Spin-dependent confinement limit of Dirac particles in three dimensions

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(Received 27 December 2013; published 18 September 2015)

Unanyan, Otterbach, and Fleischhauer [Phys. Rev. A **79**, 044101 (2009)] found that the confinement limit of a one-dimensional Dirac particle can be derived from the Dirac equation. The generalization of this problem to three dimensions is discussed in this paper. It shows that the three-dimensional Dirac particle in vector and scalar potentials has a confinement limit proportional to the modulus of expectation value of spin. This result obtained in Dirac equation is applicable for any Dirac particle confined in a finite region of space, even when vector and scalar potentials of quite general character are present. In addition, a Dirac particle confined in Lorentz scalar potential is discussed.

DOI: 10.1103/PhysRevA.92.032120 PACS number(s): 03.65.Pm

I. INTRODUCTION

Quantum uncertainty is one of the most extensively studied notions in quantum physics. Interest in coordinate uncertainty has been stimulated recently in the context of the analysis of one-dimensional Dirac particles, partly because it has a possible application in various systems which exhibit Dirac-type behavior, but chiefly because it reminds us that the Hamiltonian formalism of a Dirac particle may contain the information about its coordinate uncertainty. Unanyan, Otterbach, and Fleischhauer [1] found that the confinement limit of a one-dimensional Dirac particle in a symmetric scalar potential is half its corresponding Compton length and can be derived from the Dirac equation. Based on a detailed analysis of point interaction and finite-ranged potentials, Toyama and Nogami [2] conjectured that a more stringent confinement limit holds for any symmetric potential. It was shown that [3,4] the confinement limit conjectured by Toyama and Nogami can be derived from the Dirac equation. This result does not depend on the Heisenberg uncertainty relation and the explicit form of the potentials. In two and three dimensions the confinement situation with a central square well potential has been investigated in Ref. [5]. There it was found that we can make coordinate uncertainty of bound states as small as we like by choosing the potential well with a very small range and a very high walls.

However, the calculation results of the coordinate uncertainty in Ref. [5] does not mean that Dirac particles in three dimensions can be confined to an arbitrarily small spatial region by a scalar potential. It is a well-known fact [6] that in the presence of a very strong potential the vacuum of quantum electrodynamics becomes unstable due to the spontaneous creation of particle-antiparticle pairs which cannot be confined to a region of a radius much smaller than Compton wavelength. In the models of hadrons, in order to get a confining solution of the Dirac equation, we must introduce position-dependent mass term through the so-called Lorentz scalar potential as was done in the MIT bag model [7] of quark confinement.

The behavior of a Dirac particle, like the electron, is distinguished from that of a scalar particle by its spin structure, which can be used for storage and transport of information [8,9]. The applications in spintronics depend strongly on the control and manipulation of the spin degree of freedom. On the other hand, the confinement of Dirac particles is crucial for the realization of nanoelectronic devices [10]. In this paper we derive a confinement limit from the Dirac equation in three dimensions. We find that the confinement limit of a three-dimensional Dirac particle has a direct relation to its spin angular momentum.

II. PROOF

For a Dirac particle with rest mass M moving in three dimensions in the presence of a vector potential $\boldsymbol{A}$ and a scalar potential U, the time-independent Dirac equation is given as

$$[c\boldsymbol{\alpha}\cdot(\hat{\boldsymbol{p}}+q\boldsymbol{A})+\beta Mc^2+U]\psi=E\psi, \tag{1}$$

where c is the speed of light, E is the relativistic energy of the system, and $\boldsymbol{\alpha}$ and β are the well-known 4×4 Dirac matrices expressed in terms of the three 2×2 Pauli spin matrices $\boldsymbol{\sigma}$ and the 2×2 unit matrix I,

$$\alpha_i=\begin{pmatrix}0 & \sigma_i\\ \sigma_i & 0\end{pmatrix},\quad \beta=\begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix}, \tag{2}$$

where $i=x,y,z$, and the Dirac matrices satisfies the anticommutation algebra $\alpha_i\alpha_j+\alpha_j\alpha_i=2\delta_{ij}\mathbb{I}$, $\alpha_i\beta+\beta\alpha_i=0$, and $\alpha_i^2=\beta^2=\mathbb{I}$.

