*Research Letter*

# Quantum Transitions by Change of Parameters and in Noninertial Motion

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As it is well known, a quantum system depending on parameters exhibits the (geometric) Berry phase when parameters are varying in the adiabatic limit. A generalization of the Berry phase is given in the present paper for a nonadiabatic change of parameters, which leads to quantum transitions in the system. This generalization is applied to noninertial motions and it is shown that such motions may induce quantum transitions for a system in an external field governed by Schrodinger's equation.

## 1. INTRODUCTION

As it is well known [1], a quantum system subjected to a change of parameters exhibits the (geometric) Berry phase, providing the change proceeds in the adiabatic limit. A careful examination of the derivation of the Berry phase suggests that a nonadiabatic change in parameters may induce quantum transitions in the system. It is shown in the present paper that the Berry phase can be generalized in such a way as to describe quantum transitions for such nonadiabatic changes in parameters. Moreover, it is shown that the displacement vector in a (nonuniform) translation or the rotation angle in a (nonuniform) rotation may play the role of such nonadiabatic parameters, such that a noninertial motion may cause quantum transitions for a system placed in an external field.

## 2. BERRY PHASE

Let the hamiltonian $H$, its (orthogonal) eigenfunctions $\varphi_k$, and energy eigenvalues $E_k$ depend on a parameter denoted generically by $\mathbf{R}$. This dependence is written explicitly in the eigenvalue equation

$$H(\mathbf{R})\varphi_k(\mathbf{R}) = E_k(\mathbf{R})\varphi_k(\mathbf{R}). \tag{1}$$

A time dependence $\mathbf{R}(t)$ is assumed for the parameter $\mathbf{R}$, and Schrodinger's equation is written as

$$\frac{i\hbar\partial\psi(t)}{\partial t} = H(\mathbf{R})\psi(t). \tag{2}$$

In the adiabatic limit $\dot{\mathbf{R}} \to 0$, the original eigenstate $\varphi_n(\mathbf{R})$ is preserved during the temporal evolution, and the solution of (2) reads

$$\psi_n(t) = \exp\left[ -\frac{i}{\hbar}\int_0^t E_n(\mathbf{R}(t'))\,dt' \right]\cdot e^{i\gamma_n(t)}\varphi_n(\mathbf{R}(t)), \tag{3}$$

where $\gamma_n(t)$ is given by

$$\dot{\gamma}_n(t) = i\left( \varphi_n, \frac{\partial\varphi_n}{\partial\mathbf{R}} \right)\dot{\mathbf{R}}. \tag{4}$$

The bracket in (4) indicates a scalar (inner) product. For a circuit $C$ described by the parameter $\mathbf{R}$, this is Berry's geometric phase $\gamma_n$ [1].

## 3. TRANSITIONS BY CHANGE OF PARAMETERS

This result implies that, in general, for nonvanishing $\dot{\mathbf{R}}$, the quantum system may exhibit transitions between its various states. Indeed, the general solution of (2) can be written as

$$\psi(t) = \sum_k a_k(t)\exp\left[ -\frac{i}{\hbar}\int_0^t E_k(\mathbf{R}(t'))\,dt' \right]\varphi_k(\mathbf{R}(t)), \tag{5}$$

where the coefficients $a_k(t)$ obey the equation

$$\dot{a}_n = i\sum_k a_k \gamma_{nk}(t)\dot{\mathbf{R}}$$
$$\cdot \exp\left[\frac{i}{\hbar}\int_0^t \left[E_n(\mathbf{R}(t')) - E_k(\mathbf{R}(t'))\right]dt'\right], \tag{6}$$

$$\gamma_{nk}(t) = i\left(\varphi_n, \frac{\partial\varphi_k}{\partial\mathbf{R}}\right). \tag{7}$$

This $\gamma_{nk}(t)$ is a generalization of the Berry phase; the latter corresponds to

$$\gamma_n(t) = \int_0^t d\mathbf{R}(t')\gamma_{nn}(t'), \tag{8}$$

where the integration is performed along the path described by the parameter $\mathbf{R}$ in its motion from $\mathbf{R}(t = 0)$ to $\mathbf{R}(t)$. The $\gamma_{nk}(t)$ are the matrix elements of the operator $-\mathbf{P}/\hbar$, $\gamma_{nk} = -\mathbf{P}_{nk}/\hbar$, where $\mathbf{P}$ may be viewed formally as the momentum associated with the parameter $\mathbf{R}$. Then (6) gives the transition amplitudes caused by a perturbation $H_1 = \mathbf{VP}$, where $\mathbf{V} = \dot{\mathbf{R}}$ is the velocity of the parameter $\mathbf{R}$.

