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Localization of two-level systems

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The quantum dynamics of the two-level system under a periodic external potential is mapped to the classical one of a charged particle moving in the harmonic-oscillator potential plus a magnetic field in a plane. The behavior of tunneling and localization is fully described by the radial trajectory of the particle. It is shown that localization may happen only if the radial trajectory is periodic. The possible period is an integral multiple of that of the external force. Three models are studied.

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Tunneling plays a central role in quantum mechanics [1]. Although localization, a complementary concept to tunneling, is extremely important in solid-state physics [2], it was not until the discovery of the coherent destruction of tunneling by Hänggi's group [3–6] that attention has been paid to the study of localization of a single particle in the double-well potential under a periodic acting field. Since this external control of tunneling will be practically valuable in many research fields such as laser physics, chemical reactions, etc. [7,8], a full understanding of tunneling and/or localization mechanisms is desired.

Both classical and quantum dynamics of a particle in a quartic double-well potential perturbed by a periodic monochromatic field have been investigated extensively [9]. Because this model is not analytically solvable, one often resorts to the numerical calculation that sometimes avoids physical insights. It was demonstrated [6,10] that a two-level system may also show localization if the parameters of the acting field are justified, which represents a common feature of the double-well system. The influence of an external periodic field on the two-level system has always been the focal subject in laser physics, and the main mathematical technique developed in the study, the Floquet theory [11], was used later to discover the localization for a double-well model in the deep quantum regime by Hänggi's group. It should be pointed out that the first report of the destruction of tunneling seems to be in the study of a two-level system plus a sinusoidal field; the transition probability from the lower-energy level to the higher one is strongly decreased if suitable field parameters are chosen [12]. This observation was overlooked then.

In this Rapid Communication, on the one hand, we shall map quantum dynamics of the two-level system under the periodic acting field to a classical one. In other words, we will show that the time evolution of the system can be described by a classical equation of motion of a charged particle in two fields simultaneously. One of the fields is time independent and the other is periodic. The periodic field can be recognized as a magnetic one. The particle moves in a plane. Its distance to the origin represents the extent of one specified state in the state at that moment. Thus, tunneling or localization is obviously shown in the trajectory of the particle. On the other hand, the system can be viewed as a classical, linear dynamical system of two variables; thus we can obtain information of tunneling from the study of stability.

The Hamiltonian of the two-level system in the external periodic potential is

$$\hat{H}=-(\Delta_0/2)(|1\rangle\langle 1|-|2\rangle\langle 2|)+V(t)(|1\rangle\langle 2|+|2\rangle\langle 1|)\ , \tag{1}$$

where Δ_0 is the energy splitting between the states $|1\rangle$ and $|2\rangle$, and $V(T+t)=V(t)$, a periodic function of time.

Define the left state and the right state, respectively, as

$$|l\rangle\equiv(|1\rangle+|2\rangle)/\sqrt{2}$$

and

$$|r\rangle\equiv(|1\rangle-|2\rangle)/\sqrt{2}\ .$$

The wave function $|\Psi(t)\rangle$ can be expanded in the basis $(|l\rangle,|r\rangle)$. Denote

$$|\Psi(t)\rangle=c_l(t)|l\rangle+c_r(t)|r\rangle\ . \tag{2}$$

Then $\mathbf{C}\equiv(c_l(t),c_r(t))^T$ satisfy the equation of motion

$$\dot{\mathbf{C}}=\mathbf{MC}\ , \tag{3}$$

where

$$\mathbf{M}=\begin{bmatrix}-iV(t) & i\Delta_0/2\\ i\Delta_0/2 & iV(t)\end{bmatrix}.$$

Note that $c_l(t)$ and $c_r(t)$ are complex. We introduce two pairs of real functions of time (γ,θ) and (ρ,ϕ). Applying the following variable transformations

$$c_l(t)=\gamma(t)\exp\left[i\theta(t)-i\int^t V(t)dt\right]\ ,$$

$$c_r(t)=\rho(t)\exp\left[i\phi(t)+i\int^t V(t)dt\right]$$

and the normalization condition

$$|c_l(t)|^2+|c_r(t)|^2=1\ ,$$

we obtain

$$(\dot{\gamma})^2+\gamma^2(\dot{\theta})^2+\frac{\Delta_0^2}{4}\gamma^2=\frac{\Delta_0^2}{4}\ , \tag{4}$$