In Eq. (1) the Dirac particle is described by the Dirac four-component spinor wave function

$$\psi=\begin{pmatrix}\varphi_1\\ \varphi_2\\ \chi_1\\ \chi_2\end{pmatrix}=\begin{pmatrix}\varphi\\ \chi\end{pmatrix}. \tag{3}$$

By multiplying Eq. (1) on the left by matrix $\left(\begin{smallmatrix}0 & I\\ I & 0\end{smallmatrix}\right)$, we have

$$c\boldsymbol{\Sigma}\cdot(-i\hbar\nabla+q\boldsymbol{A})\psi=\begin{pmatrix}0 & I\\ I & 0\end{pmatrix}(E-U-\beta Mc^2)\psi, \tag{4}$$

where

$$\Sigma_i=\begin{pmatrix}\sigma_i & 0\\ 0 & \sigma_i\end{pmatrix} \tag{5}$$

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are the four-dimensional Pauli spin matrices. We take the Hermitian conjugates of Eq. (4) to obtain

$$c\psi^{\dagger}(i\hbar\overleftarrow{\nabla}+q\boldsymbol{A})\cdot\boldsymbol{\Sigma}=\psi^{\dagger}(E-U-\beta Mc^2)\begin{pmatrix}0 & I\\ I & 0\end{pmatrix}, \quad (6)$$

where $\overleftarrow{\nabla}$ differentiates the wave function to the left. By multiplying Eqs. (4) and (6) with $\psi^{\dagger}$ and ψ, respectively, we can obtain

$$\frac{\lambda_C\nabla\cdot(\psi^{\dagger}\boldsymbol{\Sigma}\psi)}{2}=i(\bar{\varphi}_1\chi_1-\varphi_1\bar{\chi}_1+\bar{\varphi}_2\chi_2-\varphi_2\bar{\chi}_2), \quad (7)$$

where Compton length $\lambda_C=\hbar/(Mc)$, $\bar{\varphi}$, and $\bar{\chi}$ are the complex conjugates of φ and χ, respectively.

If Z_1, Z_2 are any two complex numbers, then

$$|Z_1|^2+|Z_2|^2\geqslant|i(\bar{Z}_1Z_2-\bar{Z}_2Z_1)|. \quad (8)$$

Using this inequality and Eq. (7) we obtain

$$\rho\geqslant\frac{\lambda_C}{2}\left|\frac{\partial(\psi^{\dagger}\Sigma_x\psi)}{\partial x}+\frac{\partial(\psi^{\dagger}\Sigma_y\psi)}{\partial y}+\frac{\partial(\psi^{\dagger}\Sigma_z\psi)}{\partial z}\right|, \quad (9)$$

where ρ is the normalized density distribution corresponding to the wave function ψ : $\rho=|\varphi|^2+|\chi|^2$. Using the integral inequality $\int_a^b dx|f(x)|\geqslant|\int_a^b dxf(x)|$ and expressing the expectation value of $|x|$ in the form $\langle|x|\rangle$, we find

$$\langle|x|\rangle=\int_V dV|x|\rho\geqslant\frac{\lambda_C}{2}\left|\int_V dVx\left[\frac{\partial(\psi^{\dagger}\Sigma_x\psi)}{\partial x}+\frac{\partial(\psi^{\dagger}\Sigma_y\psi)}{\partial y}+\frac{\partial(\psi^{\dagger}\Sigma_z\psi)}{\partial z}\right]\right|. \quad (10)$$

Here the symbol $\int_V dV$ denotes an integration over the whole space: $\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dy\int_{-\infty}^{+\infty}dz$. The integration by parts over x in the first term in the modulus in Eq. (10) yields

$$\int_V dVx\frac{\partial(\psi^{\dagger}\Sigma_x\psi)}{\partial x}=\int_{-\infty}^{+\infty}dy\int_{-\infty}^{+\infty}dz[x\psi^{\dagger}\Sigma_x\psi]_{-\infty}^{+\infty}-\langle\Sigma_x\rangle, \quad (11)$$

where $\langle\Sigma_x\rangle=\int_V dV\psi^{\dagger}\Sigma_x\psi$ is the expectation value of Σ_x. When the Dirac particle is in an appropriate bound state, the boundary term in the integrand in Eq. (11) vanishes. Similarly, by discarding the boundary term we get

$$\int_V dVx\frac{\partial(\psi^{\dagger}\Sigma_y\psi)}{\partial y}=0,\qquad\int_V dVx\frac{\partial(\psi^{\dagger}\Sigma_z\psi)}{\partial z}=0. \quad (12)$$

Finally, Eq. (10) can be reduced to $\langle|x|\rangle\geqslant\lambda_C|\langle\Sigma_x\rangle|/2$. Our purpose is to obtain a limit of coordinate uncertainty, $\Delta x=\sqrt{\langle x^2\rangle-\langle x\rangle^2}$. Using the Cauchy-Schwarz inequality $\langle x^2\rangle=\langle|x|^2\rangle\geqslant\langle|x|\rangle^2$, it follows that $\sqrt{\langle x^2\rangle}\geqslant\lambda_C|\langle\Sigma_x\rangle|/2$. Similar inequalities also hold in the y and z directions. In the case that the vector potential $\boldsymbol{A}$ and the scalar potential U are all symmetric, the probability density ρ is also symmetric and, thus, we have $\langle x\rangle=\langle y\rangle=\langle z\rangle=0$. In this case, we arrive at the following inequalities for confinement limit:

$$\Delta x\geqslant\frac{|\langle\hat{s}_x\rangle|}{Mc},\quad\Delta y\geqslant\frac{|\langle\hat{s}_y\rangle|}{Mc},\quad\Delta z\geqslant\frac{|\langle\hat{s}_z\rangle|}{Mc}. \quad (13)$$

