Fig. 4. We see that for the different potentials shown in that figure the classical average probability of crossing is smaller than the quantum one, but for stronger potentials this classical probability, coming from the spin contribution, becomes relatively important.

4. Discussion

From (13) and (14) it is clear that the quantum probability of tunneling is independent of the spin. However, from the classical point of view there is a nonvanishing crossing which is related to the spin structure.

To test experimentally if there is a spin contribution, it will be necessary to perform separate experiments with spinning and spinless particles of the same mass and charge. Thus, the difference in the outcome will be related to the spin contribution. No elementary particles of the same mass and charge and different spins are known. A possibility is to use electrons polarized perpendicular or along the direction of motion. Those polarized in the direction of motion will have the zitterbewegung, according to the classical model, in a plane orthogonal to the linear momentum with no influence in the crossing, and therefore the probability will be smaller than in the other case. Is this a possible interpretation of the quoted spin-polarized tunneling in magnetoresistive materials [7]? The colossal magnetoresistance of polycrystalline thin films at certain temperature is decreased when there is applied a magnetic field in the direction of the thin layers, and therefore the conduction electrons are polarized in that direction. This effect is interpreted by the increase of the mobility of electrons that cross adjacent layers by spin-polarized tunneling.

Another experiment that can be performed is to use ions of the type A^{++} that could be in a singlet or triplet state either. In this kind of experiment it can be argued that ions are not elementary objects and the dipole structure of the atom might therefore contribute with another energy term, not included in the previous quantum analysis. If this is the case and there is some difference in the outcome it will be related to the different dipole structure for the different atomic spin states.

Then, what is the quantum analog of this additional contribution to tunneling? When considered from the classical point of view, and for the center of mass observer, the spin structure of our model suggests that the elementary particle can be interpreted as a point charge at the center of mass plus a magnetic moment $\boldsymbol{\mu}$ in the spin direction produced by the charge motion, but also an oscillating electric dipole $\boldsymbol{d} = e(\boldsymbol{r} - \boldsymbol{q})$, orthogonal to the spin. This produces two additional energy terms $-\boldsymbol{\mu} \cdot \boldsymbol{B} - \boldsymbol{d} \cdot \boldsymbol{E}$, that were already found by Dirac (see Ref. [4], p. 267) in his analysis of the electron structure, but only the magnetic moment term survived in the non-relativistic approach to give rise the magnetic term of the Schrödinger–Pauli equation. It is clear that the oscillating electric dipole has a vanishing time-average value and probably in low energy processes it can be neglected. But in high intensity fields and high energy processes, or in condensed matter physics where there are sharp variations of the fields in short distances of the order R , it has to be taken into account. In the case of atoms the addition of an electric dipole term leads to the usual interpretation of the Stark effect, and in the case of elementary particles, we need it because of the electric dipole structure associated to the spin.

Therefore, to be consistent with the above analysis, the Schrödinger–Pauli equation should be modified to include an additional electric dipole term. A term of the form $-eER \cos \omega t$, where E is the external electric field, should be considered to solve the corresponding quantum wave function. This term is of the order of magnitude of the separation R between the center of mass and center of charge, which is responsible for

the classical crossing. This makes the quantum problem time dependent and its analysis more difficult and whether or not it is equivalent to the classical contribution, is left to a subsequent paper.

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