Hierarchical theory of quantum adiabatic evolution

Qi Zhang[1,2], Jiangbin Gong[3,4] and Biao Wu[1,5,6]

[1] Wilczek Quantum Center and College of Science, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China
[2] International Joint Research Laboratory for Quantum Functional Materials of Henan Province and School of Physics and Engineering Zhengzhou University, Henan 450001, People's Republic of China
[3] Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, 117542, Singapore
[4] NUS Graduate School for Integrative Sciences and Engineering, Singapore 117597, Singapore
[5] International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, People's Republic of China
[6] Collaborative Innovation Center of Quantum Matter, Beijing 100871, People's Republic of China
E-mail: wubiao@pku.edu.cn

Abstract

Quantum adiabatic evolution is a dynamical evolution of a quantum system under slow external driving. According to the quantum adiabatic theorem, no transitions occur between nondegenerate instantaneous energy eigenstates in such a dynamical evolution. However, this is true only when the driving rate is infinitesimally small. For a small nonzero driving rate, there are generally small transition probabilities between the energy eigenstates. We develop a classical mechanics framework to address the small deviations from the quantum adiabatic theorem order by order. A hierarchy of Hamiltonians is constructed iteratively with the zeroth-order Hamiltonian being determined by the original system Hamiltonian. The kth-order deviations are governed by a kth-order Hamiltonian, which depends on the time derivatives of the adiabatic parameters up to the kth-order. Two simple examples, the Landau–Zener model and a spin-1/2 particle in a rotating magnetic field, are used to illustrate our hierarchical theory. Our analysis also exposes a deep, previously unknown connection between classical adiabatic theory and quantum adiabatic theory.

1. Introduction

Quantum evolution under external adiabatic driving has been of fundamental interests to physicists. Born and Fock proved the quantum adiabatic theorem shortly after the discovery of the Schrödinger equation [1]. This theorem states that no transition occurs between instantaneous energy eigenstates in a system under adiabatic driving. However, this is only true when the external driving is infinitesimally slow. With a slow but finite external driving, there is generally small probability of transition between energy levels. There has been a great deal of effort to address this small deviation from the quantum adiabatic theorem [2–13]. Throughout the many studies on this issue, a controversy on the validity of the quantum adiabatic theorem arises [14–25]. With the success of the quantum adiabatic algorithm in quantum computing, this issue has also become important in a practical sense [26, 27]. It is hence important to make an effort towards a better assessment and control of the errors in quantum adiabatic computing.

In this work we present a theory to address the deviation from the quantum adiabatic theorem. Based on a classical mechanics framework, we construct iteratively a hierarchy of Hamiltonians with the zeroth-order Hamiltonian being determined by the original Hamiltonian. The deviations of the kth-order are the adiabatic invariants of the kth-order Hamiltonian while the adiabaticity of the kth-order Hamiltonian is determined by the time derivatives of the external parameters (denoted R) up to the kth-order. Within this theoretical framework, the deviations from the quantum adiabatic theorem can be computed to arbitrary order iteratively. The theory breaks down at the kth-order when the kth-order time derivative of the external parameters becomes relatively large. We use two simple examples, the Landau–Zener model and the spin-1/2 under a rotating magnetic field, to illustrate our hierarchical theory.

Our hierarchical theory establishes an intuitive picture for quantum adiabatic evolution. At the zeroth-order, the adiabatic evolution is a smooth curve of instantaneous eigenstates in the projective Hilbert space where the overall phase is removed. We call the smooth curve adiabatic trajectory (see figure 1). At the first order, this adiabatic trajectory is shifted by a small amount that is proportional to the first-order time derivative of external parameters ($\dot{R} = dR/dt$). At the second order, the adiabatic trajectory is shifted again by a small amount that is proportional to $\dot{R}^2$ or other possible second-order small parameters, such as $\ddot{R}$. Predicting and understanding such type of net shift of a certain order from perfect adiabatic following is one noteworthy feature of our theory. A schematic picture is presented in figure 1. Depending on the explicit time dependence of R, an actual time evolving state may or may not have small oscillations around a trajectory that is systematically shifted from the idealized adiabatic trajectory.

Technically we take advantage of two facts to develop our theory. First, we use the superposition principle, which allows us to focus on the adiabatic evolution of each individual energy eigenstate. Second, we use the classical Hamiltonian formulation of the Schrödinger equation [28–30]. In this formalism, an energy eigenstate is mapped into an elliptic fixed point in the corresponding projective Hilbert space. Note that this classical formulation is purely mathematical and is *not* the traditional semiclassical limit $\hbar \to 0$. Our classical mechanics framework exposes a deep, previously unknown connection between classical adiabatic theory and the quantum adiabatic theory. The relation between classical adiabatic theory and the
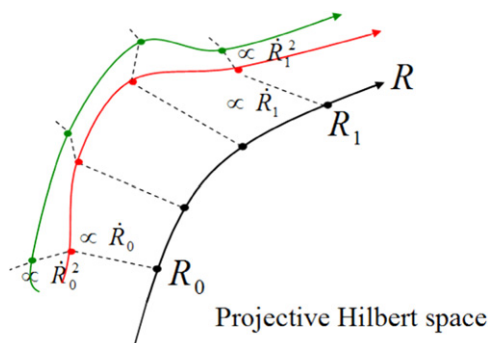
Figure 1. The adiabatic trajectories of different orders in the projective Hilbert space. The black line is for the zeroth-order, the red line for the first-order, and the green line for the second-order. The difference between the zeroth-order and the first-order trajectories is proportional to $\dot{R}$ while the difference between the first-order and the second-order trajectories is proportional to $\dot{R}^2$. The possible small oscillations around the adiabatic trajectories of the first and second orders are omitted for clarity.

quantum adiabatic theory was explored in [30] but not as deeply as in this work. In particular, a high-order deviation in the quantum adiabatic following still has a classical mechanics structure and may be still understood using classical adiabatic theory.

2. Classical Hamiltonian formulation of the Schrödinger equation

We consider a quantum system described by the Hamiltonian $\hat{H}_0(R)$, where $R = R(t)$ represents time-dependent parameters in an adiabatic protocol. As normally assumed for quantum adiabatic evolutions [1], $\hat{H}_0(R)$ has a discrete nondegenerate spectrum during the entire control protocol. Further, the rate of change in R is small as compared with the transition frequencies of the system. Deviations from the quantum adiabatic theorem are expected so long as the protocol is not executed in the mathematical limit $\dot{R} \to 0$. The aim of this work is to develop a general and systematic framework to quantitatively describe such deviations.

Though our consideration can be extended to cases with a Hilbert space of infinite dimensions, for convenience we assume $\hat{H}_0(R)$ lives in a finite n-dimensional Hilbert space. $\hat{H}_0(R)$ can thus be expressed as a R-dependent $n{\times}n$ Hermitian matrix. We find it mathematically more convenient to use the classical Hamiltonian formulation for the Schrödinger equation [28–30]. We express the quantum state with an n-component wavefunction $|\psi\rangle = (c_1, c_2, \ldots, c_n)^T$ and define $n - 1$ pairs of canonical variables

$$p_i = \arg(c_{i+1}) - \arg(c_1), \quad q_i = \left| c_{i+1} \right|^2, \tag{1}$$

with $i = 1, 2, \ldots, n - 1$. By construction, the Schrödinger equation then yields the following Hamilton's equations of motion,

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H_0(R)}{\partial q_i}, \frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial H_0(R)}{\partial p_i}, \tag{2}$$

where the classical Hamiltonian $H_0(R)$ is obtained from the quantum Hamiltonian $\hat{H}_0(R)$ as

$$H_0(R) = \langle \psi | \hat{H}_0(R) | \psi \rangle . \tag{3}$$

As the overall phase is removed, the phase space in this classical formalism is just the projective Hilbert space. This alternative formalism of the Schrödinger equation will allow us to exploit powerful and familiar tools in classical mechanics in our analysis. The overall phase of the wavefunction, or equivalently $\arg(c_1)$, is removed in equation (2) [28–30].

It is particularly interesting to look at eigenstates. In the original Schrödinger equation picture, an energy eigenstate of $\hat{H}_0(R)$ at a fixed R simply develops a trivial overall phase. Since the overall phase is discarded in our formalism, such an eigenstate evolution is mapped to a fixed point in the classical phase space of $H_0(R)$. The issue of the adiabatic following with the instantaneous energy eigenstates of $\hat{H}_0[R(t)]$ now becomes the issue of the adiabatic following with the instantaneous fixed points of $H_0[R(t)]$.

