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Plane rotor with time-dependent magnetic flux in a multivalued representation

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Abstract. A quantum mechanical plane rotor with time-dependent magnetic flux on its axis is considered in a representation in which the wavefunction is multivalued. If the representation is chosen such that the new kinetic angular momentum is equal to the old canonical angular momentum, the Schrödinger equation is simplified. An energy eigenfunction expansion in the new representation is used to solve the Schrödinger equation exactly.

1. Introduction

The relationship between gauge transformations and the change of representation of the generalised coordinates and their conjugate canonical momentum has recently been discussed in connection with the Aharonov-Bohm effect (Bocchieri and Loinger 1978, 1981, Rowe 1980, Zeilinger 1979, Mignaco and Novaes 1979, Bawin and Burnel 1980, Bohm and Hiley 1979, Rothe 1981, Roy and Singh 1984, Klein 1980). A problem in which the difference between gauge invariance and change of representation is well illustrated is the plane rotor with time-dependent magnetic flux on its axis (Kobe 1982b, Home and Sengupta 1983). In a previous paper, (Kobe 1983a) the problem was solved exactly in an arbitrary gauge. The Aharonov-Bohm effect was shown to exist because eigenvalues of the energy operator depend on the instantaneous magnetic flux. Some workers (Bocchieri and Loinger 1978, 1981, Wilczek 1982, Jackiw and Redlich 1983) have attempted to solve this problem by using 'singular' gauge transformations. These 'singular' gauge transformations are not valid, but their effect can be realised by a change of representation of the canonical momentum operators (Kobe 1982a).

In this paper it is shown that a change of representation (Kretzschmar 1965, Asorey *et al* 1983) of the canonical momentum operators can be used to simplify the Schrödinger equation. In the new representation the new kinetic angular momentum is equal to the old canonical angular momentum (Kobe 1982a). The new wavefunction is no longer single valued but multivalued. The new Schrödinger equation does not depend on the magnetic flux, but only on its time derivative. The magnetic flux is now taken into account by the boundary condition on the new wavefunction (Kretzschmar 1965).

The energy operator eigenvalue problem was solved by Merzbacher (1962) in the static case using the standard single-valued representation. For the time-dependent case the energy operator eigenvalue equation has the same form, since the kinetic momentum involves the instantaneous flux (Yang 1976, Kobe and Smirl 1978). In the new representation the energy operator no longer involves the magnetic flux. The

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magnetic flux is now taken into account by the boundary condition on the energy eigenfunctions. The energy eigenvalues are consequently the same as in the standard representation in which the eigenfunctions are single valued (Kretzschmar 1965). An eigenfunction expansion is used to solve the Schrödinger equation exactly. The wavefunction in the multivalued representation is transformed to the single-valued representation.

A number of workers (Bocchieri and Loinger 1978, 1981, Roy and Singh 1984) have questioned whether the wavefunction must be single valued in the standard representation of the canonical momentum ($\boldsymbol{p} = -\mathrm{i}\hbar\nabla$). If it is not, the Aharonov-Bohm effect can be made to vanish. The single valuedness of the wavefunction depends on the eigenvalues of the z-component of the orbital angular momentum being integers. The integer values of the z-component of orbital angular momentum eigenvalues were proved by Louck (1963) and Buchdahl (1962) using the algebra of the commutation relations and the form of orbital angular momentum ($\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$).

In § 2 the potentials and the Schrödinger equation for the plane rotor are reviewed. The change of representation to a multivalued wavefunction for which the new kinetic angular momentum is equal to the old canonical angular momentum is made in § 3. In § 4 the energy eigenvalue equation is solved in the new representation and in § 5 the Schrödinger equation is solved in the new representation. The conclusion is given in § 6.

2. Plane rotor with time-dependent magnetic flux

The vector and scalar potentials for a time-dependent magnetic field confined to the z axis are given in a general gauge. The Schrödinger equation for a plane rotor in an orbit about the z-axis is given in the standard representation in which the wavefunction is single valued.

