PRAMANA — journal of physics
© Indian Academy of Sciences
Vol. 72, No. 5
May 2009
pp. 777–785

Quantum-classical correspondence of the Dirac equation with a scalar-like potential

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MS received 24 September 2006; revised 6 December 2008; accepted 23 December 2008

Abstract. Quantum matrix elements of the coordinate, momentum and the velocity operator for a spin-1/2 particle moving in a scalar-like potential are calculated. In the large quantum number limit, these matrix elements give classical quantities for a relativistic system with a position-dependent mass. Meanwhile, the Klein–Gordon equation for the spin-0 particle is discussed too. Though the Heisenberg equations for both the spin-0 and spin-1/2 particles are unlike the classical equations of motion, they go to the classical equations in the classical limit.

Keywords. Quantum-classical correspondence; scalar-like potential; Dirac equation; Klein–Gordon equation.

PACS Nos 03.65.-w; 03.65.Pm; 03.65.Ca

1. Introduction

There have been many investigations on the quantum-classical correspondence in the literature [1–10]. The most often mentioned correspondence principle is perhaps the Bohr correspondence principle, which states that a quantum system behaves like the corresponding classical system in large quantum limit. Recently, the Heisenberg correspondence principle (HCP) has aroused much interest [6–10]. HCP says that in the classical limit, the quantum matrix elements correspond to the Fourier components of the classical motion. As is well known, the Heisenberg equations of motion in quantum mechanics are similar to the classical equations. For example, for the harmonic oscillator the Heisenberg equations of the coordinate and momentum operators are

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{p}{\mu}, \quad \frac{\mathrm{d}p}{\mathrm{d}t} = -\mu\omega_0^2 x, \tag{1.1}$$

where μ and ω_0 are the mass and frequency respectively. The mean values of the coordinate and momentum for an eigenstate are zero and eq. (1.1) becomes $0 = 0$. No useful information can be obtained from the mean values. HCP deals with the problem of quantum-classical correspondence from the aspect of quantum matrix elements. Using the Schrödinger equation, it is not difficult to show that the matrix elements

$$x_{mn}(t) = \int \psi_m^*(x,t) x \psi_n(x,t) \mathrm{d}V$$
$$p_{mn}(t) = \int \psi_m^*(x,t) p \psi_n(x,t) \mathrm{d}V \tag{1.2}$$

satisfy the following equations of motion:

$$\frac{\mathrm{d}x_{mn}(t)}{\mathrm{d}t} = \frac{p_{mn}(t)}{\mu}, \quad \frac{\mathrm{d}p_{mn}(t)}{\mathrm{d}t} = -\mu\omega_0^2 x_{mn}(t) \tag{1.3}$$

which are similar to (1.1). Making sum over m in (1.3), one sees that the sum of the possible matrix elements $\sum_m x_{mn}(t) = x_n(t), \sum_m p_{mn}(t) = p_n(t)$ also satisfy (1.3)

$$\frac{\mathrm{d}x_n(t)}{\mathrm{d}t} = \frac{p_n(t)}{\mu}, \quad \frac{\mathrm{d}p_n(t)}{\mathrm{d}t} = -\mu\omega_0^2 x_n(t). \tag{1.4a}$$

At finite n, the quantities $x_n(t), p_n(t)$ are complex. But, in the limit $n \to \infty$, they become real. By some calculations one gets

$$x_n(t) = \sqrt{\hbar/(2\mu\omega_0)}\left[\sqrt{n}\exp(-i\omega_0 t) + \sqrt{n+1}\exp(i\omega_0 t)\right] \tag{1.4b}$$

which is complex. In the limit $n \to \infty$, we have $x_n(t) = A\cos\omega_0 t$, with the amplitude $A \to \sqrt{2n\hbar/(\mu\omega_0)}$ and the energy $E_n = (n+1/2)\hbar\omega_0 \to n\hbar\omega_0$. The energy and the amplitude now obey the classical relation $E_n = (1/2)\mu\omega_0^2 A^2$. In the classical limit, one needs to treat $n\hbar$ as a classical quantity.