$$(\dot{\rho})^2+\rho^2(\dot{\phi})^2+\frac{\Delta_0^2}{4}\rho^2=\frac{\Delta_0^2}{4}\ , \tag{5}$$

and

$$\ddot{\gamma}+2i\dot{\gamma}\dot{\theta}-\gamma(\dot{\theta})^2+i\gamma\ddot{\theta}-2iV(t)(\dot{\gamma}+i\gamma\dot{\theta})+\frac{\Delta_0^2}{4}\gamma=0\ , \tag{6}$$

$$\ddot{\rho}+2i\dot{\rho}\dot{\phi}-\rho(\dot{\theta})^2+i\rho\ddot{\phi}+2iV(t)(\dot{\rho}+i\rho\dot{\phi})+\frac{\Delta_0^2}{4}\rho=0\ . \tag{7}$$

These equations can be interpreted by the terminology in classical mechanics. In fact, if we define

$$\mathbf{R}_l\equiv\gamma\mathbf{e}_\gamma,\quad V_l\equiv\dot{\mathbf{R}}_l=\dot{\gamma}\mathbf{e}_\gamma+\gamma\dot{\theta}\mathbf{e}_\theta\ ,$$

$$\mathbf{R}_r\equiv\rho\mathbf{e}_\rho,\quad \mathbf{V}_r\equiv\dot{\mathbf{R}}_r=\dot{\rho}\mathbf{e}_\rho+\rho\dot{\phi}\mathbf{e}_\phi\ ,$$

where $(\mathbf{e}_\gamma,\mathbf{e}_\theta)$ and $(\mathbf{e}_\rho,\mathbf{e}_\phi)$ are the unit vectors of two two-dimensional (2D) spaces in the polar coordinate system, respectively, then Eqs. (6) and (7) are nothing but the Newtonian equations describing the dynamics of a particle experiencing a harmonic force in a magnetic field that is perpendicular to the plane formed by any pair of the two sets of unit vectors:

$$\frac{d\mathbf{V}_l}{dt}=-\frac{\Delta_0^2}{4}\gamma\mathbf{e}_\gamma-\mathbf{V}_l\wedge\mathbf{B}\ , \tag{8}$$

$$\frac{d\mathbf{V}_r}{dt}=-\frac{\Delta_0^2}{4}\rho\mathbf{e}_\rho+\mathbf{V}_r\wedge\mathbf{B}\ , \tag{9}$$

where $\mathbf{B}=2V(t)\mathbf{e}_z$. Thus the time evolution of $c_l(t)$ and $c_r(t)$ is equivalent to the classical movement of a charged particle in the harmonic-oscillator potential under a periodic acting magnetic field. As a consequence, Eqs. (4) and (5) are expressions of the conservation of energy. Since $|c_l(t)|^2=\gamma^2$ and $|c_r(t)|^2=\rho^2$, γ and ρ are the square roots of the probabilities for the system to be found in the left state and in the right state, respectively, it is required that $0\le\gamma\le1$ and $0\le\rho\le1$. It follows that *the motion of the particle is constrained to the interior of a unit circle in the same plane.* Moreover, a clear physical picture of tunneling can be taken from the trajectory of the motion: if the particle always runs in a narrow concentric ring within the unit circle, then the particle is localized; otherwise, it tunnels from one state to the other. Note that γ and ρ *contain* the same amount of information about the evolution of the system. To study the characteristic of tunneling, therefore, we only need to consider one trajectory of the particle, $\mathbf{R}_l(t)$ or $c_l(t)$, say.

The description of the two-level system above reminds us of the Feynman-Vernon-Hellwarth (FVH) [13] stratagem. By defining the Bloch vector in terms of the elements in the density matrix, they were able to transform the quantum dynamics to the precession of the Bloch vector (with unit length) around a moving pseudofield. The difference between FVH theory and our method lies in the fact that the former results in a 3D classical dynamics and the latter describes the dynamics in a 2D *configuration space* plus two additional momentum spaces which can be reduced to one when the conservation of energy is taken into account. Although the equation of motion in 2D configuration space is not simpler than that of FVH, a 2D picture appeals to one's intuition in some cases.

