Higher-order adiabatic approximations for classical evolution

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(Received 26 May 1989)

The higher-order adiabatic approximation method of solving the Schrödinger equation for slowly transported quantum systems, which contains Berry's improved adiabatic theorem as its zeroth-order step, is generalized to solve evolution equations for a wide class of slowly transported classical systems. It is shown how the adiabatic condition is broken and transitions between different modes take place. Selection rules for such transitions are shown to be a topological property of the evolution path in parameter space.

I. INTRODUCTION

The geometrical phase factor found by Berry in his study of the quantum adiabatic theorem has attracted great attention among both theoretical and experimental physicists.[1-3]

Hannay and Berry have studied the analogous classical holonomy effect.[4,5] For more quantal systems that are transported less slowly, a few higher-order adiabatic approximation (HOAA) methods have been proposed.[6,7] In an earlier paper the author developed a formalism which provided a general method of solving the Schrödinger equation for slowly (not necessarily extremely slowly) transported systems.[8] By using it, one can calculate the evolution operator to any degree of accuracy, provided the eigenvalues and the eigenvectors of the slowly changing Hamiltonian are known. Its zeroth-order approximation gives Berry's improved quantal adiabatic theorem. The validity of this HOAA method is mathematically related to the hermiticity of the slowly changing Hamiltonian which appears in the Schrödinger equation. Therefore if a classical evolution equation can be reduced to the following form:

$$\frac{d}{dt}X(t)=A(t)X(t) , \tag{1}$$

where $X(t)$ is a vector and $A(t)$ is anti-Hermitian operator changing slowly with time, then the above HOAA method can be used to solve it. However, most classical evolution equations cannot be reduced to the form (1). In the following we will show that a wide class of classical evolution equations can be written as

$$\frac{d}{dt}X(t)=S(t)X(t) , \tag{2}$$

where $S(t)$ is a slowly changing matrix similar to an anti-Hermitian one, or equivalently, a slowly changing operator satisfying the following conditions.

(i) All its eigenvalues are purely imaginary.
(ii) Its eigenvectors span the whole space.

In this case, the above HOAA method applies with some modification being made.

II. CLASSICAL EVOLUTION EQUATIONS

Let us start by examining an undamped linear oscillating system with N degrees of freedom. Suppose the system is slowly transported. Its motion equation is

$$\frac{d}{dt}[M(t)\dot{Y}(t)]=-K(t)Y(t) , \tag{3}$$

where $Y(t)$ is the $N\times 1$ displacement vector, $M(t)$ is the $N\times N$ mass matrix, and $K(t)$ is the $N\times N$ rigidity matrix. $M(t)$ and $K(t)$ are both real symmetric positively definite matrices. Introducing the $N\times 1$ momentum vector

$$P(t)=M(t)\dot{Y}(t) , \tag{4}$$

we rewrite the motion equation as follows:

$$\frac{d}{dt}\begin{bmatrix}Y(t)\\P(t)\end{bmatrix}=\begin{bmatrix}0 & [M(t)]^{-1}\\-K(t) & 0\end{bmatrix}\begin{bmatrix}Y(t)\\P(t)\end{bmatrix} . \tag{5}$$

It is easy to prove that the $2N\times 2N$ matrix

$$\begin{bmatrix}0 & [M(t)]^{-1}\\-K(t) & 0\end{bmatrix}$$

is similar to an anti-Hermitian one, or equivalently, satisfies the above conditions (i) and (ii). From the eigenequation

$$\begin{bmatrix}0 & [M(t)]^{-1}\\-K(t) & 0\end{bmatrix}\begin{bmatrix}Y(t)\\P(t)\end{bmatrix}=\lambda(t)\begin{bmatrix}Y(t)\\P(t)\end{bmatrix} , \tag{6}$$

it follows that

$$[M(t)]^{1}P(t)=\lambda(t)Y(t) ,$$
$$-K(t)Y(t)=\lambda(t)P(t) .$$

Hence

$$\begin{aligned}&-K(t)Y(t)=\lambda^2(t)M(t)Y(t) ,\\&-Y(t)^{\dagger}K(t)Y(t)=\lambda^2(t)Y(t)^{\dagger}M(t)Y(t) .\end{aligned} \tag{7}$$

