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Quantum transitions by change of parameters and in non-inertial motion

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Abstract

A quantum system may suffer transitions by varying parameters which, in the adiabatic limit, give the Berry phase. Similarly, non-inertial motion may cause quantum transitions for a system in an external field governed by Schrodinger's equation.

Key words: Berry phase, quantum transitions, non-inertial motion

Berry phase. Let the hamiltonian H, its (orthogonal) eigenfunctions φ_k and energy eigenvalues E_k depend on a parameter denoted generically by $\mathbf{R}$. This dependence in 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

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

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 equation (2) reads

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

where $\gamma_n(t)$ is given by

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

For a circuit C described by the parameter $\mathbf{R}$, this is Berry's geometric phase γ_n (Berry 1985).

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

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

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

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

and

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

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, equation (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

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

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 γ_{kn} and energy eigenvalues in the exponential factor in (9) may be neglected. The transition amplitudes can then be written as

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

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

For a uniform change of parameters, *i.e.* 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 φ_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

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

The first term in the *rhs* of this equation corresponds to the change in the wavefunction 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 equation (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 ω, $\mathbf{V}(t) = \mathbf{V}e^{i\omega t} + c.c.$, 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 ω 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.[1]

A few examples. Let a particle of mass m moving 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 $n = 1, 2, ...$ 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 ω as described by $a = a_0 + \varepsilon\cos\omega t$, where $\varepsilon/a_0 \ll 1$. Making use of equation (11) we get the transition probabilities $w_{kn} = 2\pi\hbar\left[\varepsilon\omega kn/a_0(k^2-n^2)\right]^2\delta(E_k - E_n \pm \hbar\omega)$ per unit time, in the limit of the infinite time. The diagonal matrix element γ_{nn} is vanishing in this case, $\gamma_{nn} = 0$.

Following Berry (1984), 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 μ is the Bohr magneton. The energy eigenvalues are given by $E_n = -g\mu Bn$, where $n = -S, ...S$. In order to calculate the matrix elements entering equation (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 θ and ϕ as parameters R. First, we set $\phi = 0$ and let θ describe a circuit according to $\theta = \omega t$, where $\omega \ll g\mu B/\hbar$. Making use of equation (9) we get transition probabilities $w_{kn} = (\pi\hbar\omega^2/8)\left[S(S+1) - n(n\pm 1)\right]\delta_{k,n\pm 1}\delta(E_n - E_k \pm \hbar\omega)$, 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 equation (11). We may also set $\theta = const$ and let $\phi = \omega t$ describe a conical circuit of semiangle θ. The results are similar, the amplitudes containing now the factor $\sin\theta$.[2]

Translations. A similar analysis can be carried out for non-inertial motion. Let $\mathbf{r} = \mathbf{r}' + \mathbf{R}(t')$, $t = t'$ be a translation. In this case, the hamiltonian, its eigenfunctions and energy eigenvalues do not depend on the parameter $\mathbf{R}$. Schrodinger's equation (2) becomes

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

where $\mathbf{V} = \dot{\mathbf{R}}$. The last term in the *rhs* of equation (13) can be viewed as an interaction $H_1 = -\mathbf{Vp}$, where $p = -i\hbar\partial/\partial\mathbf{r}'$ is the momentum associated to the coordinate $\mathbf{r}'$. The transition amplitudes are given by equation (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, *i.e.* 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 not a determined energy (it is not a stationary state, in general). For constant velocity $\mathbf{V} = const$, 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

[1] 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 ω 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 (Unruh 1976).

[2] 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 $H_1 \sim (m/M)E_{el}$, where E_{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.

$\psi'(t,\mathbf{r}') = \exp[-(i/\hbar)(MV^2t/2 + M\mathbf{Vr})]\psi(t,\mathbf{r})$, where M is the mass of the ensemble, preserves Schrodinger's equation, in accordance with Galileo's principle of relativity.[3]

The situation is different for particles in an external field. There, in general, the off-diagonal matrix elements $\mathbf{p}_{kn}$ of the momentum of the particles are non-vanishing, 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 become now an external field for the latter, whose motion depend parametrically on the positions of the former. The coordinates of the heavy particles do not appear anymore in the momentum, so there may exist non-vanishing matrix elements of this momentum between states of the moving particles. It follows that non-inertial motion may give rise to quantum transitions for particles in an external field.

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 α_{ij} is a rotation matrix of angle ϕ 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 ε_{ijk} is the totally antisymmetric unit tensor, we get easily that an interaction $H_1 = \mathbf{\Omega l}$ appears in hamiltonian, similar with the interaction given by (13), where $\mathbf{l}$ is the total (orbital) angular momentum. 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 not off-diagonal matrix elements. The coefficient a_{nn} may generate a gauge transformation, which reflects, in general, the non-stationarity of the rotating state. For uniform rotations, *i.e.* for $\mathbf{\Omega} = const$, the gauge transformation $\psi'(t,\mathbf{r}') = \exp[-(i/\hbar)(m\rho^2\Omega^2/2 - m\rho^2\mathbf{\Omega}\phi/\hbar)]\psi(t,\mathbf{r})$, where ρ 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 non-vanishing off-diagonal matrix elements, so non-uniform (accelerated) rotations may induce quantum transitions.

Conclusion. The main conclusion of the results described herein is that non-inertial motion may cause quantum transitions for systems in external fields governed by Schrodinger's equation. It follows that an observer who is set in non-inertial 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.

The analysis can be extended to fields, with similar conclusions. For similarities with quantization in gravitational fields we refer to Cai&Papini (1991), Casini&Montemayor (1994), Singh (2005) and Singh&Mobed (2006).

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[3]The unitary transformation $\psi = \exp(-i\mathbf{Rp}/\hbar)\psi'$ takes the Schrodinger equation $i\hbar\partial\psi/\partial t = H\psi$ into $i\hbar\partial\psi'/\partial t = H\psi - \mathbf{Vp}\psi' + \mathbf{R}(\partial H/\partial\mathbf{r})\psi' + ...$ 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.

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