Here $\hat{s}_i=\hbar\Sigma_i/2$ is spin angular momentum. Equation (13) implies that the confinement limit of a Dirac particle in a direction is proportional to the modulus of expectation value of spin in this direction. The spin angular momentum does not commute with the Hamiltonian and hence it does not provide a good quantum number.

From Eq. (8) the equality $|Z_1|^2+|Z_2|^2=\pm i(\bar{Z}_1Z_2-\bar{Z}_2Z_1)$ only holds if $Z_1=\pm iZ_2$. Similarly, in Eq. (9) the condition of the equality is $\varphi=\pm i\chi$. However, it is by no means the case that the limiting case $\Delta x=|\langle\hat{s}_x\rangle|/Mc$ holds only if $\varphi=\pm i\chi$. In different integral interval, the condition of the limiting case may be $\varphi=i\chi$ or $\varphi=-i\chi$, for example, $\varphi=i\chi$ for $x>0$, $\varphi=-i\chi$ for $x<0$, and so forth. A direct calculation indicates that it would be impossible to satisfy the limiting case if $\varphi=\pm i\chi$. To see this, assuming that $\Delta x=|\langle\hat{s}_x\rangle|/Mc$ holds for $\varphi=i\chi$, we obtain, from Eq. (7),

$$\frac{\lambda_C}{2}\int_V dV\nabla\cdot(\psi^{\dagger}\boldsymbol{\Sigma}\psi)=\int_V dV|\psi|^2=1, \quad (14)$$

which is incorrect, since the left-hand side of Eq. (14) is always equal to zero in a bound state.

III. NONSYMMETRIC POTENTIALS

The main difference between symmetric and nonsymmetric potentials is that, in nonsymmetric potentials, the expectation value of the coordinate is not zero in general. However, the confinement limit does not depend on the position of a Dirac particle being localized. For any finite $\boldsymbol{r}_0$, it is easy to see that

$$\int_V dV\boldsymbol{r}^2\rho(\boldsymbol{r}-\boldsymbol{r}_0)-\left(\int_V dV\boldsymbol{r}\rho(\boldsymbol{r}-\boldsymbol{r}_0)\right)^2=\int_V dV\boldsymbol{r}^2\rho(\boldsymbol{r})-\left(\int_V dV\boldsymbol{r}\rho(\boldsymbol{r})\right)^2. \quad (15)$$

Thus, in nonsymmetric potentials, if the expectation value of the coordinate x is not zero, we can always make a shift in x, the coordinate variable of the physical system, so that the new particle wave function ψ' satisfies

$$\int_V dVx\rho'(\boldsymbol{r})=0, \quad (16)$$

with $\rho'=|\psi'|^2$. Here, the new wave function ψ' is related to the original wave function ψ by a shift along the x axis,

$$\psi'(x,y,z)=\psi(x-x_0,y,z), \quad (17)$$

where

$$x_0=-\int_V dVx\rho(r). \quad (18)$$

x_0 defined in this way can finally give us Eq. (16).

It can be seen that in fact the new wave function ψ' is also the solution of the Dirac equation

$$[c\boldsymbol{\alpha}\cdot(\hat{\boldsymbol{p}}+q\boldsymbol{A}')+\beta Mc^2+U']\psi'=E\psi', \quad (19)$$

where

$$\boldsymbol{A}'(x,y,z) = \boldsymbol{A}(x - x_0,y,z), \quad U'(x,y,z) = U(x - x_0,y,z). \tag{20}$$

By repeating the same analysis for Eq. (13) we can obtain

$$\sqrt{\int_V dV x^2 \rho'} \geqslant \frac{\lambda_C |\langle \Sigma_x' \rangle|}{2}, \tag{21}$$

where

$$\Sigma_x' = \int_V dV \psi'^{\dagger} \Sigma_x \psi' = \Sigma_x. \tag{22}$$

By combining Eqs. (16), (21), and (15) we can finally obtain the same confinement limit $\Delta x \geqslant |\langle \hat{s}_x \rangle|/Mc$ for nonsymmetric vector potential $\boldsymbol{A}$ and nonsymmetric scalar potential U. Similar conclusion is also true of course for y and z directions.