In principle, the time evolution emanating from an arbitrary initial state as a superposition of different energy eigenstates can be considered. However, the linearity of the original Schrödinger equation indicates that it suffices to study initial states that are energy eigenstates of $\hat{H}_0[R(0)]$ at $t = 0$. As such, in our classical formalism we only need to consider those initial conditions that are fixed points in the phase space.

One final technical comment is in order. The mapping from the wavefunction components c_i to phase space variables (p_i, q_i) [see equation (1)] becomes ambiguous when any one of the wavefunction component c_i becomes zero. Fortunately, this ambiguity can be easily overcome by adopting a different representation to re-express the wavefunction. For example, c_1 in equation (1) is used to remove the overall wavefunction phase. If $c_1 = 0$, one can always select another nonzero c_i to carry out a similar mapping.

3. First order deviations

As the generalization to arbitrary dimensions is straightforward, we consider a quantum system with a two-dimensional Hilbert space for the rest of the paper. With $n = 2$ the Hamilton's equations of motion in equation (2) only involve one pair of canonical variables q_1 and p_1. The phase space is hence also two-dimensional. For clarity we drop the subscript 1 hereafter. A R-dependent fixed point in the phase space is denoted as $[\bar{p}(R), \bar{q}(R)]$. There are two fixed points corresponding to two energy eigenstates of $\hat{H}_0(R)$.

According to the quantum adiabatic theorem, under a sufficiently slow protocol $R = R(t)$, the dynamics emanating from an energy eigenstate will follow the instantaneous energy eigenstates. With the removal of the overall phase, this dynamics is completely described by the smooth curve of instantaneous energy eigenstates in the projective Hilbert space. We shall call it adiabatic trajectory (see figure 1). However, in a realistic protocol where $R(t)$ changes slowly with a nonzero rate, there should be a deviation from this picture of perfect adiabatic following.

There have been studies on the small deviations from what the adiabatic theorem predicts. These were done in special classical systems and the small deviations were found to pollute the Hannay's angle [31–33]. Recently, the first-order deviation was studied in nonlinear quantum adiabatic evolutions [34, 35], where the result was used successfully to predict a new kind of geometric phase beyond the traditional Berry phase. As their focus was on the global effects of the deviations, detailed dynamics of the deviation was not considered. Our work conducts a

systematic study of the quantum adiabatic evolution and reveals its hierarchical structure. Our results can be easily generalized to classical systems and nonlinear quantum systems.

With possible deviations from the instantaneous fixed points $[\bar{q}(R), \bar{p}(R)]$, the actual adiabatic trajectory in the phase space can be written as

$$p(t) = \bar{p}[R(t)] + \delta p, \quad q(t) = \bar{q}[R(t)] + \delta q, \tag{4}$$

with $(\delta p, \delta q)$ being time-dependent deviations from the ideal adiabatic trajectory $[\bar{p}(R), \bar{q}(R)]$. This section is mainly to develop a theory to understand the behavior of $(\delta p, \delta q)$ to the first order of $\dot{R}$.

As a preparation we first consider the case when R is fixed. Using Hamilton's equations of motion and Taylor expanding $\frac{\partial H_0(R)}{\partial p}$ and $\frac{\partial H_0(R)}{\partial q}$ to the first order of $(\delta p, \delta q)$, we have

$$\begin{pmatrix} \dfrac{dp}{dt} \\ \dfrac{dq}{dt} \end{pmatrix} = \Gamma_0 \begin{pmatrix} \delta p \\ \delta q \end{pmatrix}, \tag{5}$$

where

$$\Gamma_0 = \begin{pmatrix} -\dfrac{\partial^2 H_0}{\partial q \partial p} & -\dfrac{\partial^2 H_0}{\partial q \partial q} \\ \dfrac{\partial^2 H_0}{\partial p \partial p} & \dfrac{\partial^2 H_0}{\partial p \partial q} \end{pmatrix}_{p=\bar{p}, q=\bar{q}} \tag{6}$$

is an R-dependent matrix obtained from the second-order derivatives of $H_0(R)$. The terms with first-order derivatives of $H_0(R)$ do not appear on the right-hand side of equation (5) simply because $[\bar{q}(R), \bar{p}(R)]$ is a fixed point. All higher-order terms are neglected here.

We now consider the dynamics of $(\delta q, \delta p)$ in the control protocol where $R = R(t)$ changes slowly with time. In this case, we have

$$\frac{dp}{dt} = \frac{\partial \bar{p}(R)}{\partial R} \dot{R} + \frac{d\delta p}{dt}$$

$$\frac{dq}{dt} = \frac{\partial \bar{q}(R)}{\partial R} \dot{R} + \frac{d\delta q}{dt}. \tag{7}$$

Equation (5) consequently becomes

$$\begin{pmatrix} \dfrac{d\delta p}{dt} \\ \dfrac{d\delta q}{dt} \end{pmatrix} = \Gamma_0(R) \left[\begin{pmatrix} \delta p \\ \delta q \end{pmatrix} - \Gamma_0^{-1}(R) \begin{pmatrix} \dfrac{\partial \bar{p}}{\partial R} \\ \dfrac{\partial \bar{q}}{\partial R} \end{pmatrix} \dot{R} \right]. \tag{8}$$

Two remarks are necessary for this equation of $(\delta p, \delta q)$. First, because it is already assumed that throughout the protocol $R = R(t)$ the studied energy eigenstates never become degenerate, the corresponding fixed points in the phase space do not vanish or collide. It is therefore legitimate to always associate the deviations with one fixed point so long as $(\delta p, \delta q)$ is

small. Second, it can be shown that the determinant $|\Gamma_0|$ does not vanish with nondegenerate energy eigenstates. Γ_0^{-1} in equation (8) hence exists for all R.

Remarkably, equation (8) possesses a canonical structure. The variables $(\delta p, \delta q)$ are a canonical pair and equation (8) can be derived from the following Hamiltonian

$$H_1\big(\delta p, \delta q; R, \dot{R}\big) = \frac{1}{2}\left(\frac{\partial^2 H_0}{\partial q^2}\right)_{\bar{p},\bar{q}} \big(\delta q - B_1\big)^2 + \left(\frac{\partial^2 H_0}{\partial q \partial p}\right)_{\bar{p},\bar{q}} \big(\delta q - B_1\big)\big(\delta p - A_1\big)$$
$$+ \frac{1}{2}\left(\frac{\partial^2 H_0}{\partial p^2}\right)_{\bar{p},\bar{q}} \big(\delta p - A_1\big)^2, \tag{9}$$

where $A_1 = A_1(R, \dot{R})$ and $B_1 = B_1(R, \dot{R})$ are defined as

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \Gamma_0^{-1}(R) \begin{pmatrix} \dfrac{\partial \bar{p}}{\partial R} \\ \dfrac{\partial \bar{q}}{\partial R} \end{pmatrix} \dot{R} . \tag{10}$$

This expression was previously obtained by Fu and Liu [34, 35]. It is clear that the first-order Hamiltonian (9) describes harmonic oscillations around the central point (A_1, B_1).

The first-order Hamiltonian H_1 generating the dynamics of $(\delta p, \delta q)$ depends upon two parameters $R(t)$ and $\dot{R}(t)$. We assume that $\dot{R}(t)$ also changes slowly with time. In this case, the dynamics of $(\delta p, \delta q)$ becomes the adiabatic evolution of H_1 and can be understood with the help of the classical adiabatic theorem. We define the action for $(\delta p, \delta q)$ as

$$I_1 = \frac{1}{2\pi} \oint \delta p \cdot d(\delta q). \tag{11}$$

This action is the adiabatic invariant possessed by H_1 [36]. (A_1, B_1) is the fixed point of H_1 with $I_1 = 0$. The dynamics of $(\delta p, \delta q)$ can be viewed as a spiral motion along the adiabatic trajectory specified by fixed point (A_1, B_1). The amplitude of the spiral oscillations is determined by the action I_1. With this analysis, it becomes clear that when both $R(t)$ and $\dot{R}(t)$ change slowly with time (A_1, B_1) describes an adiabatic trajectory shifted from the ideal trajectory of fixed point $[\bar{p}(R), \bar{q}(R)]$ as shown in figure 1.