Generally, writing the wave function for a quantum system as

$$\psi_q(x,y,z,t) = \psi_q(x,y,z)\exp(-iE_q t), \tag{1.5}$$

where q stands for all the possible quantum numbers, the following quantity

$$\Omega_q(t) = \sum_Q \int \psi_Q^*(x,y,z,t)\Omega\psi_q(x,y,z,t)\mathrm{d}V \tag{1.6}$$

with Ω being the Hermitian operator for a physical observable and $\mathrm{d}V = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ being a small volume in space, should generate the classical result in the large quantum number limit (which is the Bohr correspondence principle) according to the idea of HCP. In the next section, a general explanation that the quantity (1.6) is real in the classical limit is given (see (2.13–2.16)).

In non-relativistic case and the relativistic case discussed in [10], the Heisenberg equation of motion for the momentum operator can be written as

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}, \tag{1.7}$$

where $\vec{F}$ represents the external force. For a charged particle moving in a magnetic field, $\vec{F}$ has the form $q\vec{v} \times \vec{B}$; for a particle moving in an external potential, $\vec{F}$ is $-\nabla V$. Clearly, eq. (1.7) is similar to the corresponding classical equation. So, it may not be difficult to understand why eq. (1.7) reduces to the classical equation in the classical limit. However, for the relativistic case, the problem is more complicated. The Heisenberg equation of motion is not always similar to the classical equation. For the scalar-like confining potential, the Hamiltonian is [11,12]

$$H = \vec{\alpha} \cdot \vec{p}c + \beta(mc^2 + Az) \tag{1.8}$$

and the Heisenberg equations of motion take the form

$$\frac{\mathrm{d}p_x}{\mathrm{d}t} = \frac{\mathrm{d}p_y}{\mathrm{d}t} = 0, \quad \frac{\mathrm{d}p_z}{\mathrm{d}t} = -\beta A, \tag{1.9}$$

where $p_j, j = x, y, z$ are the three components of the momentum. The form of the equation for p_z in (1.9) is different from that in (1.7). On the right-hand side in (1.9), there is a 4×4 matrix β. Hence, it is interesting to see if the equation for p_z can give the classical equation in the classical limit.

This article is arranged as follows. The next section gives the matrix elements and the classical limits for the scalar-like potential, where the spin-0 particle is discussed too. The final section is the conclusion.

2. Matrix elements and the classical limits

For the scalar-like confining potential, the energy eigenvalues are [11,12]

$$E_n = \pm\sqrt{2(n+1)\hbar cA + p_1^2c^2 + p_2^2c^2}. \tag{2.1}$$

In quantum field theory, the positive and negative energy solutions correspond to particle and antiparticle respectively and there are particle creations and annihilations. However, when we discuss the quantum-classical correspondence in quantum mechanics, we should restrict to one particle each time. Next we focus on the particle or positive energy solution. For the antiparticle, discussions are similar. Introducing the function

$$\phi_n(\xi) = N_n H_n(\xi) \exp\left(-\frac{1}{2}\xi^2\right), \quad N_n = \left(\frac{\sqrt{A}}{\sqrt{\hbar c\pi} n! 2^n}\right)^{1/2} \tag{2.2}$$

the eigenfunctions can be written in the form

$$\psi_q(x,y,z,t) = C_n \begin{bmatrix} \frac{\phi_{n+1}(\xi)}{N_{n+1}} + \frac{E_n}{\sqrt{\hbar cA}}\frac{\phi_n(\xi)}{N_n} \\ (p_2 - ip_1)\sqrt{\frac{c}{\hbar A}}\frac{\phi_n(\xi)}{N_n} \\ i\left(\frac{\phi_{n+1}(\xi)}{N_{n+1}} - \frac{E_n}{\sqrt{\hbar cA}}\frac{\phi_n(\xi)}{N_n}\right) \\ -(p_2 + ip_1)\sqrt{\frac{c}{\hbar A}}\frac{\phi_n(\xi)}{N_n} \end{bmatrix} \exp\left[i\frac{p_1x + p_2y - E_nt}{\hbar}\right], \tag{2.3}$$