It should be pointed out that the confinement limit obtained here may also have a classical explanation. Møller has shown that [11] (see also Ref. [12] for a discussion of position operators) a classical system with nonvanishing internal angular momentum J must have an extension or size R greater than a minimum value proportional to the internal angular momentum, $R \geqslant J/Mc$, where M is the rest mass of the classical system. Equation (13) is quite similar in form to this result, but with an essential difference in approach on which we elaborate.

IV. LORENTZ SCALAR POTENTIAL

The interest in studying the Dirac equation with Lorentz scalar potential was mainly motivated by the attempt to understand quark confinement. In this section we investigate the confinement limit of a Dirac particle in a central, Lorentz scalar potential $S(r)$. The Dirac equation is given by

$$[c\boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} + \beta(Mc^2 + S(r))]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{23}$$

The solution of the Dirac equation (23) in spherical coordinates can be generally written as

$$\psi(\mathbf{r}) = \begin{pmatrix} i\frac{G(r)}{r} y_j^l\left(\frac{\mathbf{r}}{r}\right) \\ \frac{F(r)}{r}\frac{\sigma\cdot\mathbf{r}}{r} y_j^l\left(\frac{\mathbf{r}}{r}\right) \end{pmatrix}, \tag{24}$$

where G and F are two radial parts, and y_j^l is a normalized function which depends on the spin and angle only. Here j and l are the total and orbital angular momenta.

The Dirac equation (23) can be reduced to a two-component radial equation,

$$\hbar c \frac{d}{dr}\begin{pmatrix} G(r) \\ F(r) \end{pmatrix} = \begin{bmatrix} -\frac{\kappa\hbar c}{r} & Mc^2 + S(r) + E \\ Mc^2 + S(r) - E & \frac{\kappa\hbar c}{r} \end{bmatrix}\begin{pmatrix} G(r) \\ F(r) \end{pmatrix}, \tag{25}$$

where the quantum number κ is related to the total angular momentum j by

$$\kappa = \mp\left(j + \tfrac{1}{2}\right), \tag{26}$$

with $j = l \pm 1/2 = 1/2, 3/2, \ldots$.

We now multiply the upper and lower equations of Eq. (25) by rG and rF, respectively. Then we can obtain the following identity for two radial parts:

$$\frac{r}{2}\frac{d}{dr}(G^2 - F^2) + \kappa(G^2 + F^2) = \frac{2Er}{\hbar c}GF. \tag{27}$$

The normalization of the wave function (24) implies the normalization condition

$$\int_0^\infty (G^2 + F^2)dr = 1. \tag{28}$$

Using integration by parts and discarding two boundary terms we obtain from Eq. (27),

$$\left|\frac{2E}{\hbar c}\int_0^\infty rGF dr\right| \geqslant |\kappa| - \frac{1}{2}\left|\int_0^\infty (F^2 - G^2)dr\right| \geqslant j. \tag{29}$$

Note that two boundary terms

$$rG^2(r)|_0^\infty = rF^2(r)|_0^\infty = 0, \tag{30}$$

since the integral of $r(G^2 + F^2)$ is assumed to be finite and because the wave function (24) is normalizable when $r \to 0$.

Furthermore, using Cauchy-Schwarz inequality and arithmetic mean inequality we have

$$\frac{|E|}{\hbar c}\sqrt{\langle r^2 \rangle} \geqslant \frac{|E|}{\hbar c}\int_0^\infty r(G^2 + F^2)dr \geqslant \left|\frac{2E}{\hbar c}\int_0^\infty rGF dr\right|. \tag{31}$$

This gives us the confinement limit

$$\sqrt{\langle r^2 \rangle} \geqslant j\frac{\hbar c}{|E|}. \tag{32}$$

This inequality tells us that Dirac particles cannot be confined to an arbitrarily small spatial region by the Lorentz scalar potential as long as E is finite. For discussing quark confinement, the energy of quantum systems is a parameter depending on the experimental value of the proton mass.

V. CONCLUSIONS

We derived the confinement limit of the three-dimensional Dirac particle in vector and scalar potentials. We arrived at the conclusion that the spin of a three-dimensional Dirac particle prevents its localization to be confined in an arbitrarily small region. It shows that the lower bound on the measurability of the position of a three-dimensional Dirac particle in a space direction is proportional to its corresponding Compton length and the modulus of the expectation value of the spin in this space direction. This conclusion does not depend on the Heisenberg uncertainty relation and the explicit form of the potentials.

Although the main interest of this paper is in the vector and scalar potentials, we discuss the Lorentz scalar potential, showing that the Dirac particle confined in a central Lorentz scalar potential also has a confinement limit that is proportional to total angular momentum and is inversely proportional to the modulus of eigenenergy.

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