We now consider two typical cases. In the first case, $\dot{R}$ is increased slowly from zero. In this case, as A_1 and B_1 are zero initially, the action I_1 is zero and the adiabatic evolution to the first order will follow exactly the adiabatic trajectory specified by (A_1, B_1). This is illustrated in figure 2(a). In the second case, the external driving rate $\dot{R}$ is finite and small at the beginning. This means that (A_1, B_1) is not zero initially and the action I_1 has a finite and small value. In this second case, the adiabatic evolution will become a spiral motion around the trajectory of (A_1, B_1) as shown in figure 2(b). This analysis of the second case in fact implies that infrequent sudden but small jump of $\dot{R}$ will not break down the adiabaticity of the evolution. Note that the smallness of the jump in $\dot{R}(t)$ is implicitly guaranteed by the slow change of $R(t)$. We mention it explicitly in our discussion just for clarity.

Our first-order adiabatic theory shows that a small quantum transition to other energy eigenstates always occurs with probability determined by $\dot{R}$. The probability is zero only in special cases where the coefficients in equation (10) vanish.
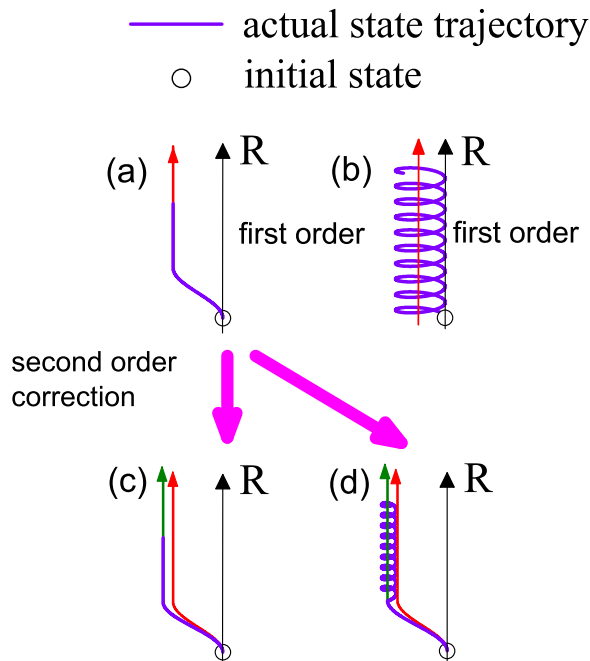
Figure 2. Adiabatic evolutions at first and second orders. The black line is the zeroth-order adiabatic trajectory, the red line the first-order adiabatic trajectory, and the dark green line is the second-order adiabatic trajectory. (a) The evolution follows the first-order adiabatic trajectory when the adiabatic manipulation is gradually launched (continuous increasing of $\dot{R}$ from zero); (b) it becomes a spiral oscillatory motion when the process is started with a finite $\dot{R}$. (c) The state follows the second-order adiabatic trajectory when $\ddot{R}$ is changed slowly from zero; (d) it becomes a spiral-like motion when $\ddot{R}$ is started with a finite value.

Our first-order theory offers a deep insight into the generic subtlety of how the adiabatic following breaks down. Let us consider a situation where $\dot{R}(t)$ is small but changes with a great rate, i.e. $\ddot{R}(t)$ is large. In this case, the dynamics governed by H_1 is not adiabatic; I_1 is not an adiabatic invariant and can not stay small for a long time. When the evolution is long enough, the dynamical evolution of the first-order deviations $(\delta p, \delta q)$ will no longer be bounded: the small deviations $(\delta p, \delta q)$ can accumulate and eventually be amplified to the zeroth-order level. This breakdown due to the largeness of $\ddot{R}(t)$ clearly depends on the detail of the protocol $R(t)$ and the Hamiltonian; general conclusions will be difficult to reach.

We note that our theory can be naturally extended to a Hilbert space of larger dimension $n > 2$, where the matrix Γ_0 becomes $2(n - 1) \times 2(n - 1)$ dimension and the first-order Hamiltonian has $(n - 1)$ pairs of canonical variables.

4. Second-order deviations

In the previous section we have found that the first-order correction $(\delta p, \delta q)$ evolves according to a first-order Hamiltonian H_1. It is natural to wonder whether we can find a similar Hamiltonian for the second-order deviations. We find that if the system follows the first-order adiabatic trajectory (see figure 2(a)), we can indeed find such a Hamiltonian. We write

$$p = \bar{p} + A_1 + \delta^2 p , \qquad q = \bar{q} + B_1 + \delta^2 q . \tag{12}$$

After substituting it into H_0 and with straightforward calculation, we obtain the second-order Hamiltonian

$$
\begin{aligned}
H_2\left(\delta^2 p, \delta^2 q; R, \dot{R}, \ddot{R}\right) = &\frac{1}{2}\left(\frac{\partial^2 H_0}{\partial q \partial q}\right)_{\bar{p}+A_1, \bar{q}+B_1} \left(\delta^2 q - B_2\right)^2 \\
&+ \left(\frac{\partial^2 H_0}{\partial q \partial p}\right)_{\bar{p}+A_1, \bar{q}+B_1} \left(\delta^2 q - B_2\right)\left(\delta^2 p - A_2\right) \\
&+ \frac{1}{2}\left(\frac{\partial^2 H_0}{\partial p \partial p}\right)_{\bar{p}+A_1, \bar{q}+B_1} \left(\delta^2 p - A_2\right)^2,
\end{aligned}
\tag{13}
$$

where

$$
\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \Gamma_0^{-1} \left[\begin{pmatrix} \dfrac{\partial A_1}{\partial R} \\[2mm] \dfrac{\partial B_1}{\partial R} \end{pmatrix} \dot{R} + \begin{pmatrix} \dfrac{\partial A_1}{\partial \dot{R}} \\[2mm] \dfrac{\partial B_1}{\partial \dot{R}} \end{pmatrix} \ddot{R} \right] - \frac{1}{2}\Gamma_0^{-1} \delta\Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}.
\tag{14}
$$

Here $\delta\Gamma$ is defined as

$$\delta\Gamma = \left(\frac{\partial \Gamma}{\partial p}\right)_{\bar{p},\bar{q}} A_1 + \left(\frac{\partial \Gamma}{\partial q}\right)_{\bar{p},\bar{q}} B_1 \tag{15}$$

with

$$
\Gamma \equiv \begin{pmatrix} -\dfrac{\partial^2 H_0}{\partial q \partial p} & -\dfrac{\partial^2 H_0}{\partial q \partial q} \\[3mm] \dfrac{\partial^2 H_0}{\partial p \partial p} & \dfrac{\partial^2 H_0}{\partial p \partial q} \end{pmatrix}.
\tag{16}
$$

The detailed derivation of this second-order Hamiltonian (13) can be found in appendix A along with some subtlety involved in the derivation.

The second-order Hamiltonian H_2 has a similar structure as H_1 and describes a generalized harmonic oscillator. The significant difference is that H_2 depends on three parameters $(R, \dot{R}, \ddot{R})$ while H_1 depends on only two parameters $(R, \dot{R})$. In the following, we conduct a similar analysis for H_2 as for H_1. We focus on the case where $\ddot{R}$, along with $R, \dot{R}$, changes slowly with time. In this case, the dynamics of the second-order deviation $(\delta^2 p, \delta^2 q)$ as governed by H_2 is adiabatic. We define the action for $(\delta^2 p, \delta^2 q)$ as

$$I_2 = \frac{1}{2\pi} \oint \delta^2 p \cdot d\left(\delta^2 q\right), \tag{17}$$

which is the adiabatic invariant possessed by H_2 [36]. (A_2, B_2) is the fixed point of H_2 with $I_2 = 0$. The dynamics of $(\delta^2 p, \delta^2 q)$ can be viewed as a spiral motion along the adiabatic trajectory specified by fixed point (A_2, B_2). The amplitude of the spiral oscillations is

determined by the action I_2. It is clear from this analysis that (A_2, B_2) describes an adiabatic trajectory shifted from the first-order one that is specified by $[\bar{p} + A_1, \bar{q} + B_1]$ (see figure 1).