Considering that $K(t)$ and $M(t)$ are positive definite, we conclude that $\lambda^2(t)$ is real and negative. Therefore $\lambda(t)$ is purely imaginary. Now let us prove the completeness of

the eigenvector set. There exists a real symmetric positive definite $N\times N$ matrix $L(t)$ such that

$$[L(t)]^2=M(t) . \tag{8}$$

Equation (7) can be rewritten as follows:

$$-[L(t)]^{-1}K(t)[L(t)]^{-1}L(t)Y(t)=\lambda^2(t)L(t)Y(t) .$$

The $N\times N$ matrix $[L(t)]^{-1}\,K(t)[L(t)]^{-1}$ is real symmetric positive definite, so it has N real normalized eigenvectors orthogonal to each other:

$$Z_m^{\dagger}(t)Z_n(t)=\delta_{mn} ,$$

$$[L(t)]^{-1}K(t)[L(t)]^{-1}Z_n(t)=\omega_n^2(t)Z_n(t) ,$$

where eigenvalues $\omega_n^2(t)$ are positive real numbers. It can be seen that the N linearly independent vectors

$$[L(t)]^{-1}Z_n(t)\equiv Y_n(t)$$

satisfy Eq. (7),

$$K(t)Y_n(t)=\omega_n^2(t)M(t)Y_n(t) .$$

Let

$$P_n^{\dagger}(t)=\pm i\omega_n(t)M(t)Y_n(t) .$$

Direct calculation shows

$$\begin{bmatrix} 0 & [M(t)]^{-1} \\ -K(t) & 0 \end{bmatrix}\begin{bmatrix} Y_n(t) \\ P_n^{\pm}(t) \end{bmatrix}=\pm i\omega_n(t)\begin{bmatrix} Y_n(t) \\ P_n^{\pm}(t) \end{bmatrix} . \tag{9}$$

These $2N$ eigenvectors, each of which has $2N$ components, are linearly independent. In fact, suppose

$$\sum_{n=1}^{N}\left[a_n\begin{bmatrix} Y_n(t) \\ P_n^{\dagger}(t) \end{bmatrix}+b_n\begin{bmatrix} Y_n(t) \\ P_n^{-}(t) \end{bmatrix}\right]=0 .$$

This is a $2N\times 1$ matrix equality. The upper N components being zero requires that

$$a_n+b_n=0 \quad \text{for } n=1,2,\ldots,N ,$$

and the lower N components being zero requires that

$$a_n-b_n=0 \quad \text{for } n=1,2,\ldots,N ,$$

so that all the $2N$ coefficients a_n and b_n are zeros.

From the above typical example, one would be convinced that unlike the quantal case where the Schrödinger equations for all slowly transported systems have the form (2), not all the classical evolution equations for slowly transported classical systems can be reduced to the form (2). However, a wide class of classical evolution equations can be reduced to the form (2). Undamped linear oscillating systems with slowly changing parameters are met frequently in classical physics and engineering.

III. FORMALISM

Suppose the $S(t)$ in Eq. (2) depends on a set of real parameters $\{R_1,R_2,\ldots,R_F\}$ which vary with time slowly. Let T be a quantity of time dimension much greater than the natural oscillation periods of the system. Symbolically,

$$S=S(R_1,\ldots,R_F)=s(R) ,$$

$$R_q=R_q(t) \quad (q=1,\ldots,F) .$$

Let $\tau=t/T$. $dR_q/d\tau=T(dR_q/dt)$ are not very large. Suppose that the eigenequation of $S(R)$,

$$S(R)X_n(R)=i\omega_n(R)X_n(R)$$

is nondegenerate. We expand the $X(t)$ in Eq. (2) in terms of $X_n(R)$:

$$X(t)=\sum_n c_n(t)x_n(R(t))\exp\left[i\int_{t_0}^{t}\omega_n(t')dt'\right] .$$

Substituting the above expression into Eq. (2), we obtain

$$\sum_n \dot{c}_n(t)X_n(R(t))\exp\left[i\int_{t_0}^{t}\omega_n(t')dt'\right]$$
$$=-\sum_n c_n(t)\dot{X}_n(R(t))\exp\left[i\int_{t_0}^{t}\omega_n(t')dt'\right] .$$