where the parameter $\xi = \sqrt{A/(\hbar c)}(mc^2/A + z)$, the normalization constant $C_n = N_n \hbar c \left(\sqrt{A/(\hbar c)}\right)^{3/2}/(2E_n)$, $H_n(\xi)$ is the Hermitian polynomial, q represents p_1, p_2 and n. Through some calculations, we have

$$x_q(t) = \frac{p_1 c^2}{E_n} t, \quad y_q(t) = \frac{p_2 c^2}{E_n} t \tag{2.4}$$

$$\begin{aligned} z_q(t) = &-\frac{mc^2}{A} + \frac{\sqrt{n\hbar c}(E_n + E_{n-1})}{2\sqrt{2A}E_{n-1}} \exp\left[i\frac{E_{n-1} - E_n}{\hbar} t\right] \\ &+ \frac{\sqrt{(n+1)\hbar c}(E_n + E_{n+1})}{2\sqrt{2A}E_n} \exp\left[i\frac{E_{n+1} - E_n}{\hbar} t\right] \end{aligned} \tag{2.5}$$

and

$$p_{xq}(t) = p_1, \quad p_{yq}(t) = p_2 \tag{2.6}$$

$$\begin{aligned} p_{zq}(t) = &-i\frac{\sqrt{n\hbar A/c}\,(E_n + E_{n-1})}{2\sqrt{2}E_{n-1}} \exp\left[i\frac{E_{n-1} - E_n}{\hbar} t\right] \\ &+ i\frac{\sqrt{(n+1)\,\hbar A/c}\,(E_n + E_{n+1})}{2\sqrt{2}E_n} \exp\left[i\frac{E_{n+1} - E_n}{\hbar} t\right]. \end{aligned} \tag{2.7}$$

In the large quantum number limit, (2.4)–(2.7) become

$$x_c(t) = \frac{p_1 c^2}{E_c} t, \quad y_c(t) = \frac{p_2 c^2}{E_c} t, \tag{2.8}$$

$$z_c(t) = -\frac{mc^2}{A} + \sqrt{\frac{2n\hbar c}{A}} \cos \omega t, \tag{2.9}$$

$$p_{xc}(t) = p_1, \quad p_{yc}(t) = p_2, \tag{2.10}$$

$$p_{zc}(t) = -\sqrt{\frac{2n\hbar A}{c}} \sin \omega t, \tag{2.11}$$

where $\omega = Ac/E_n = \partial E_n/\partial(n\hbar)$, E_c is the energy when n is very large. In the derivations, the following relations are used:

$$\begin{aligned} E_{n\pm1} - E_n &= \sqrt{2\,(n + 1 \pm 1)\,\hbar c A + p_1^2 c^2 + p_2^2 c^2} - E_n \\ &= \sqrt{E_n^2 \pm 2\hbar c A} - E_n = E_n(1 \pm 2A\hbar c/E_n^2)^{1/2} - E_n \\ &\to E_n \pm \hbar c A/E_n - E_n = \pm \hbar c A/E_n = \pm \hbar\omega. \end{aligned} \tag{2.12}$$

At finite quantum number, quantities in (2.5) and (2.7) are complex functions of time. But, in the large quantum number limit, they become real as shown in (2.9) and (2.11). Now we give a general explanation that in the large quantum limit the quantity (1.6) becomes real. To be mathematically simple, we use the Dirac notation. The wave function is written as $|\psi_q(t)\rangle$ and the sum of the possible matrix elements become $\Omega_q(t) = \sum_Q \langle\psi_Q(t)|\Omega|\psi_q(t)\rangle$. The sum can be divided into two parts: One is that $Q > q$ and the other is $Q < q$

$$\begin{aligned}\Omega_q(t) &= \sum_{Q>q} \langle\psi_Q(t)|\Omega\,|\psi_q(t)\rangle + \sum_{Q<q} \langle\psi_Q(t)|\Omega\,|\psi_q(t)\rangle \\ &= \sum_{k=0}^{\infty} \langle\psi_{q+k}|\Omega\,|\psi_q(t)\rangle + \sum_{k=0}^{q} \langle\psi_{q-k}(t)|\Omega\,|\psi_q(t)\rangle\,. \end{aligned} \tag{2.13}$$

