Localization conditions for two-level systems

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Abstract

The dynamics of two-level systems in an external periodic field are investigated in general. The necessary conditions of localization are obtained through analysing the time-evolving matrix. It is found that localization is possible if not only is the dynamics of the system periodic, but also its period is the same as that of the external potential. A model system in a periodic $\delta$-function potential is studied thoroughly.

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Tunneling and localization play a central role in quantum mechanics [1]. They are the two aspects of one quantum phenomenon. The two concepts are extremely important in solid state physics [2]. The great achievements of Anderson et al. are focused on the localization of electrons while much progress on resonant tunneling has been made since Esaki’s group proposed the model of superlattice [3, 4]. It is not until the discovery of the coherent destruction of tunneling by Hänggi’s group [3, 5, 6, 7, 8] 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 reaction, macroscopic quantum mechanics etc [3, 11, 12, 13], we need more knowledge about this type of localization or the suppression of tunneling.

To study the localization, the most popular model is a quartic double-well system perturbed by a periodic monochromatic field. Such a model has been investigated extensively using the Floquet theory [14, 15]. Because it is not analytically solvable, one often recourses to the numerical calculation that sometimes avoids physical insights. Recently it has been demonstrated [5, 16, 17] that a two-level system shows localization if the parameters of the acting field are adjusted, which represents a common feature of the double-well system. In a recent paper [17] it is shown that the quantum dynamics of the two-level system under a periodic external potential can be mapped to the classical one of a charged particle moving in the harmonic oscillator potential plus an magnetic field in a plane. The behavior of tunneling and localization is fully described by the radial trajectory of the particle. This gives us an interesting physical picture although the difficulties of mathematical treatments are not lessened at all.

In this letter, we shall consider the dynamical behavior of two-level systems in the external periodic field which is antisymmetric with respect to time in one period. Although the dynamics has been generally discussed through time-advancing matrix in [17] there are still some features unexplored. By the same procedure we will study the evolution of the particle in the two states and give the necessary condition of localization. We will also derive the explicit results when the external field is a periodic $\delta$-function potential.

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

$$\hat{H} = -(\Delta_0/2)(|1> <1| - |2> <2|) + V(t)(|1> <2| + |2> <1|),$$

where $\Delta_0$ is the energy splitting between the states $|1>$ and $|2>$, $V(t)$ is the coupling between them induced by the external periodic driving force, and

$$V(T + t) = V(t), V(t) = -V(t + T/2),$$
with $T$ being the period of the external field. We call $V(t)$ a *generalized-parity* potential.

Define the left state and the right state as, respectively

$$|l > = (|1 > + |2 >)/\sqrt{2},$$

and

$$|r > = (|1 > - |2 >)/\sqrt{2}.$$  

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

$$|\Psi(t) > = c_l(t)|l > + c_r(t)|r >.$$  

Then $C = (c_l(t), c_r(t))^T$ satisfy the equation of motion:

$$\dot{C} = MC,$$

where

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

Since $\text{Tr}M = 0$, the time-advancing mapping or propagator $A$ over a single period is a 2D area-preserving one ($\det A = 1$) [18]. Apparently this conclusion does not depend on the form of $V(t)$.

Defining

$$A(t) : C(t) = A(t)C(0)$$

for $0 \leq t < T$ and $A \equiv A(T)$, we have

$$C(nT + t) = A(t)A^nC(0).$$

Consider three states $C(0)$, $C(T/2)$ and $C(T)$ at three times $0, T/2$ and $T$ respectively. The initial state $C(0)$ is arbitrary except that its components must satisfy the normalization condition, $|c_l(0)|^2 + |c_l(0)|^2 = 1$. We can write

$$C(T) = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} C(T/2),$$  

$$C(T/2) = \begin{pmatrix} p & q \\ s & t \end{pmatrix} C(0).$$

According to the normalization condition, the matrix elements should satisfy

$$|\alpha|^2 + |\beta|^2 = 1.$$
and

\[ |\gamma|^2 + |\delta|^2 = 1. \]  \hspace{1cm} (8)

Replacing \( t \) by \( -t \) in (3) and taking its complex conjugate we get

\[ \dot{C} = \begin{pmatrix} -iV(-t) & i\Delta_0/2 \\ i\Delta_0/2 & iV(-t) \end{pmatrix} C. \]  \hspace{1cm} (9)

Note that \( V(t) \) is antisymmetric with respect to \( t = T/2 \). If we move the origin \( t = 0 \) to \( t = T/2 \), then \( V(t) = -V(t) \). Inserting it into (9) and after some analysis one can easily find the following relations

\[ p = \alpha^*, \quad q = -\gamma^* \]
\[ s = -\beta^*, \quad t = \delta^*. \]

Thus, we have

\[ A = \begin{pmatrix} |\alpha|^2 - |\beta|^2 & \beta\delta^* - \alpha\gamma^* \\ \gamma\alpha^* - \delta\beta^* & |\delta|^2 - |\gamma|^2 \end{pmatrix}. \]  \hspace{1cm} (10)

Together with (3) and (7), we obtain

\[ A = \begin{pmatrix} a & -b + ic \\ b + ic & a \end{pmatrix}, \]

where \( a, b \) and \( c \) are real numbers determined by the system and \( a^2 + b^2 + c^2 = 1 \) from \( \det A = 1 \).