We again consider two typical cases. (*i*) When both $\dot{R}$ and $\ddot{R}$ are started continuously from zero, I_2 is zero and the dynamics of $(\delta^2 p, \delta^2 q)$ follows exactly (A_2, B_2). This means that the state follows exactly the adiabatic trajectory deviating from original instantaneous eigenstate by $(A_1 + A_2, B_1 + B_2)$ (see figure 2(c)). (*ii*) When the system starts with a finite $\ddot{R}$, I_2 is nonzero and the system undergoes a spiral motion around (A_2, B_2) (see figure 2(d)). The amplitude of the spiral motion is determined by I_2.

We can continue this procedure and construct a *k*th-order Hamiltonian for the *k*th-order deviation. The result and the detailed derivation can be found in appendix B. A general feature is that the *k*th-order Hamiltonian will depend on $k + 1$ parameters, $R, \dot{R}, \ddot{R}, \cdots, \mathrm{d}^k R/\mathrm{d}t^k$, and the adiabaticity of its dynamics is controlled by these parameters. We note that a *k*th-order Hamiltonian can be constructed only when the dynamics of the deviations of order $(k - 1)$ follows the $(k - 1)$ th-order adiabatic trajectory (the scenarios illustrated in figures 2(a), (c)).

In brief, we have developed a hierarchical theory for quantum adiabatic evolution. In this theory, a hierarchy of Hamiltonians can be constructed: the *k*th-order deviation from quantum adiabatic theorem is governed by a *k*th-order Hamiltonian. This theory not only offers an explicit formula to compute the deviations of various orders but also presents an intuitive insight into the intricacy of adiabatic evolution. To illustrate the latter, we use the second-order Hamiltonian $H_2(R, \dot{R}, \ddot{R})$ as an example. We assume that $R, \dot{R}$ is small while $\ddot{R}$ is large. In this case the dynamics of the second-order deviation $(\delta^2 p, \delta^2 q)$ governed by H_2 is not adiabatic. As a result, the second-order deviation $(\delta^2 p, \delta^2 q)$ can grow, reach the first-order level, and continue to grow even bigger. The evolution of the first-order deviations is adiabatic due to the smallness of R and $\dot{R}$. However, this conclusion is only true when the deviation is small. If the second-order deviation grows so large that the deviation is no longer small, the adiabticity at the first-order level is then broken. Eventually, the growth starting from the second-order level can even break down the zeroth-order adiabaticity. This example suggests that the adiabatic evolution can be maintained for an arbitrarily long time only when all orders of time derivative of R are small. However, such growth of a high-order deviation to an appreciable quantity at a low-order level can take a long time scale beyond our practical interest. As the exact time scale needed for this growth depends on the detail of the control protocol $R(t)$, it can only be examined case by case. However, there are cases where a breakdown of adiabaticity at a higher order may not pass on to a lower level and then cause the breakdown of adiabaticity at the lower level.

In figure 3, we illustrate a specific case in which, for $(A_1, B_1) \neq (0, 0)$, the spiral-like motions are in tangency with the trajectory of the instantaneous eigenstate on both the starting and ending times of the adiabatic process. If the duration of the adiabatic process is precisely chosen such that the final state is just on the instantaneous eigenstate, then the adiabaticity is accidently restored, a situation different from the true adiabaticity maintained throughout the whole process. Because the adiabatic curve itself is derived within the first-order approximation, to the second-order accuracy the final state is not exactly on the instantaneous eigenstate (see point 1 in figure 3). On the other hand, if the duration T is chosen such that the final state is on point 2 (see figure 3), then the final state will deviate from the instantaneous eigenstate with a first-order deviation. For a higher-order case, e.g. $(A_1, B_1) = (0, 0)$ but $(A_2, B_2) \neq (0, 0)$ at the starting and ending times of the protocol, we will have an analogous
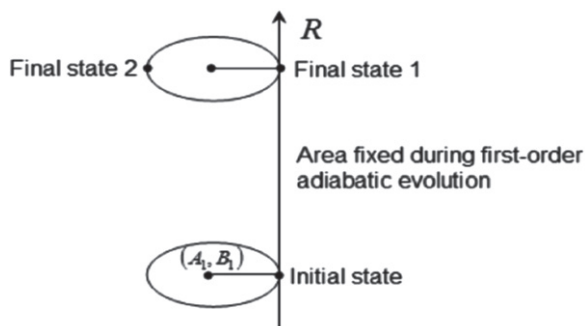
Figure 3. Illustration of initial and final states due to spiral-like motion, where the initial state is exactly the instantaneous eigenstate and, at the initial and final times, the spiral-like motions are all in tangency with the trajectory of the instantaneous eigenstate. The mean first-order deviations (A_1, B_1) are not zero on the starting and ending points of the adiabatic process and the area enclosed by orbit, or I_1, determined by (A_1, B_1) on the starting point is conserved according to the first-order adiabatic theory. The orbits here in the first-order approximation permit second-order errors.

situation. These qualitative insights are fully consistent with early results in [37] based on a different approach.

We can now also see the possibility of higher-order deviations not accumulating to a lower-order deviation from the perfect adiabatic following. Suppose we divide the whole protocol into many segments. If, at the end of each segment, the state rotates (with kth-order spiral-like motion when $(A_i, B_i) = (0, 0)$ for $i = 1, 2, \ldots k - 1$ but $(A_k, B_k) \neq (0, 0)$) back to the instantaneous eigenstate, then this kth-order deviation is unable to accumulate to the $(k - 1)$ th order. By contrast, if the state at the ending times of many segments always rotates away, say, to the farthest point from the instantaneous eigenstate, then the deviation can become larger and larger and eventually its value may accumulate to reach the $(k - 1)$th-order.

For the hierarchical expressions of adiabatic errors detailed in appendix B, we have assumed that the higher time derivatives of R possess a higher-order (and hence smaller) magnitude, e.g. the term proportional to $(\mathrm{d}^m R/\mathrm{d}t^m)^n$ belongs to the group of terms of $m \cdot n$-order. This grouping scheme, mainly for convenience, is intuitive and can be reasonable in a vast variety of adiabatic protocols. However, this order grouping scheme may be problematic in some protocols of $R(t)$. Consider, for example, the protocol $R = \sin(\epsilon t)$ with a small ϵ, then all the higher-order derivatives will be small, and $(\mathrm{d}^m R/\mathrm{d}t^m)^n \propto \epsilon^{mn}$ is indeed a $m \cdot n$-order term. However, for the protocol $R = \epsilon \sin(t)$ with a small ϵ, all orders of time derivatives of R, e.g. $\dot{R}, \ddot{R}, \ldots, \mathrm{d}^k R/\mathrm{d}t^k$, are of the same order of magnitude. As such, for this situation a term containing $(\mathrm{d}^m R/\mathrm{d}t^m)^n \propto \epsilon^n$ is of the n-order. On one hand, this is fully consistent with early observations that sometimes terms associated with higher-order derivatives of R can be important [37, 38]. On the other hand, it is clear now that the many terms arising from our hierarchical theory may not automatically be an expansion cast in terms of their orders of magnitude. To analyze the details we still need to make use of the explicit $R(t)$ to assess the actual importance (or weightage) of the many different terms emerging from our theory. In any case, we have learned from our classical mechanics framework that the dynamics of quantum adiabatic following can be digested in terms of adiabatic following of various orders occurring in parallel.

5. Two examples

We now use two simple systems to illustrate our hierarchical theory. One is a spin-1/2 particle in an external rotating magnetic field; the other is the Landau–Zener model. They are chosen because they are either exactly solvable or their numerical solutions can be found with great accuracy. In this way, there will be no ambiguity in checking the validity of our hierarchical theory. In this section, we always assume $\hbar = 1$.

5.1. Spin-1/2 particle under a rotating field

In the hierarchical theory, the first-order deviation and its dynamics is of the most importance. In this subsection, we employ the simple model of a spin-1/2 particle in a rotating magnetic field to illustrate the first-order adiabatic theory. The Hamiltonian for a spin-1/2 particle in an external rotating field is

$$\hat{H}_0 = \frac{1}{2}\begin{pmatrix} 0 & L\exp(-i\alpha) \\ L\exp(i\alpha) & 0 \end{pmatrix}, \tag{18}$$

where $\alpha(t)$ changes slowly with time for a rotating field. We use $|\psi\rangle = (c_1, c_2)^T$, where c_1 and c_2 are complex, to denote the quantum state of this spin-1/2 particle. We turn to the classical formulation by introducing a pair of conjugate variables, $p = \arg(c_2) - \arg(c_1)$ and $q = |c_2|^2$. The corresponding classical Hamiltonian is

$$H_0 = \langle\psi|\,\hat{H}_0\,|\psi\rangle = L\sqrt{q - q^2}\,\cos(\alpha - p). \tag{19}$$

The classical Hamiltonian in equation (19) has two elliptic fixed points, namely, $(\bar{q} = 1/2, \bar{p} = \alpha)$ and $(\bar{q} = 1/2, \bar{p} = \alpha + \pi)$, corresponding respectively to the two eigenstates of equation (18). We focus on the adiabatic following of the fixed point $\bar{q} = 1/2, \bar{p} = \alpha$ as α (rotating field) changes slowly. The conventional adiabatic theorem states that the actual state will accurately follow the instantaneous state $(\bar{q} = 1/2, \bar{p} = \alpha)$.