Equation (6) is solved in the first order of the perturbation theory, with the initial conditions $a_n(0) = 1$, $a_k(0) = 0$ for $k \neq n$. The transition amplitudes

$$a_{kn}(t) = i\int_0^t d\mathbf{R}(t')\gamma_{kn}(t')$$
$$\cdot \exp\left[\frac{i}{\hbar}\int_0^{t'}\left[E_k(\mathbf{R}(t'')) - E_n(\mathbf{R}(t''))\right]dt''\right] \tag{9}$$

are obtained, where an additional label $k$ has been given to the coefficient $a_n$ in order to indicate the transition from state $n$ to state $k$. At the same time,

$$a_{nn}(t) = 1 + i\int_0^t d\mathbf{R}(t')\gamma_{nn}(t') = 1 + i\gamma_n(t). \tag{10}$$

From (9) and (10), one can see that in the adiabatic limit $\dot{\mathbf{R}} \to 0$ the Berry phase $\gamma_n = \gamma_n(T)$ is recovered in $a_{nn}(T) = e^{i\gamma_n(T)}$ for a circuit $C$, where $T$ is the period during which the parameter $\mathbf{R}$ describes the circuit $C$.

In the first order of the perturbation theory, the $\mathbf{R}$-dependence of the matrix elements $\gamma_{kn}$ and energy eigenvalues in the exponential factor in (9) may be neglected. The transition amplitudes can then be written as

$$a_{kn}(t) = -\frac{i}{\hbar}\int_0^t dt'\cdot\mathbf{V}(t')\mathbf{P}_{kn}\exp\left(i\omega_{kn}t'\right), \tag{11}$$

where $\omega_{kn}(t) = (E_k - E_n)/\hbar$.

For a uniform change of parameters, that is, for $\mathbf{V} = $ const, the transition amplitudes are vanishing ($a_{kn}(t) = 0$, $k \neq n$). The diagonal amplitude $a_{nn}(t) = 1 - (i/\hbar)\mathbf{VP}_{nn}t \simeq \exp(-i\mathbf{VP}_{nn}t/\hbar)$ given by (10) contains the correction $\mathbf{VP}_{nn}$ to the energy of the state $\varphi_n$ in the first order of the perturbation theory. The gauge transformation $\psi'_n = \exp(-i\mathbf{VP}_{nn}t/\hbar)\psi_n$ leaves Schrodinger's equation unchanged.

Let velocity $\mathbf{V}$ have a sudden variation from $\mathbf{V} = 0$ for $0 < t < t_0$ to $\mathbf{V} = $ const for $t_0 < t$, such that $\partial\mathbf{V}/\partial t = \mathbf{V}\delta(t-t_0)$. The transition amplitudes given by (11) become

$$a_{kn}(t) = -\frac{\mathbf{VP}_{kn}e^{i\omega_{kn}t}}{E_k - E_n} + \left[\frac{\mathbf{VP}_{kn}}{E_k - E_n}\right]e^{i(E_k-E_n)t_0/\hbar}. \tag{12}$$

The first term in the *rhs* of this equation corresponds to the change in the wave function under the action of the constant perturbation $\mathbf{VP}$ for $t > t_0$. The transition amplitude is given by the second term in the *rhs* of (12), so the transition probability is $w_{kn} = [\mathbf{VP}_{kn}/(E_k - E_n)]^2$.

If the velocity is periodic in time with frequency $\omega$, $\mathbf{V}(t) = \mathbf{V}e^{i\omega t} + $ c.c., the transition probability per unit time is given by $w_{kn} = (2\pi/\hbar)(\mathbf{VP}_{kn})^2\delta(E_k - E_n \pm \hbar\omega)$ in the limit of the infinite time. The calculations are not restricted to the discrete spectrum, so there may appear transitions in the continuum. It is worth noting that frequencies $\omega$ in the variation spectrum of the parameter $\mathbf{R}$ must be comparatively high of the order of the frequencies of the quantum system in order to have such quantum transitions. For a quantum-statistical system with a characteristic spectrum $\hbar\omega \times$ integer, the quantum transitions described above may induce an increase $\delta T \sim \hbar\omega$ in temperature. For a periodic change of parameters, the frequency $\omega$ is proportional to the ratio of the average acceleration $a$ to the average velocity $v$, so the increase in temperature is $\delta T \sim \hbar v/a$. It is similar with the Unruh temperature [2].