Because \( -2 \leq \text{Tr} A = 2a \leq 2 \), the dynamics of the system is strongly stable \[8\]. In other words, the future behavior of the two-level model is insensitive to the initial condition. Roughly speaking, localization means that the state of the system evolves near the initial state. To investigate the rule of localization, thus, we can choose any initial state as we like. But what we are interested in practice is related to the evolution of either the left state or the right one. Therefore, we suppose \( C(0) = (1, 0)^T \) in the following discussion. The state at the \( n \)th stroboscopic point \( nT \) is given by

\[ C(nT) = A^n C(0). \]  \hspace{1cm} (11)

The power of \( A \) can be determined by the Caley-Hamilton theorem (see, e.g. \[19\]):

\[ A^{n-1} = P_{n-2}(a) A - P_{n-3}(a) I, \]  \hspace{1cm} (12)

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

After a simple calculation we obtain the modulus of \( c_r(nT) \):

\[ |c_r(nT)| = |\sin(n\sigma)|. \]  \hspace{1cm} (13)
Localization requires that for any integer $n$ the probability of finding the system in the right state should be small, i.e., $|c_r(t)| \ll 1$. This is only a qualitative statement. Quantitatively, we define localization as $|c_r| < 1/2$ for all the time. As a necessary condition for localization, therefore, we must have $|c_r(nT)| = |\sin(n\sigma)| < 1/2$. Mathematically if

$$\sigma \neq \frac{Q\pi}{P}$$  \hspace{1cm} (14)

where $P$ and $Q$ are two mutually prime integers, then the set $\{\sin(n\sigma) : n \in \mathbb{N}\}$ is dense in the interval $[0, 1]$. In other words, for arbitrary $\sigma$ there must exist such an integer $n$ that $\sin(n\sigma)$ is very near to 1, as a consequence, localization is destroyed. To guarantee localization, thus it is needed

$$\sigma = \frac{Q\pi}{P}$$  \hspace{1cm} (15)

for some integers $P$ and $Q$, i.e., there must be a set of integers $m$ to satisfy

$$\sin(m\sigma) = 0.$$  \hspace{1cm} (16)

Suppose $m > 1$ and $m$ is the smallest one in the set. Thus $\sigma$ can be written as

$$\sigma = \frac{l\pi}{m},$$  \hspace{1cm} (17)

where $l$ and $m$ are mutually prime integers. If $m$ is even, then

$$\left|\sin\left(\frac{m\sigma}{2}\right)\right| = 1,$$  \hspace{1cm} (18)

which is forbidden for localization because $mT/2$ is also a stroboscopic point. If $m$ is odd, since $m$ and $l$ is mutually prime, there is an integer $n$ less than $m$ such that $\text{mod}(nl, m) = \frac{m-1}{2}$. Then we have

$$|\sin(n\sigma)|^2 = \left|\sin\left(\frac{(m-1)\pi}{2}\right)\right|^2 > \frac{1}{2}. $$  \hspace{1cm} (19)

Taking account of (18) and (19), we conclude that only if $m = 1$ localization may arise. Namely, we have proved that

**Theorem:** The necessary conditions for localization of two-level systems in external periodic fields are 1) its dynamics should be periodic; 2) the period should equal to that of the external fields. In mathematical language, these conditions are simply described as

$$\mathbf{A} = \pm \mathbf{I}.$$  \hspace{1cm} (20)

This result strengthens the conclusion in reference [17] in which only the first localization condition is given. Note that this observation was obtained by Großmann and
Hänggi in [8], using the Floquet approach. In the following, this theorem will be applied to the treatment of the periodic \( \delta \)-function potential or pulse acting on a two-level system.

The \( \delta \)-function potential is very important in physics because it is simply representing the most physical features of other acting potentials. We find that it is difficult to solve directly, and so we treat the \( \delta \)-function field as the limited case, \( \epsilon \to 0 \), of the rectangular potential or pulse, namely,

\[
V(t) = \begin{cases} 
0 & \text{if } 0 \leq t < T/4 - \epsilon \\
V_0/2\epsilon & \text{if } T/4 - \epsilon \leq t < T/4 + \epsilon \\
0 & \text{if } T/4 + \epsilon \leq t < 3T/4 - \epsilon \\
-V_0/2\epsilon & \text{if } 3T/4 - \epsilon \leq t < 3T/4 + \epsilon \\
0 & \text{if } 3T/4 + \epsilon \leq t < T 
\end{cases}
\]

and \( V(T + t) = V(t) \) (see Fig. 1). If we define the time-advancing matrix \( \mathcal{T} \) of one \( \delta \)-function potential \( V_0 \delta (t) \) as

\[
\mathbf{C}(0^+) = \mathcal{T} \mathbf{C}(0^-),
\]

we can derive

\[
\mathcal{T} = \begin{pmatrix} \exp(iV_0) & 0 \\ 0 & \exp(-iV_0) \end{pmatrix}.
\]