An important feature of the system under consideration is the *periodicity*. We scrutinize some properties concerning this property according to the Newtonian equation (8). Suppose $\mathbf{R}_l$ is a periodic solution of t with period $\mathcal{T}$. It is not difficult to show that the only possible values for $\mathcal{T}$ are nT $(n\in\mathbb{N})$. Furthermore, we can demonstrate that the dynamics must be periodic if the parameters of the magnetic field are appropriately matched. In fact, one can explicitly construct four special, independent solutions of (8). For instance, written in the Cartesian coordinates $(x,y),(\dot{x},\dot{y})$, these solutions $\mathbf{R}_l^{(i)}(t)$ $(i=1,2,3,4)$ may be chosen to satisfy the following initial conditions:

$$\mathbf{R}_l^{(1)}=(1,0),\quad \dot{\mathbf{R}}_l^{(1)}=(0,0),\quad \mathbf{R}_l^{(2)}=(0,1)\ ,$$

$$\dot{\mathbf{R}}_l^{(2)}=(0,0),\quad \mathbf{R}_l^{(3)}=(0,0),\dot{\mathbf{R}}_l^{(3)}=(\Delta_0/2,0)\ ,$$

$$\mathbf{R}_l^{(4)}=(0,0),\quad \dot{\mathbf{R}}_l^{(4)}=(0,\Delta_0/2)\ ,$$

respectively. We can verify that if one of the four solutions is periodic, then all four are periodic with the same period. Therefore, the periodic condition requires that one of the four independent solutions be periodic. Using the properties $V(t+T/2)=-V(T/2-t)$, $V(T/4+t)=V(T/4-t)$, one can figure out the periodic conditions more physically. For instance, if we want the period of the motion to be T, then it is necessary that $\dot{\gamma}(T/4)=0$ for the four special solutions mentioned above. In this case, γ reaches an extremity at $T/4$. From the continuity of classical movement, one can always realize this requirement if the parameters of the external field are carefully adjusted.

An extremely important question is: *What is the relation between localization and periodic movement?* A related problem is when the periodicity is a necessary condition for localization. Let us answer this question by considering Eq. (3) directly or by the direct method. We should stress that the periodicity of $c_l(t)$ is equivalent to that of $\mathbf{R}_l(t)$. Since $\mathrm{Tr}\mathbf{M}=0$, the time-advance mapping or propagator $\mathbf{A}$ over a single period $(0,T)$ is a 2D area-preserving one ($\det\mathbf{A}=1$) [14]. This conclusion does not depend on the form of $V(t)$. We suppose that the Hamiltonian of the studied system is invariant under the operation of $\hat{P}(V(t)\rightarrow -V(t),\ t\rightarrow t+T/2)$. Defining

$$\mathbf{A}(t){:}\mathbf{C}(t)=\mathbf{A}(t)\mathbf{C}(0)$$

for $0\le t<T$ and $\mathbf{A}=\mathbf{A}(T)$, we have

$$\mathbf{C}(nT+t)=\mathbf{A}(t)\,\mathbf{A}^n\mathbf{C}(0)\ . \tag{10}$$

It can be shown that

$$\mathbf{A}=\begin{bmatrix} a & -b+ic \\ b+ic & a \end{bmatrix}\ ,$$

where a, b, and c are real numbers determined by the system and $a^2+b^2+c^2=1$. Because $-2\leq \mathrm{Tr}\,\mathbf{A}=2a\leq 2$, *the dynamics of the system is strongly stable* [14]. In other words, the future behavior of the two-level model is insensitive to the initial condition. The power of $\mathbf{A}$ can be determined by the Caley-Hamilton theorem (see, e.g., [15]):

$$\mathbf{A}^{n-1}=P_{n-2}(a)\,\mathbf{A}-P_{n-3}(a)\mathbf{I}\ , \tag{11}$$

where P is the Chebyshev polynomial and $\mathbf{I}$ is the identity matrix. Take $\sigma\equiv\arccos a$, then $P_n=\sin[(n+1)\sigma]/\sin\sigma$.

For simplicity, we still assume that the initial state is $\mathbf{C}(0)-(1,0)^T$. Localization means $\mathbf{C}(nT+1)=([1-\delta(n,t)]e^{i\eta_1},\delta'(n,t)e^{i\eta_2})^T$, where $\delta(n,t),\delta'(n,t)\ll 1$ for any n. Using the Cayley-Hamilton theorem, we can prove that this will be *possible* only if $\mathbf{A}^m=\mathbf{I}$ for a finite integer m, i.e., for a periodic dynamics. In the following, three special forms of $V(t)$ will be treated either by tackling the Newtonian equation or the direct method.