In the classical limit $q \to \infty$, the quantity (1.6) or (2.13) becomes

$$\begin{aligned}\Omega_q(t) \;&\to \sum_{k=0}^{\infty} \langle\psi_{q+k}|\Omega\,|\psi_q(t)\rangle + \sum_{k=0}^{\infty} \langle\psi_{q-k}(t)|\Omega\,|\psi_q(t)\rangle \\ &= \sum_{k=0}^{\infty} [\langle\psi_{q+k}|\Omega\,|\psi_q(t)\rangle + \langle\psi_{q-k}(t)|\,\Omega\,|\psi_q(t)\rangle\,. \end{aligned} \tag{2.14}$$

Let us focus our attention on each term $\langle\psi_{q+k}|\,\Omega\,|\psi_q(t)\rangle + \langle\psi_{q-k}(t)|\,\Omega\,|\psi_q(t)\rangle$ in the sum (2.14). Setting $q = q' + k$ in the second term, one has

$$\begin{aligned}&\langle\psi_{q+k}|\,\Omega\,|\psi_q(t)\rangle + \langle\psi_{q-k}(t)|\,\Omega\,|\psi_q(t)\rangle \\ &\quad = \langle\psi_{q+k}|\,\Omega\,|\psi_q(t)\rangle + \langle\psi_{q'}(t)|\,\Omega\,|\psi_{q'+k}(t)\rangle\,. \end{aligned} \tag{2.15}$$

The limit $q \to \infty$ results in $q' \to \infty$. Thus, under the classical limit, there is the relation $\langle\psi_{q'}(t)|\,\Omega\,|\psi_{q'+k}(t)\rangle = \langle\psi_q(t)|\,\Omega\,|\psi_{q+k}(t)\rangle$. Or, in the large number limit

$$\begin{aligned}&\langle\psi_{q+k}|\,\Omega\,|\psi_q(t)\rangle + \langle\psi_{q'}(t)|\,\Omega\,|\psi_{q'+k}(t)\rangle \\ &\to \langle\psi_{q+k}|\,\Omega\,|\psi_q(t)\rangle + \langle\psi_q(t)|\,\Omega\,|\psi_{q+k}(t)\rangle\,. \end{aligned} \tag{2.16}$$

Each term of these two terms is the complex conjugate of the other and so the quantity (2.16) is real. Thus (1.6) is real too in the classical limit. By some calculations, we also obtain

$$\begin{aligned}(-\beta A)_q(t) = -\frac{A}{E_n}\Bigg\{&\sqrt{\frac{n\hbar cA}{2}}\exp\!\left[i\frac{E_{n-1}-E_n}{\hbar}t\right] \\ &-\sqrt{\frac{(n+1)\hbar cA}{2}}\exp\!\left[i\frac{E_{n+1}-E_n}{\hbar}t\right]\Bigg\}. \end{aligned} \tag{2.17}$$

In the large quantum number limit

$$(-\beta A)_c(t) \to -\frac{A}{E_c}\sqrt{2n\hbar cA}\cos\omega t = F_c. \tag{2.18}$$

The momentum (2.11) and the force (2.18) obey

$$\frac{\mathrm{d}p_{zc}(t)}{\mathrm{d}t} = F_c. \tag{2.19}$$

In the next, we will see that (2.19) is in fact the classical equation of motion.