　　On top of the conventional adiabatic theorem, there are first-order corrections. To that end we now derive the effective first-order Hamiltonian H_1. According to equations (9), (10) and (19), one finds for fixed point $(q = 1/2, p = \alpha)$,

$$H_1 = -\frac{L}{2}\left[2\left(\delta q - \frac{\dot{\alpha}}{2L}\right)^2 + \frac{1}{2}(\delta p)^2 \right]. \tag{20}$$

Interestingly, for this example, H_1 happens to be independent of the adiabatic parameter α. The first-order fixed point is located at $A_1 = 0, B_1 = \dot{\alpha}/2L$. In the following we consider three different control protocols $\alpha(t)$ with $\alpha(0) = 0$ and the initial state emanating exactly from the fixed point $q(0) = 1/2, p(0) = \alpha$.

　　(*i*) Let us first consider the simplest protocol in which $\alpha = \omega t$ with ω being constant. At $t = 0$, the initial state is $q = 1/2, p = 0$ while the first-order fixed point is at $(A_1 = 0, B_1 = \omega/2L)$. So, the state starts off the first-order fixed point and the first-order action is
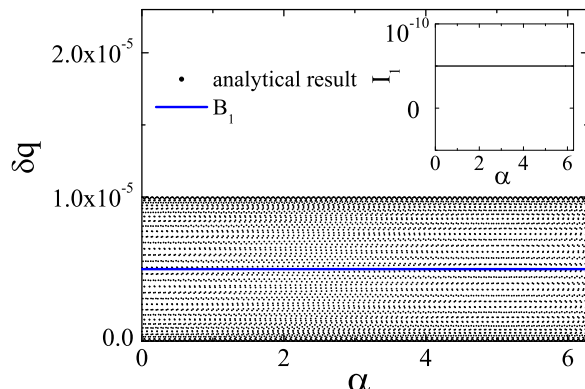
$$I_1 = \frac{\omega^2}{4L^2}. \tag{21}$$

Figure 4. The first-order solution of a spin-1/2 particle in a slowly rotating magnetic field. The dots are δq computed from the analytical solution to the first-order equation (22). The solid line is B_1 of the first-order fixed point. The inset shows the first-order action I_1 computed from the analytical solution equation (22). $\omega = 10^{-5}$.

According to our theory, the first-order deviation will undergo a spiral motion, similar to what is depicted in figure 2(b), with its amplitude determined by I_1.

The validity of our theory can be checked by directly integrating the Schrödinger equation governed by (18). This solution can be found exactly. With the omission of higher orders, the solution can be written as

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 - \dfrac{\omega}{2L}[1 - \cos{(Lt)}] \\ \left[1 + \dfrac{\omega}{2L}(1 - \cos{(Lt)})\right] e^{i\left[\omega t + \frac{\omega}{L}\sin(Lt)\right]} \end{pmatrix}. \tag{22}$$

This solution is plotted in figure 4 by mapping $|\psi\rangle$ to (p,q) and thus to $(\delta p, \delta q)$. In this figure, we clearly see oscillations around the fixed point ($A_1 = 0$, $B_1 = \omega/2L$), consistent with our first-order theory. As shown in the inset of this figure, our direct computation also confirms that the first-order action I_1 is a constant. We point out that this is equivalent to a system under the following control protocol

$$\alpha = 0 \quad \text{for} \quad t < 0\,; \quad \alpha = \omega t \quad \text{for} \quad t > 0\,. \tag{23}$$

That is, there can be a small sudden jump in $\dot{\alpha}$ at $t = 0$. Analytically, the first-order deviation can be readily computed from the solution (22)

$$\delta p = p - \bar{p} = \frac{\omega}{L}\sin{(Lt)},$$

$$\delta q = q - \bar{q} = \frac{\omega}{2L}(1 - \cos{(Lt)}), \tag{24}$$

which is indeed consistent with the first-order Hamiltonian dynamics predicted by H_1 in equation (20).

According to the mapping (1) between δp and δq and wavefunction, we can write down the adiabatic error during the whole adiabatic process in terms of the quantum state,

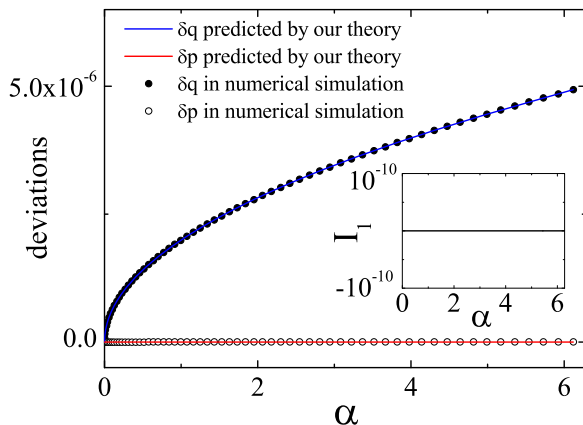**Figure 5.** Numerical results for the first-order correction $(\delta p, \delta q)$ obtained from the Hamilton's equation of motion governed by (19). The control protocol is $\alpha = \frac{1}{2}at^2$ with $a = 7.96 \times 10^{-12}$. The dots and circles are numerical results while the solid lines are for the first-order fixed point $(A_1 = 0, B_1 = at/2L)$. The inset shows the numerically computed I_1.

$$\text{Err} = 1 - \left| \left\langle \psi(\bar{p}, \bar{q}) | \psi(\bar{p} + \delta p, \bar{q} + \delta q) \right\rangle \right|^2 = \frac{\dot{\alpha}^2}{4L^2} \propto \dot{\alpha}^2, \tag{25}$$

which is consistent with an earlier result based on exact calculations [39].

(*ii*) In the second protocol, the speed $\dot{\alpha}$ increases gradually from zero. To be specific, we choose $\alpha = \frac{1}{2}at^2$ with $a = 7.96 \times 10^{-12}$. For this protocol, the first-order fixed point is $(A_1 = 0, B_1 = 0)$ at $t = 0$. Therefore, according to our first-order theory, the action $I_1 = 0$ and the dynamics of the first-order deviation $(\delta p, \delta q)$ follows exactly the first-order fixed point $(A_1 = 0, B_1 = at/2L)$. We have numerically solved the Hamilton's equations of motion governed by equation (19) for this second protocol. The numerical results for $(\delta p, \delta q)$ and I_1 are shown in figure 5 and an excellent agreement with our first-order theory is found.

(*iii*) In the third protocol, we change the sign of $\dot{\alpha}$ frequently while keeping $|\dot{\alpha}|$ small. This is to ensure that the second-order time derivative $\ddot{\alpha}$ can be quite large. We use this protocol to illustrate an insight offered by our hierarchical theory: a high-order time derivative of R can also lead to the breakdown of adiabaticity. For this spin-1/2 system, the smallness of $|\dot{\alpha}|$ does not guarantee the accuracy of the quantum adiabatic theorem. When $\ddot{\alpha}$ is large, then the first-order dynamics governed by H_1 is no longer adiabatic, and the accumulation of $(\delta p, \delta q)$ will eventually lead to the breakdown of adiabaticity at the zeroth orders. We have solved numerically the equations of motion governed by equation (19). The results are plotted in figure 6, where we see that δq can indeed grow and destroy the adiabaticity. The solid line seen in the middle of the pattern shown in figure 6 demonstrates that the action I_0 is no longer a constant.