Example 1. Suppose $V(t)=V_0$, $\mathbf{R}_l(0)=1$, and $\mathbf{R}_l(0)=0$. It is a trivial model for observing localization, since this model is something like an asymmetric double-well system. In this case, the generalized parity transformation $\hat{P}$ *does not* leave the Hamiltonian (1) invariant. This problem is easier to solve directly from Eq. (3) than from the Newtonian equations (8) and (9). However, more physical insight will be obtained if (8) and (9) are tackled. For instance, we want to know the minimum of $c_l(t),c_{l,\min}$ and at what time τ from the beginning this value is reached. Classical mechanics tells us that the change rate of angular momentum equals the torque provided by the magnetic field. The torque is $2V_0\gamma\dot{\gamma}\mathbf{e}_z$ and the angular momentum reads $\gamma_{\min}\mathbf{e}_\gamma\wedge\gamma_{\min}\dot{\theta}(\tau)\mathbf{e}_\theta$. Noticing that $\dot{\gamma}(\tau)=0$, we have from conservation of energy (4),

$$|\gamma_{\min}\dot{\theta}(\tau)|=\frac{\Delta_0}{2}\sqrt{1-\gamma_{\min}^2}\ . \tag{12}$$

Thus, we find

$$-\int_0^\tau 2V_0\dot{\gamma}\gamma\,dt=\frac{\Delta_0}{2}\sqrt{1-\gamma_{\min}^2}\ , \tag{13}$$

which leads to

$$\gamma_{\min}^2=\frac{4V_0^2}{4V_0^2+\Delta_0^2}\ .$$

Note that in general *it is not the motion of the particle, $\mathbf{R}_l(t)$, but $\gamma(t)$ that is periodic* (see Fig. 1). The period reads

$$\mathcal{T}=\frac{2\pi}{\sqrt{\Delta_0^2+4V_0^2}}\ .$$

γ takes the minimum value at the half period.

Example 2. Suppose

$$V(t)=\begin{cases}V_0 & \text{if } 0\leq t<T/2\\ -V_0 & \text{if } T/2\leq t<T\end{cases}$$

and $V(T+t)=V(t)$. $\hat{P}$ does leave the Hamiltonian (1) invariant in this case.

The solution of (3) in the nth period can be written as

$$\mathbf{C}(nT+t)=\begin{cases}\mathbf{A}_1(t)\,\mathbf{A}^n\mathbf{C}(0) & \text{if } 0\leq t<T/2\\ \mathbf{A}_2(t-T/2)\,\mathbf{A}_1(T/2)\,\mathbf{A}^n\mathbf{C}(0) & \text{if } T/2\leq t<T\ ,\end{cases}$$

where

$$\mathbf{A}_{1,2}(t)=\begin{bmatrix}\cos\omega t\mp i\alpha\sin\omega t & i\beta\sin\omega t\\ i\beta\sin\omega t & \cos\omega t\pm i\alpha\sin\omega t\end{bmatrix}$$

with $\alpha=2V_0/\sqrt{\Delta_0^2+4V_0^2}$, $\beta=(1+4V_0^2/\Delta_0^2)^{-1/2}$, and $\omega=\Delta_0/(2\beta)$, and

$$\mathbf{A}=\mathbf{A}_2(T/2)\,\mathbf{A}_1(T/2)=\begin{bmatrix}\cos^2\frac{\omega T}{2}+(\alpha^2-\beta^2)\sin^2\frac{\omega T}{2} & i\beta\sin\omega T-2\alpha\beta\sin^2\frac{\omega T}{2}\\ i\beta\sin\omega T+2\alpha\beta\sin^2\frac{\omega T}{2} & \cos^2\frac{\omega T}{2}+(\alpha^2-\beta^2)\sin^2\frac{\omega T}{2}\end{bmatrix}.$$