Now, we show that (2.8)–(2.11) are the classical coordinates and momenta of a classical system with the Hamiltonian

$$H = \sqrt{p_x^2c^2 + p_y^2c^2 + p_z^2c^2 + (mc^2 + Az)^2}. \tag{2.20}$$

It can be proved that the squared classical Hamiltonian is the classical limit of the squared quantum Hamiltonian (1.8). The classical Hamiltonian (2.20) describes a system with position-dependent mass. From this Hamiltonian, it is easy to get the classical equations of motion

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= \frac{p_x c^2}{H}, \quad \frac{\mathrm{d}p_x}{\mathrm{d}t} = 0 \\ \frac{\mathrm{d}y}{\mathrm{d}t} &= \frac{p_y c^2}{H}, \quad \frac{\mathrm{d}p_y}{\mathrm{d}t} = 0 \end{aligned} \tag{2.21}$$

and

$$\begin{aligned} \frac{\mathrm{d}p_z}{\mathrm{d}t} &= F, \quad F = -\frac{A\left(mc^2 + Az\right)}{H} \\ \frac{\mathrm{d}z}{\mathrm{d}t} &= \frac{p_z c^2}{H}. \end{aligned} \tag{2.22}$$

Notice that $\mathrm{d}H/\mathrm{d}t = \partial H/\partial t = 0$, or the energy is conserved. Equations (2.21) have the solutions

$$x = \frac{p_1 c^2}{E_c}t, \quad y = \frac{p_2 c^2}{E_c}t \tag{2.23}$$

$$p_x = p_1, \quad p_y = p_2 \tag{2.24}$$

which agree with (2.8) and (2.10) respectively. From (2.22), one obtains

$$\frac{\mathrm{d}^2 z}{\mathrm{d}t^2} + \omega^2\left(z + \frac{mc^2}{A}\right) = 0, \quad \omega = \frac{Ac}{E_c} \tag{2.25}$$

which has the solution

$$z(t) = -mc^2/A + z_0 \cos\omega t. \tag{2.26}$$

Compared to (2.9), one gets the amplitude $z_0 = \sqrt{2n\hbar c/A}$. The classical momentum $p_z(t) = E_c\,\mathrm{d}z/\mathrm{d}t$ agrees with (2.11). The classical force

$$F = -\frac{A\left(mc^2 + Az\right)}{H} = -\frac{A}{E_c}\sqrt{2n\hbar cA}\cos\omega t \tag{2.27}$$

is the same as (2.18). So, eq. (2.22) is the classical equation for p_z in (2.22).

For the Hamiltonian (1.8), there is also the velocity operator

$$\vec{\alpha} = \frac{\mathrm{d}\vec{r}}{\mathrm{d}t}, \tag{2.28}$$

where $r = (x, y, z)$. Calculations show that quantum matrix elements satisfy this equation, as pointed out in [10] for other systems.

In the following, we turn to the spin-0 particle, which obeys the Klein–Gordon equation

$$[(mc^2 + Az)^2 + \vec{p}^2c^2]\psi(x, y, z, t) = E^2\psi(x, y, z, t). \tag{2.29}$$

The wave functions are found to be

$$\psi_n(x, y, z, t) = \frac{\phi_n(\xi)}{2\pi} \exp\left(i\frac{p_1}{\hbar}x + i\frac{p_2}{\hbar}y - i\frac{E_n}{\hbar}t\right). \tag{2.30}$$

By some calculations, we have

$$\begin{aligned} z_n(t) &= \sqrt{\frac{n\hbar c}{2A}} \exp\left[i\frac{E_{n-1} - E_n}{\hbar}t\right] \\ &\quad + \sqrt{\frac{(n+1)\hbar c}{2A}} \exp\left[i\frac{E_{n+1} - E_n}{\hbar}t\right], \\ p_{zn}(t) &= -i\sqrt{\frac{n\hbar A}{2c}} \exp\left[i\frac{E_{n-1} - E_n}{\hbar}t\right] \\ &\quad + i\sqrt{\frac{(n+1)\hbar A}{2c}} \exp\left[i\frac{E_{n+1} - E_n}{\hbar}t\right]. \end{aligned} \tag{2.31}$$

These are complex quantities. In the large quantum number limit, eqs (2.31) become real and agree with (2.9) and (2.11). One may write the squared quantum Hamiltonian for the spin-0 particle as

$$H^2 = \vec{p}^2c^2 + \left(mc^2 + Az\right)^2. \tag{2.32}$$

The Heisenberg equations

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \frac{1}{i}[z, H], \quad \frac{\mathrm{d}p_z}{\mathrm{d}t} = \frac{1}{i}[p_z, H] \tag{2.33}$$

are actually very complicated due to the non-commutation between z and p_z. But, through the quantum matrix elements, we have obtained the classical solutions without much difficulty.