5.2. Hierarchy of adiabatic corrections in the Landau–Zener model

In this subsection, we consider a different model, the Landau–Zener (LZ) model, and use it to demonstrate higher-order deviations. The LZ Hamiltonian can be written as
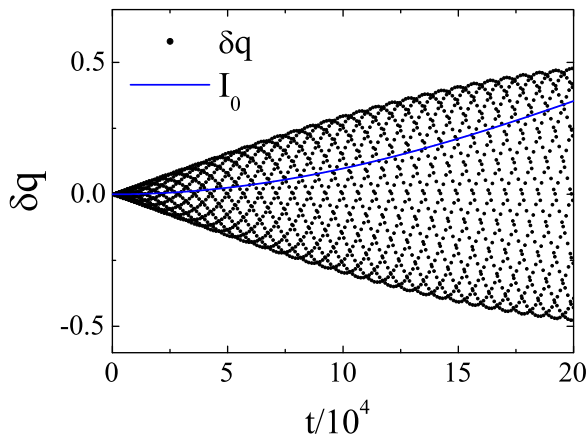
Figure 6. Numerical solution of δq and $I_0 = \frac{1}{2\pi} \oint p \cdot dq$ with Hamilton's equation of motion governed by (19). For the control protocol, we have $|\dot{\alpha}| = 10^{-5}$. The sign of $\dot{\alpha}$ oscillates with the frequency $\nu = 1$.

$$\hat{H}_0^{\mathrm{LZ}} = \frac{1}{2}\begin{pmatrix} z & x \\ x & -z \end{pmatrix}, \tag{26}$$

where the coupling term $x > 0$ is a constant whereas z changes slowly and linearly from $-Z_0$ to Z_0,

$$z = Vt, \qquad t: -Z_0/V \to Z_0/V. \tag{27}$$

Similarly, we define $c_1 = |c_1|e^{i\phi_1}$, $c_2 = |c_2|e^{i\phi_2}$, $p = \phi_{c_2} - \phi_{c_1}$, and $q = |c_2|^2$, and obtain the classical Hamiltonian (drop a constant):

$$H_0 = \langle \psi | \hat{H}_0^{\mathrm{LZ}} | \psi \rangle = x\sqrt{q - q^2} \cos (p) - zq. \tag{28}$$

This classical Hamiltonian has two fixed points at $(\bar{p} = 0, \bar{q} = \frac{1}{2} - \frac{z}{2\sqrt{x^2 + z^2}})$ and $(\bar{p} = \pi, \bar{q} = \frac{1}{2} + \frac{z}{2\sqrt{x^2 + z^2}})$. Without loss of generality, we focus on the fixed point $(\bar{p} = \pi, \bar{q} = \frac{1}{2} + \frac{z}{2\sqrt{x^2 + z^2}})$, which corresponds to the eigenstate with the lower energy. According to the quantum adiabatic theorem, i.e. zeroth-order theory, when the initial state is the ground state $\left[\cos \left(\frac{\arctan (x/Z_0)}{2}\right), -\sin \left(\frac{\arctan (x/Z_0)}{2}\right) \right]^T$ at $z = -Z_0$ the system will follow the instantaneous eigenstate and ultimately reach $\left[-\sin \left(\frac{\arctan (x/Z_0)}{2}\right), \cos \left(\frac{\arctan (x/Z_0)}{2}\right) \right]^T$ at $z = Z_0$. In what follows, we will compute explicitly the first-order deviation and the second-order deviation, and discuss some general properties of the higher-order deviations.

According to equations (9) and (28), the first-order Hamiltonian H_1 reads

$$H_1 = \sqrt{x^2 + z^2}\left(1 + \frac{z^2}{x^2}\right)(\delta q)^2 + \frac{1}{4}x^2 \frac{\left(\delta p - \frac{V}{x^2 + z^2}\right)^2}{\sqrt{x^2 + z^2}}. \tag{29}$$

The fixed point for the first-order deviation $(\delta p, \delta q)$ (or the first-order deviation from the zeroth-order adiabatic trajectory) is

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} \dfrac{V}{x^2 + z^2} \\ 0 \end{pmatrix}. \tag{30}$$

The results for the second-order deviation $(\delta^2 p, \delta^2 q)$ can be computed similarly. The second-order Hamiltonian is

$$H_2 = \sqrt{x^2 + z^2} \left(1 + \frac{z^2}{x^2} \right) \left(\delta^2 q - \frac{5x^2 z V^2}{4\left(x^2 + z^2\right)^{7/2}} \right)^2$$

$$- \frac{zV}{x^2 + z^2} \left(\delta^2 q - \frac{5x^2 z V^2}{4\left(x^2 + z^2\right)^{7/2}} \right) \delta^2 p + \frac{1}{4} x^2 \frac{\left(\delta^2 p\right)^2}{\sqrt{x^2 + z^2}}. \tag{31}$$

The fixed point (or, the deviation from the first-order adiabatic trajectory) is

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} 0 \\ \dfrac{5x^2 z V^2}{4\left(x^2 + z^2\right)^{7/2}} \end{pmatrix}; \tag{}$$

We consider the limit $Z_0 \to \infty$. At this limit, we have $A_1 = B_1 = A_2 = B_2 = 0$ at $|z| = \infty$. This means that the deviations of the first-order and the second-order are zero both at the beginning and at the end of the evolution. The higher-order deviations can also be computed with the formula in appendix B. There is no need to write them down here. We only want to mention, for all these higher-order deviations, we also have

$$A_k \to 0; \quad B_k \to 0, \quad \text{as} \quad |z| \to \infty. \tag{32}$$

This indicates that the LZ tunneling rate at $Z_0 \to \infty$ tends to zero to all orders of the small driving rate V based on our hierarchy theory. This is perfectly consistent with the standard rigorous result for the LZ tunneling rate $\exp\left(-\frac{\pi x^2}{V}\right)$ [40, 41], where any term in the Taylor expansion of $\exp\left(-\frac{\pi x^2}{V}\right)$ with respect to V is zero. This result is in sharp contrast to the previous case in the last subsection, where the leading term of the deviation from an ideal adiabatic behavior is proportional to ω^2.

6. Summary

Our hierarchical theory is summarized in table 1. We have found that the small deviations from the quantum adiabatic theorem can be analyzed in a hierarchical order (not necessarily in terms of the order of magnitude of each term): the deviations of kth-order are governed by a kth-order Hamiltonian which depends on R, $\dot{R}$, ..., $d^k R/dt^k$. When there is a large change in $d^k R/dt^k$, the dynamics governed by the kth-order Hamiltonian is no longer adiabatic and the effect of this nonadiabaticity may iteratively accumulate to affect the lower-order adiabaticity.

In many practical systems for a limited time scale, it is sufficient to consider the first-order deviation, neglecting all higher-orders. In figure 7, we have depicted schematically three typical scenarios of the first-order deviations. It is clear that the first-order deviations can be manipulated by designing $R(t)$ and $\dot{R}(t)$. This can be very useful to control the nonadiabatic
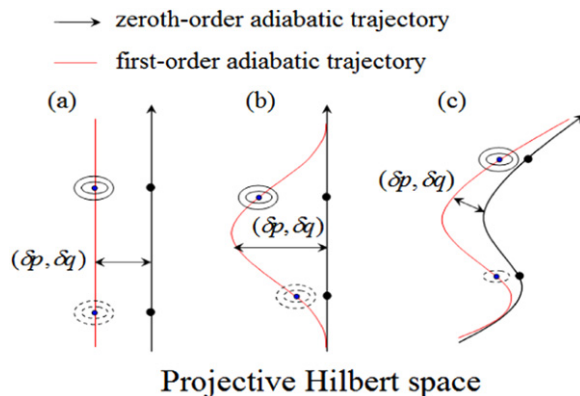
Figure 7. Schematics of different scenarios for the first-order deviation from the zeroth-order adiabatic trajectory. (a) For the case of a spin-1/2 particle under a rotating field considered in section 5.1, the first-order deviation from the zeroth-order adiabatic trajectory is a constant. (b) In the case of a LZ process considered in section 5.2, the average deviation in either the initial stage or the final stage approaches zero, but it can be appreciable at the intermediate stage. (c) The first-order deviations $(\delta p, \delta q)$ can be manipulated by designing the time dependence of $R(t)$ and $\dot{R}(t)$.

Table 1. Hierarchical adiabatic following at different orders, with the associated adiabatic Hamiltonians determined by various derivatives of the adiabatic parameter $R(t)$.