Notice that the eigenvectors of $S(R)$ are not necessarily orthonormal, for $S(R)$ is not necessarily anti-Hermitian. We have to construct the dual basis $\{\tilde{X}_m(R)\}$, such that

$$\langle\tilde{x}_m(R),X_n(R)\rangle=\delta_{mn} .$$

Using the dual basis we get

$$\dot{c}_m(t)=\sum_n\langle\tilde{x}_m(R(t)),\dot{X}_n(R(t))\rangle$$
$$\times\exp\left[i\int_{t_0^t}\omega_{mn}(R(t'))dt'\right]c_n(t) ,$$

where

$$\omega_{mn}(R(t))=\omega_n(R(t))-\omega_m(R(t)) .$$

Changing to the new variable τ, we obtain

$$\frac{dc_m(\tau)}{d\tau}=\sum_n\left\langle\tilde{X}_m(R),\frac{d}{d\tau}X_n(R)\right\rangle$$
$$\times\exp\left[iT\int_{\tau_0}^{\tau}\omega_{mn}(\tau')d\tau'\right]c_n(\tau) , \tag{10}$$

or in the matrix form,

$$\frac{dC(\tau)}{d\tau}=K(\tau)C(\tau) , \tag{11}$$

where $K(\tau)$ is a matrix with elements

$$K_{mn}(\tau)=\left\langle\tilde{x}_m(R),\frac{d}{d\tau}X_n(R)\right\rangle\exp\left[iT\int_{\tau_0}^{\tau}\omega_{mn}(\tau')d\tau'\right] . \tag{12}$$

Now what we need to do is just to follow the same steps in (8). Divide $K(\tau)$ into two parts,

$$K(\tau)=d(\tau)+O(\tau) . \tag{13}$$

$D(\tau)$ is the diagonal part of $K(\tau)$, of which the elements do not oscillate, while $O(\tau)$ inherits the off-diagonal elements which oscillate. $O_{mn}(\tau)$ themselves are not necessarily small, but they give small integrals when being

multiplied by a nonresonant function of τ and integrated over a finite interval. Introducing the evolution operator $U(\tau,\tau_0)$, we have

$$\frac{dU(\tau,\tau_0)}{d\tau}=[D(\tau)+O(\tau)]U(\tau,\tau_0)\ ,$$

$$U(\tau_0,\tau_0)=1\ .$$

Expand $U(\tau,\tau_0)$ into a perturbation series

$$U(\tau,\tau_0)=U^{(0)}(\tau,\tau_0)+U^{(1)}(\tau,\tau_0)+\cdots +U^{(n)}(\tau,\tau_0)+\ldots\ , \tag{14}$$

where $U^{(n)}(\tau,\tau_0)$ stands for the processes containing n transitions between different energy levels. The results are

$$U^{(0)}(\tau,\tau_0)=\mathcal{T}\exp\left[\int_{\tau_0}^{\tau}D(\tau')d\tau'\right]\ , \tag{15}$$

where $\mathcal{T}$ stands for the chronological product, or

$$U^{(0)}_{mm}(\tau,\tau_0)=\exp\left[\int_{\tau_0}^{\tau}D_{mm}(\tau')d\tau'\right] \tag{16}$$

and

$$U^{(n)}(\tau,\tau_0)=\int_{\tau_0}^{\tau}d\tau' U^{(0)}(\tau,\tau')O(\tau')U^{(n-1)}(\tau',\tau_0)\ . \tag{17}$$

It is notable what when $S(R)$ is not anti-Hermitian, the $U(\tau,\tau_0)$ is not unitary. This does not cause any trouble. Because the $X(t)$ here is not a state vector, and we do not need probability conservation. In addition, an undamped oscillating system with changing parameters is no longer a closed and conservative system.