## 4. SOME SIMPLE APPLICATIONS

Let a particle of mass $m$ move in an infinite square potential well in one dimension. The eigenfunctions are $\varphi_n(x) = \sqrt{2/a}\sin(\pi nx/a)$ and the energy eigenvalues are given by $E_n = \pi^2\hbar^2 n^2/2ma^2$, where $n = 1, 2, \ldots$. The width $a$ of this potential well is taken as parameter $R$. The wall of the potential well, placed at distance $a$ from the origin, is subjected to an oscillatory motion of frequency $\omega$ as described by $a = a_0 + \varepsilon\cos\omega t$, where $\varepsilon/a_0 \ll 1$. Making use of (11), we get the transition probabilities $w_{kn} = 2\pi\hbar[\varepsilon\omega kn/a_0(k^2 - n^2)]^2\delta(E_k - E_n \pm \hbar\omega)$ per unit time in the limit of the infinite time. The diagonal matrix element $\gamma_{nn}$ is vanishing in this case, $\gamma_{nn} = 0$.

Following Berry [1], we consider a spin $\mathbf{S}$ placed in a magnetic field $\mathbf{B}$. The hamiltonian reads $H = -g\mu\mathbf{BS}$, where $g$ is the gyromagnetic factor and $\mu$ is the Bohr magneton. The energy eigenvalues are given by $E_n = -g\mu Bn$, where $n = -S, \ldots, S$. In order to calculate the matrix elements entering (11), it is convenient to use the identity $(E_n - E_k)(\varphi_k, \partial\varphi_n/\partial\mathbf{R}) = (\varphi_k, (\partial H/\partial\mathbf{R})\varphi_n)$ for $k \neq n$. We write then $\mathbf{BS} = B(S_x\sin\theta\cos\phi + S_y\sin\theta\sin\phi + S_z\cos\theta)$ and take the angles $\theta$ and $\phi$ as parameters $R$. First, we set $\phi = 0$ and let $\theta$ describe a circuit according to $\theta = \omega t$, where $\omega \ll g\mu B/\hbar$. Making use of (9), we get transition probabilities $w_{kn} = (\pi\hbar\omega^2/8)[S(S+1) - n(n\pm1)]\delta_{k,n\pm1}\delta(E_n - E_k \pm \hbar\omega)$ in the limit of the infinite time. Since $\omega \ll g\mu B/\hbar$, these transition probabilities are vanishing, in fact, as we get by using (11). We may also set $\theta = $ const and let $\phi = \omega t$ describe a conical circuit of semiangle $\theta$. The results are similar, the amplitudes containing now the factor $\sin\theta$.

Another example is provided by the electronic terms of the molecules, which depend parametrically on the nuclear coordinates $\mathbf{R}$. The interaction $H_1 = \mathbf{VP}$ can easily be estimated as $H_1 \sim (m/M)E_{\text{el}}$, where $E_{\text{el}}$ is a characteristic electronic term of the molecule and $m/M$ is the ratio of the

electron mass $m$ to the nuclear mass $M$. It is of the same order of magnitude as the accuracy of the adiabatic decoupling of the electronic motion from the nuclear motion, so it gives a natural width of the electronic terms in molecules.

## 5. NONINERTIAL MOTION TRANSLATIONS

A similar analysis can be carried out for noninertial motion. Let $\mathbf{r} = \mathbf{r}' + \mathbf{R}(t')$, $t = t'$, be a translation, where $\mathbf{r}$, $\mathbf{r}'$ denote the position of the system and $\mathbf{R}$ is the displacement vector. The hamiltonian, its eigenfunctions, and energy eigenvalues do not depend on the displacement $\mathbf{R}$, so it can be taken as the general parameter $\mathbf{R}$ in the previous sections. Schrodinger's (2) becomes

$$\frac{i\hbar \partial \psi(t', \mathbf{r}')}{\partial t'} = H(\mathbf{r}')\psi(t', \mathbf{r}') + \frac{i\hbar \mathbf{V} \partial \psi(t', r')}{\partial \mathbf{r}'}, \qquad (13)$$

where $\mathbf{V} = \dot{\mathbf{R}}$. The last term in the *rhs* of (13) can be viewed as an interaction $H_1 = -\mathbf{V}\mathbf{p}$, where $p = -i\hbar \partial/\partial \mathbf{r}'$ is the momentum associated to the coordinate $\mathbf{r}'$. The transition amplitudes are given by (11), where $\mathbf{P}$ is replaced by $\mathbf{p}$.