2.1. Potentials

The magnetic field is confined to the z-axis, and is infinite in such a way that the magnetic flux is $\Phi(t)$. The magnetic induction is

$$\boldsymbol{B} = \Phi(t)\delta(x)\delta(y)\hat{z}. \tag{2.1}$$

A vector potential $\boldsymbol{A}$ which gives the magnetic induction field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ in (2.1) is

$$\boldsymbol{A} = \hat{\theta}\Phi(t)g(\theta, t)/2\pi\rho, \tag{2.2}$$

where the function $g(\theta, t)$ is an arbitrary function of θ ($0 \leq \theta < 2\pi$) and time t subject to the constraint

$$\int_0^{2\pi} \mathrm{d}\theta'\, g(\theta', t) = 2\pi. \tag{2.3}$$

For $\rho > 0$ $\boldsymbol{B}$ is zero, but by Stokes's theorem the flux at $\rho = 0$ is $\Phi(t)$ when (2.3) is used.

If the flux $\Phi(t)$ is changing in time, there is an induced electric field by Faraday's law, EMF $= -\dot{\Phi}/c$, so

$$\boldsymbol{E} = -\hat{\theta}\dot{\Phi}(t)/2\pi\rho c, \tag{2.4}$$

where the dot denotes the time derivative. The electric field is $\boldsymbol{E} = -\nabla A_0 - \partial\boldsymbol{A}/\partial tc$, where the scalar potential A_0 is

$$A_0 = (\dot{\Phi}/2\pi c)[\theta - f(\theta, t)] - (\Phi/2\pi c)\dot{f}(\theta, t), \tag{2.5}$$

and

$$f(\theta, t) = \int_0^\theta d\theta' g(\theta', t). \tag{2.6}$$

for $0 \leq \theta < 2\pi$. The dot over the f in (2.5) denotes the partial time derivative.

2.2. *Schrödinger equation*

In the problem of the plane rotor, the Hilbert space of wavefunctions is defined on $\mathcal{S} = \{(\rho, \theta, z)|\rho = a > 0,\ \theta \in [0, 2\pi),\ z = 0\}$, because the electron is constrained to move on a circular orbit of radius a. Since the generalised coordinate is θ, the momentum conjugate to it is the canonical angular momentum $p_\theta = -i\hbar\partial/\partial\theta$. If $A^\theta = \rho\hat{\theta}\cdot \boldsymbol{A} = -A_\theta$, the Schrödinger equation can be written as†

$$(1/2I)(p_\theta + qA_\theta/c)^2\psi(\theta, t) = -c(p_0 + qA_0/c)\psi(\theta, t), \tag{2.7}$$

where $p_0 = -i\hbar\partial/\partial x^0$, $x^0 = ct$, and the moment of inertia is $I = ma^2$.

The kinetic angular momentum is

$$p_\theta + qA_\theta/c = \hbar[-i\partial/\partial\theta - \alpha(t)g(\theta, t)] \tag{2.8}$$

by (2.2), where

$$\alpha(t) = q\Phi(t)/2\pi\hbar c \tag{2.9}$$

is dimensionless. The Schrödinger equation in (2.7) then becomes

$$(\hbar^2/2I)[-i\partial/\partial\theta - \alpha(t)g(\theta, t)]^2\psi(\theta, t)$$
$$= \hbar[i\partial/\partial t - \dot{\alpha}(t)[\theta - f(\theta, t)] + \alpha(t)\dot{f}(\theta, t)]\psi(\theta, t), \tag{2.10}$$

from (2.5). The wavefunction ψ is single valued so it satisfies the boundary condition $\psi(2\pi, t) = \psi(0, t)$. The initial wavefunction $\psi(\theta, 0)$ is assumed known. Equation (2.10) was previously solved exactly. Nevertheless by using a representation in which the new kinetic angular momentum is the old canonical angular momentum it can be significantly simplified.