IV. VIBRATION OF A STRING

Let us study the vibration of a string with two slowly moving "fixed" ends at

$$x=b(t)\ ,$$

$$x=b(t)+a(t)\ .$$

Denote by $u(x,t)$ the displacement of point x at time t, and $\pi(x,t)$ the conjugate momentum density. The canonical motion equation is

$$\frac{d}{dt}\begin{bmatrix}u(x,t)\\ \pi(x,t)\end{bmatrix}=\begin{bmatrix}0 & \rho^{-1}(x,t)\\ \frac{\partial}{\partial x}E(x,t)\frac{\partial}{\partial x} & 0\end{bmatrix}\begin{bmatrix}u(x,t)\\ \pi(x,t)\end{bmatrix}\ ,$$

$$\text{for}\quad b(t)<x<b(t)+a(t)\ , \tag{18}$$

with

$$u(b(t),t)=u(b(t)+a(t),t)=0\ , \tag{19}$$

where $\rho(x,t)$ is the density and $E(x,t)$ Young's modulus. For simplicity we suppose that $\rho(x,t)$ and $E(x,t)$ are constants. Consider the eigenequation

$$\begin{bmatrix}0 & \rho^{-1}\\ \frac{\partial}{\partial x}E\frac{\partial}{\partial x} & 0\end{bmatrix}\begin{bmatrix}u(x,t)\\ \pi(x,t)\end{bmatrix}=\lambda(t)\begin{bmatrix}u(x,t)\\ \pi(x,t)\end{bmatrix}$$

$$\text{for}\ b(t)<x<b(t)+a(t)\ . \tag{20}$$

The eigenvalues and eigenvectors are

$$\lambda_n(t)=i\frac{n\pi v}{a(t)}=i\frac{n\pi}{a(t)}\left[\frac{E}{\rho}\right]^{1/2}\quad (n=\pm1,\pm2,\ldots)$$

and

$$X_n(x,t)=\begin{bmatrix}1\\ i\frac{n\pi}{a(t)}\sqrt{E\rho}\end{bmatrix}\sin\frac{n\pi[x-b(t)]}{a(t)}\ . \tag{21}$$

The dual basis is

$$\tilde{X}_m(x,t)=\begin{bmatrix}1/a(t)\\ \frac{i}{m\pi\sqrt{E\rho}}\end{bmatrix}\sin\frac{m\pi[x-b(t)]}{a(t)}$$

such that

$$\langle\tilde{X}_m(t),x_n(t)\rangle=\int_{b(t)}^{b(t)+a(t)}dx[\tilde{X}_m(x,t)]^{\dagger}X_n(x,t)=\delta_{mn}\ .$$

We have

$$\left\langle\tilde{X}_m(a,b),\frac{\partial}{\partial a}X_n(a,b)\right\rangle=\begin{cases}0 & \text{if } m=n,\\ \frac{-1}{2a} & \text{if } m=-n,\\ \frac{(-1)^{m+n}n}{(m-n)a} & \text{otherwise,}\end{cases} \tag{22}$$

and

$$\langle\tilde{x}_m(a,b),\frac{\partial}{\partial b}X_n(a,b)\rangle=\begin{cases}0 & \text{if } m-n\equiv0(\text{mod}2)\ ,\\ \frac{-2n}{(m-n)a} & \text{otherwise}\ .\end{cases} \tag{23}$$

Considering (12), (13), and (15), we conclude that in the case at hand

$$D(\tau)=0\ ,$$

and hence

$$U^{(0)}(\tau,\tau_0)=1\ .$$

The Berry phase factors here are all zeros. From (17) we see

$$U^{(1)}(\tau,\tau_0)=\int_{\tau_0}^{\tau}O(\tau')d\tau'\ . \tag{24}$$

Let us consider the following process:

$$a(t)=\begin{cases}a_0 & \text{if } t<0,\\ a_0(i+t/T) & \text{if } 0<t<T\ ,\\ 2a_0 & \text{if } T<t\ ,\end{cases}$$

$$b(t)=0\ .$$

We obtain

$$U^{(1)}_{-n,n}(\tau,0)=\frac{1-\left[\frac{1+\tau}{1+\tau_0}\right]^{iT2n\pi/a_0\sqrt{E/\rho}}}{iT(4n\pi/a_0)\sqrt{E/\rho}} ,$$

and for $|m|\neq|n|$,

$$U^{(1)}_{m,n}(\tau,0)=\left\{(-1)^{m+n}n\left[1-\left[\frac{1+\tau}{1+\tau_0}\right]^{iT[(n-m)\pi/a_0]\sqrt{E/\rho}}\right]\right\}\Big/\left[iT\frac{(n-m)^2}{a_0}\pi\left[\frac{E}{\rho}\right]^{1/2}\right] .$$