Order	Deviations	Associated Hamiltonian	Adiabatic Parameters
0	$\bar{p}, \bar{q}, \|\bar{\psi}\rangle$	$H_0(\hat{H}_0)$	R
1	$\delta p, \delta q$	H_1	$R, \dot{R}$
2	$\delta^2 p, \delta^2 q$	H_2	$R, \dot{R}, \ddot{R}$
3	$\delta^3 p, \delta^3 q$	H_3	$R, \dot{R}, \ddot{R}, \mathrm{d}^3 R/\mathrm{d}t^3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
k	$\delta^k p, \delta^k q$	H_k	$R, \dot{R}, \ddot{R}, \ldots, \mathrm{d}^k R/\mathrm{d}t^k$

error in quantum adiabatic computation [42, 43]. We plan to pursue this issue in the near future. Moreover, by substituting the hierarchically corrected wavefunction into the original Schrödinger equation, we may study possible corrections to the overall phase of the time-evolving quantum state [34, 35].

Our approach can be directly applied to classical adiabatic processes and nonlinear quantum adiabatic evolution on the mean-field level [44–49]. For example, it is of considerable interest to apply our findings to assist in the control of adiabatic processes in both classical and quantum systems [50–52].

Appendix A. Detailed derivations for the second-order theory

The premise of dealing with the second-order deviation is that the state is around the first-order fixed point. This allows us to express $(\delta p, \delta q)$ as the following,

$$\delta p = \delta^2 p + A_1; \quad \delta q = \delta^2 q + B_1, \tag{A.1}$$

where $\delta^2 p$ and $\delta^2 q$ describe the actual dynamics of $(\delta p, \delta q)$ on top of their time-averaged values (A_1, B_1).

Note that in deriving H_1 we have only kept the first-order term when expanding the force field $\left[-\frac{\partial H_0(R)}{\partial q}, \frac{\partial H_0(R)}{\partial p} \right]$. This is adequate for the first-order theory. When considering the second-order deviation, we should also keep the second-order terms in the expansion. Specifically, substituting equation (A.1) into equations (5) and (8), keeping the second-order expansion terms

$$\frac{1}{2} \left(\delta p \frac{\partial}{\partial p} + \delta q \frac{\partial}{\partial q} \right)^2 H_0' \qquad H_0' = \frac{-\partial H_0}{\partial q} \quad \text{or} \quad \frac{\partial H_0}{\partial p}, \tag{A.2}$$

and neglecting terms containing $[\delta^2 p]^2$ or $[\delta^2 q]^2$ (which are fourth-order), one finds (employing equation (10))

$$\begin{pmatrix} \dfrac{\mathrm{d}\delta^2 p}{\mathrm{d}t} \\ \dfrac{\mathrm{d}\delta^2 q}{\mathrm{d}t} \end{pmatrix} = \frac{1}{2}\delta\Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} + (\Gamma_0 + \delta\Gamma) \begin{pmatrix} \delta^2 p \\ \delta^2 q \end{pmatrix} - \begin{pmatrix} \dfrac{\mathrm{d}A_1}{\mathrm{d}t} \\ \dfrac{\mathrm{d}B_1}{\mathrm{d}t} \end{pmatrix}, \tag{A.3}$$

where $\delta\Gamma$ is defined in equation (15) as the state under consideration shifts from $(\bar{p}, \bar{q})$ to $(\bar{p} + A_1, \bar{q} + B_1)$.

Rearranging some terms on the right-hand side of equation (A.3), we arrive at

$$\begin{pmatrix} \dfrac{\mathrm{d}\delta^2 p}{\mathrm{d}t} \\ \dfrac{\mathrm{d}\delta^2 q}{\mathrm{d}t} \end{pmatrix} = (\Gamma_0 + \delta\Gamma) \left\{ \begin{pmatrix} \delta^2 p \\ \delta^2 q \end{pmatrix} - (\Gamma_0 + \delta\Gamma)^{-1} \begin{pmatrix} \dfrac{\mathrm{d}A_1}{\mathrm{d}t} \\ \dfrac{\mathrm{d}B_1}{\mathrm{d}t} \end{pmatrix} + \frac{1}{2}(\Gamma_0 + \delta\Gamma)^{-1}\delta\Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \right\}. \tag{A.4}$$

The fixed-point solution for $\delta^2 p$ and $\delta^2 q$ can be found from equation (A.4); it is

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \Gamma_0^{-1}(R) \left[\begin{pmatrix} \dfrac{\partial A_1}{\partial R} \\ \dfrac{\partial B_1}{\partial R} \end{pmatrix} \dot{R} + \begin{pmatrix} \dfrac{\partial A_1}{\partial V} \\ \dfrac{\partial B_1}{\partial V} \end{pmatrix} \ddot{R} \right] - \frac{1}{2}\Gamma_0^{-1}\delta\Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \tag{A.5}$$

where the time derivatives of the adiabatic parameter R, $\dot{R}$ and $\ddot{R}$, are assumed to be in the first-order and second-order of magnitude, respectively. All higher-order terms, such as those terms of the order of $\dot{R}^j$ with $j \geqslant 3$, are neglected. Under this treatment, it is now seen that, in terms of their time-averaged values, a more accurate prediction of $(\delta p, \delta q)$ is given by $(A_1 + A_2, B_1 + B_2)$. Note that A_2 and B_2 are evidently proportional to and $(\ddot{R})\dot{R}^2$. Equations (A.4) and (A.5) are just the second-order dynamics and the second-order fixed point given in the main text (see equations (13) and (14)). One can now readily write down the

second-order Hamiltonian

$$
H_2\left(R, \dot{R}\right) = \frac{1}{2}\left(\frac{\partial^2 H_0}{\partial q^2}\right)_{p_1, q_1}\left(\delta^2 q - B_2\right)^2 + \left(\frac{\partial^2 H_0}{\partial q \partial p}\right)_{p_1, q_1}\left(\delta^2 q - B_2\right)\left(\delta^2 p - A_2\right)
$$

$$
+ \frac{1}{2}\left(\frac{\partial^2 H_0}{\partial p^2}\right)_{p_1, q_1}\left(\delta^2 p - A_2\right)^2.
\tag{A.6}
$$

One only need to note that (p, q) take value of $(\bar{p} + A_1, \bar{q} + B_1)$ instead of $(\bar{p}, \bar{q})$ as we are at the second-order approximation.

Appendix B. High-order deviations in quantum adiabatic evolution

The dynamics of the kth-order deviation $(\delta^k p, \delta^k q)$ can be derived iteratively by substituting $\delta p = A_1 + A_2 + \dots + \delta^k p$ and $\delta q = B_1 + B_2 + \dots + \delta^k q$ into equations (5) and (8) with the expansion up to the kth-order, provided the fixed points of all the previous $(k - 1)$ orders have been obtained. Specifically, $(\delta^3 p, \delta^3 q)$ can be described by a third-order Hamiltonian $H_3(R, \dot{R}, \ddot{R}, \frac{d^3 R}{dt^3})$. The kth-order deviation $(\delta^k p, \delta^k q)$ forms a pair of canonical variables of a kth-order Hamiltonian $H_k(R, \dot{R}, \ddot{R}, \dots, \frac{d^k R}{dt^k})$, demonstrating that the kth-order deviation will undergo adiabatic evolution only if the time derivatives of parameter R up to the kth-order are all manipulated very slowly in comparison with the intrinsic frequency ω_k of the kth-order Hamiltonian, which is proportional to $|\Gamma_k| \approx |\Gamma_0|$.

The kth-order deviation consists of k terms, with the first one associated with the ideal matrix Γ_0 and the adiabatic evolution of the $(k - 1)$th-order deviation $(\delta^{k-1} p, \delta^{k-1} q)$, the second one associated with $\delta\Gamma$ and the evolution of $(\delta^{k-2} p, \delta^{k-2} q)$, and the kth one associated with $\delta^{k-1}\Gamma$ and the zeroth order adiabatic evolution of $(\bar{p}, \bar{q})$. The sum of the k terms is the result for the dynamical fixed point of H_k.