2.3. *'Singular' gauge transformations*

Several workers (Bocchieri and Loinger 1978, 1981, Wilczek 1982, Jackiw and Redlich 1983) have attempted to simplify (2.10) by making a 'singular' gauge transformation to eliminate the vector potential. The 'singular gauge function' $\Lambda_s = -\Phi(t)f(\theta, t)/2\pi$ defined on $\mathcal{R}^3$, Euclidean three space, satisfies

$$\nabla \times \nabla\Lambda_s = -\Phi(t)\delta(x)\delta(y)\hat{z}. \tag{2.11}$$

Since any gauge function must satisfy $\nabla \times \nabla\Lambda = 0$ everywhere in $\mathcal{R}^3$, Λ_s is not a valid gauge function. The new vector potential is $\boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda$. If Λ_s is used then the new

† In Kobe (1983a) the kinetic momentum in (3.1) should read $p_\theta - qA^\theta/c$ to be consistent with the notation of this paper in which $p_\theta + qA_\theta/c$ is used. Nevertheless, the results of Kobe are correct. The scalar potential ϕ of Kobe has been replaced by A_0 in this paper.

magnetic induction field $\boldsymbol{B}'=\nabla\times\boldsymbol{A}'$ is

$$\boldsymbol{B}'=\boldsymbol{B}+\nabla\times\nabla\Lambda_s=0, \tag{2.12}$$

everywhere in $\mathscr{R}^3$ by (2.11). Since $\boldsymbol{B}'\neq\boldsymbol{B}$ the function Λ_s cannot be regarded as a valid gauge function, since a change of the gauge of the potentials must not change the electromagnetic field. If the magnetic field is changed, the problem is different from the original one (Kobe 1982a).

3. Change of representation

The Schrödinger equation can be simplified by using a representation of the momentum operator in which the vector potential is cancelled, so that the new kinetic angular momentum reduces to the old canonical angular momentum (Kobe 1982a). The wavefunction in this representation is no longer single valued (continuous) but is multivalued (discontinuous) (Kretzschmar 1965). The solution to the Schrödinger equation in an arbitrary time-dependent gauge with the new boundary condition is simpler than in the standard representation.

3.1. Unitary transformations

A unitary transformation on the generalised coordinates and their conjugate canonical momenta gives a change of representation of the operators which preserves the canonical commutation relations (Kretzschmar 1965). If Γ is a differentiable function defined on $\mathscr{S}$, then the canonical momentum operators are transformed to

$$p_\mu^{(\Gamma)}=\exp(-\mathrm{i}\Gamma)p_\mu\exp(\mathrm{i}\Gamma) \tag{3.1}$$

where $\mu=0$, θ, while θ and $x^0=ct$ are unchanged. The wavefunction ψ must also be transformed,

$$\psi_{(\Gamma)}=\exp(-\mathrm{i}\Gamma)\psi, \tag{3.2}$$

to preserve the form invariance of the Schrödinger equation.

The Schrödinger equation in (2.7) in the new representation is

$$(1/2I)(p_\theta^{(\Gamma)}+qA_\theta/c)^2\psi_{(\Gamma)}=-c(p_0^{(\Gamma)}+qA_0/c)\psi_{(\Gamma)}. \tag{3.3}$$

3.2. Representation in which new kinetic momentum is old canonical momentum

A new representation can be chosen so that the new kinetic angular momentum is equal to the old canonical angular momentum (Kobe 1982a). Choose

$$\Gamma=\alpha(t)f(\theta,t), \tag{3.4}$$

where α is defined in (2.9) and f is defined in (2.6). In this representation the new kinetic angular momentum is

$$p_\theta^{(\alpha f)}+qA_\theta/c=p_\theta+\hbar\alpha\,\partial f(\theta,t)/\partial\theta-\hbar\alpha g(\theta,t)=p_\theta, \tag{3.5}$$

where the old canonical angular momentum is $p_\theta=-\mathrm{i}\hbar\partial/\partial\theta$. The zero component of the new kinetic angular momentum is

$$p_0^{(\alpha f)}+qA_0/c=-(\hbar/c)[\mathrm{i}\partial/\partial t-\dot\alpha(t)\theta]. \tag{3.6}$$