Suppose the initial condition is

$$X(0)=\begin{bmatrix}2\sin(\pi x/a_0)\\0\end{bmatrix}=X_1(a_0,0)-X_{-1}(a_0,0) .$$

Then at the zeroth-order approximation, we have

$$X(t)=X_1(a_0(1+\tau),0)e^{iT(\pi/a_0)\sqrt{E/\rho}\ln(1+\tau)}-X_{-1}(a_0(1+\tau),0)e^{-iT(\pi/a_0)\sqrt{E/\rho}\ln(1+\tau)} .$$

It shows that the system remains in the fundamental mode, when $T(1/a_0)\sqrt{E/\rho}\to\infty$. As $T(1/a_0\sqrt{E/\rho})$ becomes smaller (but still much greater than 1), we have to take account of the first-order approximation. Then the portion of the mth harmonic is given by

$$[U^{(1)}_{m1}(\tau,0)-U^{(1)}_{m-1}(\tau,0)]X_m(t)\exp\left[iT\frac{m\pi}{a_0}\left[\frac{E}{\rho}\right]^{1/2}\ln(1+\tau)\right]$$
$$+[U^{(1)}_{-m,1}(\tau,0)-U^{(1)}_{-m,-1}(\tau,0)]X_{-m}(t)\exp\left[-iT\frac{m\pi}{a_0}\left[\frac{E}{\rho}\right]^{1/2}\ln(1+\tau)\right] .$$

The two terms above are a complex conjugate to each other. They give a real sum

$$\begin{bmatrix}\frac{(-1)^{m+1}2a_0}{T\pi\sqrt{E/\rho}}\left[\frac{\sin\theta(m)-\sin\theta(1)}{(1-m)^2}+\frac{\sin\theta(m)+\sin\theta(1)}{(1+m)^2}\right]\\ \frac{(-1)^{m+1}2m\rho}{T(1+\tau)}\left[\frac{\cos\theta(m)-\cos\theta(1)}{(1-m)^2}+\frac{\cos\theta(m)+-\cos\theta(1)}{(1+m)^2}\right]\end{bmatrix}\sin\frac{m\pi(x-a_{0)}}{a_0(1+\tau)} , \tag{25}$$

where

$$\theta(m)=T\frac{m\pi}{a_0}\left[\frac{E}{\rho}\right]^{1/2}\ln(1+\tau) .$$

Let us consider another process:

$$a(t)=a_0,\quad b(t)=\begin{cases}0 & \text{if } t<0 ,\\ a_0t/T & \text{if } 0<t<T ,\\ a_0 & \text{if } T<t .\end{cases}$$

We have, for $m-n\equiv1(\text{mod }2)$,

$$U^{(1)}_{mn}(\tau,0)=-2n\left\{\exp\left[iT\frac{(n-m)\pi}{a_0}\left[\frac{E}{\rho}\right]^{1/2}\tau\right]-1\right\}\Big/\left[(m-n)iT\frac{(n-m)\pi}{a_0}\left[\frac{E}{\rho}\right]^{1/2}\right] , \tag{26}$$

and for $4m-n\equiv O(\text{mod }2)$,

$$U^{(1)}_{mn}(\tau,0)=0 .$$

Here we see a new kind of selection rule. When the representative point of the system moves slowly along a curve C in the parameter space, the transition from

eigenvibration n to eigenvibration $m(\neq n)$ cannot take place if the differential form

$$\sum_{\sigma}\left\langle \tilde{X}_m(R), \frac{\partial}{\partial R_\sigma} X_n(R)\right\rangle dR_\sigma = 0 \tag{27}$$

is zero on C. This selection rule is a topological property, which has nothing to do with the duration of the representative point on C, provided it moves slowly enough.

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