To illustrate that a general kth-order theory is possible, we consider here only a rather simple case where $\dot{R}$ is a constant. However, even in this case our expressions appear to be complicated and hence readers may skip the technical details (we present them just for completeness). In particular, the kth-order fixed point is

$$
\begin{pmatrix} A_k \\ B_k \end{pmatrix} = \Gamma_0^{-1}\begin{pmatrix} \dfrac{\partial A_{k-1}}{\partial R} \\ \dfrac{\partial B_{k-1}}{\partial R} \end{pmatrix}\dot{R} - \Gamma_0^{-1}\sum_{j=1}^{k-1}\Delta^j\Gamma\begin{pmatrix} A_{k-j} \\ B_{k-j} \end{pmatrix}.
\tag{B.1}
$$

The deviations $\Delta^j\Gamma$ in equation (B.1) is defined as

$$
\Delta^j\Gamma = \mathcal{T}^j\left\{\sum_{i=1}^{j}\frac{1}{(i+1)!}\left[\sum_{r=1}^{j}(A_r)\frac{\partial}{\partial p} + \sum_{r=1}^{j}(B_r)\frac{\partial}{\partial q}\right]^i \Gamma\right\}
\tag{B.2}
$$

The function $\mathcal{T}^j(\dots)$ in (B.2) is to take the jth-order terms in $(\dots)$, i.e., taking the sum of all the terms of the kind $A_t^u B_s^v$ with $tu + sv = j$. For example, A_2 and B_2 are second-order terms in terms of $\dot{R}$, and A_2^2 and $A_2 B_2$ become the fourth-order terms, so

$\mathcal{T}^2(A_2 + B_2 + A_2^2 + A_2 B_2) = A_2 + B_2$, $\mathcal{T}^3(A_2 + B_2 + A_2^2 + A_2 B_2) = 0$ and $\mathcal{T}^4(A_2 + B_2 + A_2^2 + A_2 B_2) = A_2^2 + A_2 B_2$, *etc*. Specifically, when $j = 1$, $\Delta\Gamma = \frac{1}{2}\delta\Gamma$.

In the case of nonconstant adiabatic speed V, we should include the derivatives of the kind $(\mathrm{d}^0 R/\mathrm{d}t^0 \equiv R)$

$$\sum_{j=0}^{k-1} \begin{pmatrix} \dfrac{\partial A_{k-1}}{\partial\left(\mathrm{d}^j R\big/\mathrm{d}t^j\right)} \\[2ex] \dfrac{\partial B_{k-1}}{\partial\left(\mathrm{d}^j R\big/\mathrm{d}t^j\right)} \end{pmatrix} \cdot \frac{\mathrm{d}^{j+1} R}{\mathrm{d}t^{j+1}}$$

for the kth-order deviation.

Generally, the hierarchy adiabatic theory can also be naturally extended to n-mode quantum system by expanding the Γ matrix from dimension 2×2 to dimension $2(n-1) \times 2(n-1)$.

Finally, it is necessary to make two remarks on high-order deviations. First, the deviations of all orders are obtained with respect to what the usual quantum adiabatic theorem predicts. This is the reason that equation (B.2) looks complicated. Second, in deriving the kth-order deviation in (B.1), we have already assumed the adiabaticity holds for up to the kth-order Hamiltonian.

References

[1] Born M and Fock V A 1928 *Z. Phys.* A **51** 165
[2] Rigolin G, Ortiz G and Ponce V H 2008 *Phys. Rev.* A **78** 052508
[3] Nguyen-Dang T T, Sinelnikov E, Keller A and Atabek O 2007 *Phys. Rev.* A **76** 052118
[4] Sun C P 1990 *Phys. Rev.* D **41** 1318–21
[5] Wu Z 1989 *Phys. Rev.* A **40** 6852–5
[6] Maamache M and Saadi Y 2008 *Phys. Rev.* A **78** 052109
[7] Maamache M and Saadi Y 2008 *Phys. Rev. Lett.* **101** 150407
[8] Rigolin G and Ortiz G 2012 *Phys. Rev.* A **85** 062111
[9] Rigolin G and Ortiz G 2010 *Phys. Rev. Lett.* **104** 170406
[10] Tong D M, Singh K, Kwek L C and Oh C H 2005 *Phys. Rev. Lett.* **95** 110407
[11] Yukalov V I 2009 *Phys. Rev.* A **79** 052117
[12] Grandi C D, Gritsev V and Polkovnikov A 2010 *Phys. Rev.* B **81** 012303
   Grandi C D, Polkovnikov A and Sandvik A W 2011 *Phys. Rev.* B **84** 224303
   Polkovnikov A, Sengupta K, Silva A and Vengalattore M 2011 *Rev. Mod. Phys.* **83** 863
[13] Cheung D, Hoyer P and Wiebe N 2011 *J. Phys. A: Math. Theor.* **44** 415302
   Jansen S, Ruskai M B and Seiler R 2007 *J. Math. Phys.* **48** 102111
[14] Marzlin K P and Sanders B C 2004 *Phys. Rev. Lett.* **93** 160408
[15] Ortigoso J 2012 *Phys. Rev.* A **86** 032121
[16] Amin M H S 2009 *Phys. Rev. Lett.* **102** 220401
[17] MacKenzie R, Morin-Duchesne A, Paquette H and Pinel J 2007 *Phys. Rev.* A **76** 044102
[18] Comparat D 2009 *Phys. Rev.* A **80** 012106
[19] Zhao Y 2008 *Phys. Rev.* A **77** 032109
[20] Ma J, Zhang Y, Wang E and Wu B 2006 *Phys. Rev. Lett.* **97** 128902
[21] Duki S, Mathur H and Narayan O 2006 *Phys. Rev. Lett.* **97** 128901

[22] Wu Z and Yang H 2005 *Phys. Rev.* A **72** 012114

[23] Du J, Hu L, Wang Y, Wu J, Zhao M and Suter D 2008 *Phys. Rev. Lett.* **101** 060403

[24] Tong D M 2010 *Phys. Rev. Lett.* **104** 120401

[25] Ambainis A and Regev O 2006 arXiv:quant-ph/0411152

[26] Farhi E, Goldstone J, Gutmann S, Lapan J, Lundgren A and Preda D A 2000 *Science* **292** 472

[27] Childs A M, Farhi E and Preskill J 2001 *Phys. Rev.* A **65** 012322

[28] Weinberg S 1989 *Ann. of Phys., N.Y.* **194** 336–86

[29] Heslot A 1985 *Phys. Rev.* D **31** 1341

[30] Liu J, Wu B and Niu Q 2003 *Phys. Rev. Lett.* **90** 170404

[31] Berry M V and Morgan M A 1996 *Nonlinearity* **9** 787

[32] Spallicci A D A M, Morbidelli A and Metris G 2005 *Nonlinearity* **18** 45

[33] Berry M V and Robbins J M 1993 *Proc. R. Soc.* A **442** 641–58

[34] Liu J and Fu L B 2010 *Phys. Rev.* A **81** 052112

[35] Fu L B and Liu J 2010 *Ann. Phys., NY* **325** 2425

[36] Dirac P A M 1925 *Proc. R. Soc.* A **107** 725

[37] Wiebe N and Babcock N S 2012 *New J. Phys.* **14** 013024

[38] Lidar D A, Rezakhani A T and Hamma A 2009 *J. Math. Phys.* **50** 102106

[39] Bohm Mostafazadeh *et al* 2003 *The Geometric Phase in Quantum Systems* (Berlin: Springer) pp 225–43

[40] Landau L D 1932 *Phys. Z. Sowjetunion* **2** 46

[41] Zener C 1932 *Proc. R. Soc.* A **137** 696–702

[42] Cen L X, Li X Q, Yan Y J, Zheng H Z and Wang S J 2003 *Phys. Rev. Lett.* **90** 147902

[43] Shi Y and Wu Y S 2004 *Phys. Rev.* A **69** 024301

[44] Zhang Q, Gong J B and Oh C H 2013 *Phys. Rev. Lett.* **110** 130402

[45] Yukalov V I 2009 *Phys. Rev.* A **79** 052117

[46] Meng S Y, Fu L B and Liu J 2008 *Phys. Rev.* A **78** 053410

[47] Itin A P and Watanabe S 2007 *Phys. Rev. Lett.* **99** 223903

[48] Zhang Q, Gong J B and Oh C H 2012 *Ann. Phys., NY* **327** 1202

[49] Zhang Q 2012 *J. Phys.* A **45** 295302

[50] Jarzynski C 2013 *Phys. Rev.* A **88** 040101(R)

[51] Deng J W, Wang Q -H, Liu Z H, Hanggi P and Gong J B 2013 *Phys. Rev.* E **88** 062122

[52] Deffner S, Jarzynski C and del Campo A 2014 *Sci. Rep.* **4** 6208