In this new representation the Schrödinger equation in (3.3) becomes

$$(\hbar^2/2I)(-\mathrm{i}\partial/\partial\theta)^2\psi_{(\alpha f)}(\theta, t) = \hbar[\mathrm{i}\partial/\partial t - \dot{\alpha}(t)\theta]\psi_{(\alpha f)}(\theta, t), \tag{3.7}$$

where the new wavefunction $\psi_{(\alpha f)}$ is

$$\psi_{(\alpha f)}(\theta, t) = \exp[-\mathrm{i}\alpha(t)f(\theta, t)]\psi(\theta, t) \tag{3.8}$$

from (3.2).

The boundary condition for $\psi_{(\alpha f)}$ is

$$\psi_{(\alpha f)}(2\pi, t) = \exp\{-\mathrm{i}2\pi\alpha(t)\}\psi_{(\alpha f)}(0, t), \tag{3.9}$$

since $\psi_{(\alpha f)}(0, t) = \psi(0, t) = \psi(2\pi, t)$, $f(2\pi, t) = 2\pi$, and $f(0, t) = 0$ by (3.8) and (2.6). The value $\psi(2\pi, t)$ is defined as lim $\psi(2\pi - \varepsilon, t)$ as $\varepsilon > 0$ goes to zero. Similar definitions hold for $\psi_{(\alpha f)}(2\pi, t)$ and $f(2\pi, t)$. Since $2\pi\alpha = q\Phi(t)/\hbar c$ is arbitrary, (3.9) shows that the wavefunction in this new representation is not continuous at $\theta = 0$.

Equation (3.7) is equivalent to (2.10) even though it does not involve the magnetic flux but only its time derivative. The magnetic flux enters the problem through the boundary condition in (3.9). For static flux the boundary condition in (3.9) ensures the existence of the Aharonov–Bohm effect in the new representation, even though the Schrödinger equation in (3.7) does not involve the flux (Ktretzschmar 1965).

4. Energy eigenvalue equation

In the representation $\Gamma = \alpha f$ the gauge-invariant energy operator is (Yang 1976, Kobe and Smirl 1978, Kobe 1983a)

$$\mathscr{E}_{(\alpha f)} = (1/2I)(p_\theta^{(\alpha f)} + qA_\theta/c)^2 = (1/2I)p_\theta^2 \tag{4.1}$$

from (3.5). The energy operator eigenvalue equation is†

$$\mathscr{E}_{(\alpha f)}\psi_{n(\alpha f)} = \varepsilon_n\psi_{n(\alpha f)}, \tag{4.2}$$

where the energy eigenfunctions $\psi_{n(\alpha f)}$ satisfy the boundary condition in (3.9). For the energy operator in (4.1), the energy eigenfunctions are

$$\psi_{n(\alpha f)}(\theta, t) = (2\pi)^{-1/2}\exp\{\mathrm{i}[n - \alpha(t)]\theta\}, \tag{4.3}$$

where n is an integer and α is given in (2.9). From (4.2) the energy eigenvalues are

$$\varepsilon_n(t) = \hbar^2[n - \alpha(t)]^2/2I, \tag{4.4}$$

which is the same as obtained in the standard representation (Kobe 1983a).

The kinetic angular momentum in the new representation is given in (3.5) as $-\mathrm{i}\hbar\partial/\partial\theta$. Equation (4.3) is also an eigenfunction of this operator, since it commutes with $\mathscr{E}_{(\alpha f)}$ in (4.1). The eigenvalue of the kinetic angular momentum is $[n - \alpha(t)]\hbar$, the same as obtained in the standard representation (Kobe 1983a).

† Merzbacher (1962) considers only the problem of static flux and uses a time-independent gauge. He claims that only single-valued wavefunctions are valid.

5. Solution of the Schrödinger equation

In the new representation the Schrödinger equation can easily be solved if the wavefunction at time $t = 0$ is given. By making an expansion in terms of the energy eigenfunctions in (4.3), the boundary condition in (3.9) is satisfied. The energy eigenfunction expansion was used previously to solve the Schrödinger equation in the standard representation (Kobe 1983a).