For a periodic solution, with nT being the period to come out, $\mathbf{A}$ should satisfy $\mathbf{A}^n=\mathbf{I}$ and $\mathbf{A}$, $\mathbf{A}^2$,..., $\mathbf{A}^{n-1}\neq\mathbf{I}$. This allows us to derive the following *periodic condition:*

$$\sin\left[\frac{T}{4}\sqrt{\Delta_0^2+4V_0^2}\right]=\sqrt{1+4V_0^2/\Delta_0^2}\sin\frac{\pi}{n}\ . \tag{14}$$

Let $n=1$. We find $T=4m\pi/\sqrt{\Delta_0^2+4V_0^2}$; m is an integer. Here *m determines the period of $\gamma(t)$, which equals $T/(2m)$* (see Fig. 2). The $\gamma(t)$ goes to its minimum $\gamma_{\min}^2=4V_0^2/(\Delta_0^2+4V_0^2)$ at $T/(4m)$.

An interesting fact is that *not every integer n is available to construct the period nT.* $2T$, for instance, should be removed from the set of possible periods which can be seen from (14). Obviously, if the strength parameter of the magnetic field V_0 is fixed, then $\sqrt{1+4V_0^2/\Delta_0^2}\sin(\pi/n)$ must not be larger than 1 for nT to be a period of $\mathbf{C}(t)$.

Example 3. Suppose $V(t)=V_0\sin\omega t$ and $\mathbf{C}(0)=(1,0)^T$. From the physical illustration above, we know that if V_0 and ω are properly chosen, one will find localization. In this case, ρ will always be small. Thus the first term on the right-hand side of (9) may be neglected. We solve (9) to obtain

$$\rho(t)=\tfrac{1}{2}\Delta_0\left|\int_0^t\exp\left[2i\frac{V_0}{\omega}\cos\omega t'\right]dt'\right|\ . \tag{15}$$

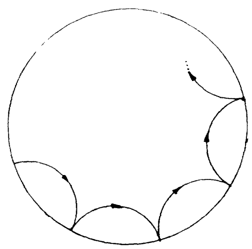

FIG. 1. The classical trajectory of a charged particle moving in a harmonic oscillator potential plus a perpendicular constant magnetic field in a plane. The particle starts at the edge of the unit circle and reaches again to the edge at multiple times of the period of $\gamma(t)$, $2\pi/\sqrt{\Delta_0^2+4V_0^2}$.

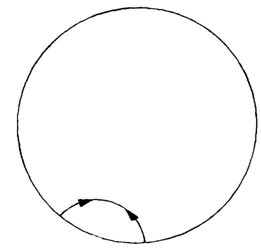

FIG. 2. The periodic classical trajectory dealing with example 2. Here the period is $4\pi/\sqrt{\Delta_0^2+4V_0^2}$, the same as the period of the external potential.

According to the discussion above, we know that $\mathbf{R}_r(t)$ must be periodic. In this case or more generally, if $V(t)$ is symmetric about $T/4$, then $\rho(t+T/2)=\rho(t)$ and $\gamma(t+T/2)=\gamma(t)$ and they reach their extremities at $T/4$. Suppose ρ possesses a period $nT/2$, then we have the periodic condition

$$\rho(nT/2)=\tfrac{1}{2}n\pi\frac{\Delta_0}{\omega}J_0(2V_0/\omega)$$
$$=0\ , \tag{16}$$

which is simplified as

$$J_0(2V_0/\omega)=0\ , \tag{17}$$

where J_0 is the zeroth-order Bessel function. This result is identical to that of the other approximation [10]. If we set V_0 and ω to the values according to the first root of (17), the maximum of ρ reads

$$\rho_{\max}^2=\rho^2(T/4)$$
$$=\frac{\Delta_0^2}{4\omega^2}\frac{\pi^2}{4}H_0^2(2V_0/\omega)\ , \tag{18}$$

where H_0 is the Struve function [16]. The minimum of γ is

$$\gamma_{\min}^2=1-\rho_{\max}^2\ . \tag{19}$$

The physical basis of our approximation, i.e., setting $\rho(t)\approx 0$ in (9) is obvious: compared to the magnetic force, the harmonic force acting on the particle is so small that its effect on the radial trajectory can be omitted. This physical picture can be used to evaluate the accuracy of the approximation. Since the harmonic force always pulls the particle to the origin, the approximate $\rho(t)$ is larger than the exact one. In other words, the particle moves in a narrower range than we estimated [see (19)]. It should be pointed out that for $\rho(t)$ there is only *one possible period in this case,* i.e., $T/2$.

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