The time-advancing mapping \( \mathbf{A} \) turns out to be

\[
\mathbf{A} = \begin{pmatrix} 1 - 2 \sin^2 \frac{T\Delta_0}{4} \cos^2 V_0 & -\sin 2V_0 \sin \frac{T\Delta_0}{4} + i \sin \frac{T\Delta_0}{2} \cos^2 V_0 \\ \sin 2V_0 \sin \frac{T\Delta_0}{4} + i \sin \frac{T\Delta_0}{2} \cos^2 V_0 & 1 - 2 \sin^2 \frac{T\Delta_0}{4} \cos^2 V_0 \end{pmatrix}.
\]

From the definition of \( \sigma \) we have

\[
\cos \sigma = 1 - 2 \sin^2 \frac{T\Delta_0}{4} \cos^2 V_0.
\]

Using the theorem above, we find the necessary condition for localization as

\[
\sin \frac{T\Delta_0}{4} \cos V_0 = 0,
\]

or

\[
\begin{cases} 
\sin V_0 = 0, \\
\cos \frac{T\Delta_0}{4} = 0.
\end{cases}
\]

If this condition is satisfied, and if the system is localized in one single period, then localization will dominate the dynamics for the whole time. In order to find the sufficient condition for localization, therefore, we only need study the dynamical features over one
period. To this end, it is required that the modulus of $c_l$ be never less than a half in one period. This requirement imposes constraints on $V_0$ and $T$ respectively, i.e.,

$$\begin{cases} V_0 = (n + \frac{1}{2})\pi, \\ 0 \leq T\Delta_0 \leq 2\pi, \end{cases}$$  \tag{27}$$

where $n$ is an integer. This gives the sufficient conditions of localization for a two-level system in the periodic $\delta$-function field.

Returning to \cite{22}, we see clearly that the applying $\delta$-function pulse only brings about changes in the phases of the left and the right states. The former is increased by $V_0$ and the latter decreased by $V_0$. Since the evolution is strongly dependent on the difference of the two phases, we can always choose a series of appropriate $\delta$-function potentials to obtain localization. For example, let us apply a periodic potential consisting of a pair of $\delta$-function pulses with opposite signs in one period to a two-level system. The two pulses are assumed to take effect at one fourth period and three fourths period (see Fig. 2). Suppose the system is in the left state at the beginning. As shown above, if and only if the positive and the negative pulses have the same amplitudes, $|V_0| = (n + \frac{1}{2})\pi$ and the period $T$ is not larger than $2\pi/\Delta_0$, then the system is localized and the probability for the system to stay in the left state will not be less than $\rho_{t,\text{min}} = \cos^2(T\Delta_0/8)$. Noticing that $T \leq 2\pi/\Delta_0$, we find that $\rho_{t,\text{min}}$ is a monotonically decreasing function of $T$, which indicates that the smaller $T$ is, the larger $\rho_{t,\text{min}}$. In other words, we can realize strong localization by taking short-period $\delta$-function pulses. The varying of the probability according to time for different periods is illustrated in Fig. 3. It should be stressed that although the period of the dynamics is identical with that of the external field, the period of the evolution of the probability in the left state is a half. In fact, this is a common feature of the two-level system perturbed by any external potential possessing the generalized parity, which can be shown via symmetry analysis \cite{17}.

In conclusion, we have derived the necessary conditions for a two-level system driven by a periodic field to be localized: not only must the system evolve periodically, but also the period is identical with that of the external potential. The necessary conditions can always be satisfied by adjusting the period and the strength of the applying field. Under these conditions the system will get localized if and only if it is localized over one single period, which becomes possible through modifying the parameters of the external field. In the case of $\delta$-function pulses, the necessary and the sufficient conditions for localization are acquired analytically. In principle, any applying potential can be imitated approximately in terms of a series of $\delta$-function pulses, and so the general localization conditions can be investigated on the basis of the results from our $\delta$-function model. Besides, we expect that this simple theory can be employed to study the process of enantiomerization,
which is of much significance in understanding the origin of life.

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Captions of figures

Fig. 1 An applied field consisting of rectangular pulses. It becomes the δ-function field by taking the limit $\epsilon \to 0$.

Fig. 2 Schematic graph of applied δ-function pulses.

Fig. 3 Calculated probabilities in the left state versus time for three periods. Here the solid line corresponds to $T\Delta_0 = 4\pi/5$, the dot dashed line $T\Delta_0 = 4\pi/3$ and the dashed line $T\Delta_0 = 2\pi$. 

\[ V(t) \quad V(t) \]

\[ V(t) \quad V(t) \]

time (unit: \(2/\Delta_0\))

\[
\begin{array}{cccccc}
2T & T/2 & 0 & T/4 & 3T/4 & 2T & 0 & 2\epsilon & V_0/2\epsilon \\
\end{array}
\]

probability in the left state

\[ V(t) \quad -V_0 \]

time (unit: \(2/\Delta_0\))

\[
\begin{array}{cccccc}
T & T/2 & 0 & T/4 & 3T/4 & T & 0 & 2\epsilon & V_0/2\epsilon \\
\end{array}
\]