If the wavefunction is given at time zero, the wavefunction at some subsequent time can be determined from the Schrödinger equation in (3.7). If $\psi_{(\alpha f)}(\theta, t)$ is expanded in terms of the eigenfunctions in (4.3),

$$\psi_{(\alpha f)}(\theta, t) = \sum_n c_n(t) \psi_{n(\alpha f)}(\theta, t), \tag{5.1}$$

the expansion coefficients are interpretable as the probability amplitudes of finding the system in an energy eigenstate (Yang 1976, Kobe and Smirl 1978). If (5.1) is substituted into the Schrödinger equation in (3.7) and the result is simplified, the equation for the probability amplitudes is

$$\mathrm{i}\hbar \dot{c}_n - \varepsilon_n c_n = \sum_m \langle \psi_{n(\alpha f)} | c(p_0^{(\alpha f)} + qA_0/c) \psi_{m(\alpha f)} \rangle c_m. \tag{5.2}$$

The matrix element in (5.2) can be evaluated from (3.6) and (4.3), which gives

$$\begin{aligned} &\langle \psi_{n(\alpha f)} | (p_0^{(\alpha f)} + qA_0/c) \psi_{m(\alpha f)} \rangle \\ &\quad = -(\hbar/c) \langle \psi_{n(\alpha f)} | (\mathrm{i}\partial/\partial t - \dot{\alpha}\theta) \psi_{m(\alpha f)} \rangle = 0, \end{aligned} \tag{5.3}$$

for all n, m. Therefore, (5.2) becomes

$$\mathrm{i}\hbar \dot{c}_n - \varepsilon_n c_n = 0, \tag{5.4}$$

which has the solution

$$c_n(t) = \exp\left(-(\mathrm{i}/\hbar) \int_0^t \mathrm{d}t' \, \varepsilon_n(t') \right) c_n(0). \tag{5.5}$$

Equation (5.5) is the same solution for the probability amplitude as obtained in the single-valued representation. For the probability that the system is in an energy eigenstate (5.5) gives $P_n(t) = |c_n(t)|^2 = P_n(0)$, a constant no matter how the flux varies in time (neglecting radiation).

The wavefunction $\psi_{(\alpha f)}$ is obtained by substituting (4.3) and (5.5) into (5.1), which gives

$$\psi_{(\alpha f)}(\theta, t) = \exp[-\mathrm{i}\alpha(t)\theta] \sum_n \exp\left(-(\mathrm{i}/\hbar) \int_0^t \mathrm{d}t' \, \varepsilon_n(t') \right) c_n(0) (2\pi)^{-1/2} \exp(\mathrm{i}n\theta). \tag{5.6}$$

From (3.8) the wavefunction in the standard representation which is the solution to (2.10) is

$$\begin{aligned} \psi(\theta, t) &= \exp\{-\mathrm{i}\alpha(t)[\theta - f(\theta, t)]\} \\ &\quad \times \sum_n \exp\left(-(\mathrm{i}/\hbar) \int_0^t \mathrm{d}t' \, \varepsilon_n(t') \right) c_n(0) (2\pi)^{-1/2} \exp(\mathrm{i}n\theta), \end{aligned} \tag{5.7}$$

which can be verified by direct substitution. This wave function was obtained previously as a solution of (2.10) using the standard representation (Kobe 1983a).

6. Conclusion

The use of a representation which gives a multivalued (or discontinuous) wavefunction may be useful at times (Kretzschmar 1965). For the plane rotor the Schrödinger equation is simplified by using a representation which makes the new kinetic angular momentum equal to the old canonical angular momentum (Kobe 1982a). The solution of the Schrödinger equation is also simplified. The wavefunction can always be transformed to the standard representation. The eigenvalues of physically observable operators like energy and kinetic angular momentum are unchanged by a change in the representation. Since expectation values of observable operators are likewise unchanged under a change of representation, the Ehrenfest theorems (Kobe 1983a,b) for observables are still satisfied.

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