3. Conclusions

For the scalar-like confining potential, we have derived the classical solutions through the calculations of quantum matrix elements, even though the Heisenberg equations are unlike the classical equations. The Klein–Gordon equation and the Dirac equation describe spin-0 and spin-1/2 particles respectively. For particles with higher spin, for example the photon, HCP can also be used. The basic equations for the electromagnetic field are the Maxwell equations, which take the form (in vacuum)

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times \vec{B} = \frac{1}{c^2}\frac{\partial \vec{E}}{\partial t}, \tag{3.1}$$

$$\nabla \cdot \vec{E} = 0, \quad \nabla \cdot \vec{B} = 0, \tag{3.2}$$

where $\vec{E}$ is the electric field and $\vec{B}$ is the magnetic field. For a long time, discussions about the photon wave functions were starting from the Maxwell equations [13,14], due to the belief that the Maxwell equations describe the wave connected with the photon according to the wave–particle duality. Through some changes, the Maxwell equations can be changed into other forms. By defining a column vector

$$|\psi\rangle = \frac{1}{\sqrt{W}}\begin{bmatrix} E_1/c + iB_1 \\ E_2/c + iB_2 \\ E_3/c + iB_3 \end{bmatrix} \tag{3.3}$$

with W being a normalization constant, the Maxwell equations in vacuum can be written as

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle, \quad H = c\vec{K}\cdot\vec{p}, \tag{3.4}$$

$$\sum_{j=1}^{3}\frac{\partial}{\partial x_j}(E_j + iB_j) = 0, \tag{3.5}$$

where

$$K_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad K_2 = \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix}, K_3 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.6}$$

Equation (3.4) is derived from (3.1) and eq. (3.5) is the conditions (3.2). It is not difficult to see that eq. (3.4) is similar to the Dirac equation for the free massless spin-1/2 particles (in this case, K_j, $j = 1, 2, 3$ are the Pauli matrices). From this sense, eq. (3.4) describes a massless particle with $\vec{S} = \hbar\vec{K}$ being the spin operator. Such a particle corresponds to the electromagnetic field and is thus the photon. So, the related function in the new form of the Maxwell equations is sometimes named the photon wave function in the literature [13,14]. One can prove the result $\vec{S}^2 = s(s+1)\hbar^2$, with $s = 1$ or the photon is a spin-1 particle. The third component operator S_3 given in (3.6) has the eigenfunctions

$$|+1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix}, \quad |-1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}, \quad |0\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{3.7}$$

which correspond to the eigenvalues +1, −1 and 0 respectively. For photon propagating in the z-direction, there are the solutions for the normalized column vector

$$|\psi_{k\sigma}(z,t)\rangle = \frac{1}{\sqrt{2\pi}}\,|\sigma\rangle \exp[i\,(kz-\omega t)]\,, \tag{3.8}$$

where $\sigma = \pm 1$ and $\omega = kc$. The state with $\sigma = 0$ is forbidden by the condition (3.5). Using (1.6) and (3.8), it is not difficult to get

$$z_{k\sigma}(t) = ct, \quad (p_z)_{k\sigma}(t) = \hbar k \tag{3.9}$$

which are the classical coordinate and momentum of a massless particle, the photon.

The basic equation in non-relativistic quantum mechanics is the Schrödinger equation. However, in relativistic quantum mechanics, different particles satisfy different forms of equations. To have a general conclusion on the quantum-classical correspondence in the relativistic regime, further studies need to be done.

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