For a free particle, the transition amplitudes are vanishing since $\mathbf{p}_{kn} = 0$ for $k \neq n$. Similarly, for an ensemble of (in general interacting) particles, the momentum $\mathbf{p}$ is the total momentum, that is, the momentum of the center of mass of the ensemble, so there are no transitions as expected. The coefficient $a_{nn}(t)$ corresponds to a gauge transformation $\exp[i \int_0^t dt_1 \mathbf{V}(t_1)\mathbf{p}_{nn}]$ of the $n$-state, which, in general, has no determined energy (it is not a stationary state in general). For constant velocity $\mathbf{V} = \text{const}$, the phase of this gauge transformation is the first-order correction to the energy of the $n$-state. It is easy to check that the gauge transformation $\psi'(t, \mathbf{r}') = \exp[-(i/\hbar)(MV^2t/2 + M\mathbf{V}\mathbf{r})]\psi(t, \mathbf{r})$, where $M$ is the mass of the ensemble, preserves Schrodinger's equation in accordance with Galileo's principle of relativity. The unitary transformation $\psi = \exp(-i\mathbf{R}\mathbf{p}/\hbar)\psi'$ takes the Schrodinger equation $i\hbar \partial \psi/\partial t = H\psi$ into $i\hbar \partial \psi'/\partial t = H\psi - \mathbf{V}\mathbf{p}\psi' + \mathbf{R}(\partial H/\partial \mathbf{r})\psi' + \cdots$. Making use of $(\varphi_k, (\partial H/\partial \mathbf{r})\varphi_n) = (E_n - E_k)(\varphi_k, \partial \varphi_n/\partial \mathbf{r})$, one can show by direct calculation that the additional interacting term in the hamiltonian has no relevance. Such a unitary transformation is different from the coordinate change.

The situation is different for particles in an external field. There, in general, the offdiagonal matrix elements $\mathbf{p}_{kn}$ of the momentum of the particles are nonvanishing, and they may cause transitions. For instance, if one or more particles in an ensemble of interacting particles acquire a large mass, then they may be viewed as being at rest during the motion of the rest of particles. Their interaction with the rest of particles becomes now an external field for the latter, whose motion depends parametrically on the positions of the former. The coordinates of the heavy particles do not appear anymore in the momentum, so there may exist nonvanishing matrix elements of this momentum between states of the moving particles. It follows that noninertial motion may give rise to quantum transitions for particles in an external field.

## 6. NONINERTIAL MOTION ROTATIONS

A similar result holds also for rotations. Let $r_i = \alpha_{ij}(t')r_j$, $t = t'$, be a change of coordinates ($i, j = 1, 2, 3$), where $\alpha_{ij}$ is a rotation matrix of angle $\phi$ and angular velocity $\dot{\phi} = \mathbf{\Omega}$ about some axis, such that $r_i' = \alpha_{ji}(t)r_j$, $\alpha_{ji}\alpha_{jk} = \delta_{ik}$. Making use of $\alpha_{li}\dot{\alpha}_{lj} = \varepsilon_{ijk}\Omega_k$, where $\varepsilon_{ijk}$ is the totally antisymmetric unit tensor, we get easily that an interaction $H_1 = \mathbf{\Omega}\mathbf{l}$ appears in hamiltonian, similar with the interaction given by (13), where $\mathbf{l}$ is the total (orbital) angular momentum. The parameter $\mathbf{R}$ introduced in the previous sections is the rotation angle $\phi$ in this case. The discussion is similar with the one given above for translations. For a free particle, or an ensemble of interacting particles, the total angular momentum has no offdiagonal matrix elements. The coefficient $a_{nn}$ may generate a gauge transformation, which reflects, in general, the nonstationarity of the rotating state. For uniform rotations, that is, for $\mathbf{\Omega} = \text{const}$, the gauge transformation $\psi'(t, \mathbf{r}') = \exp[-(i/\hbar)(m\rho^2\Omega^2/2 - m\rho^2\Omega\phi/\hbar)]\psi(t, \mathbf{r})$, where $\rho$ is the distance of particles to the axis of rotation, leaves Schrodinger's equation unchanged, in accordance with its invariance under uniform rotations. In this gauge transformation, $m\rho^2$ denotes the total momentum of inertia $I$ and the first term in the phase is the kinetic energy $l^2/2I$.

For particles in an external field, the angular momentum may have nonvanishing offdiagonal matrix elements, so nonuniform (accelerated) rotations may induce quantum transitions.

## 7. CONCLUSION

The main conclusion of the results described herein is that noninertial motion may cause quantum transitions for systems in external fields governed by Schrodinger's equation. It follows that an observer who is set in noninertial motion may record such quantum transitions. Similar transitions may be caused by changes of parameters associated with Berry's phase. The acceleration of the change of coordinates or of parameters must be fast enough in order to match the excitation spectrum of the quantum system and have such transitions.

Similar problems appear also in the field theory. For similarities with quantization in gravitational fields, we refer to [3–8].

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