Nonlinear Evolution of Quantum States in the Adiabatic Regime

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We investigate adiabatic evolution of quantum states as governed by the nonlinear Schrödinger equation and provide examples of applications with a nonlinear tunneling model for Bose-Einstein condensates. Our analysis not only spells out conditions for adiabatic evolution of eigenstates but also characterizes the motion of noneigenstates which cannot be obtained from the former in the absence of the superposition principle. We find that Aharonov-Anandan phases play the role of classical canonical actions and are conserved in the adiabatic evolution of noneigenstates.

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Adiabatic evolution has been an important method of preparation and control of quantum states [1,2]. The main guidance comes from the adiabatic theorem of quantum mechanics [3], which dictates that an initial nondegenerate eigenstate remains to be an instantaneous eigenstate when the Hamiltonian changes slowly compared to the level spacings. More precisely, the quantum eigenstate evolves only in its phase, given by the time integral of the eigenenergy (dynamical phase) and a quantity independent of the time duration (geometric phase). The linearity of quantum mechanics then immediately allows a precise statement on the adiabatic evolution of noneigenstates through the superposition principle.

Our concern here is how the adiabatic theorem gets modified in nonlinear evolution of quantum states. Nonlinearity has been introduced as possible modifications of quantum mechanics on the fundamental level [4]. Our motivation, however, derives from practical applications in current pursuits of adiabatic control of Bose-Einstein condensates (BECs) [5], which can often be accurately described by the nonlinear Schrödinger equation. Here the nonlinearity stems from a mean field treatment of the interactions between atoms. Difficulties in theoretical study of adiabatic control of the condensate arise not only from the lack of unitarity [6] but also from the absence of the superposition principle [7,8].

In this Letter we attempt to overcome these difficulties by combining ideas from classical adiabatic dynamics and quantum geometric phases. Noticing that the eigenstates correspond to extremum points of the system energy, we find that their adiabatic condition depends on the Bogoliubov excitation spectrum about such points and has nothing to do with level spacings between the eigenstates. Also, because of nonlinearity, the adiabatic evolution of noneigenstates cannot be expressed as a superposition of such eigenstates with conserved probabilities as in the linear case. We find that the Aharonov-Anandan (AA) phases [9], which can be defined for cyclic or quasicyclic quantum states (at fixed control parameters), can serve as adiabatic invariants analogous to canonical actions in classical systems [10]. As an illustration and application, we study a simple two-mode BEC system.

General formalism.—The Schrödinger equation, linear or nonlinear, can be written in the form [11] ($\hbar = 1$)

$$i\frac{d\psi_j}{dt} = \frac{\partial}{\partial \psi_j^*}\mathcal{H}(\psi, \psi^*, \boldsymbol{R}), \tag{1}$$

where ψ_j is the jth amplitude of the wave function ψ over an orthonormal basis set, $\mathcal{H}$ is the energy of the system, and $\boldsymbol{R}$ denotes all the system parameters subject to adiabatic change. It is known that the Schrödinger equation has a canonical structure of classical dynamics. One can show, for example, that for each j the probability $|\psi_j|^2$ and phase $\arg\psi_j$ form a canonical pair, which satisfies the Hamilton's equations of motion with the energy $\mathcal{H}$ serving as the classical Hamiltonian. In this sense, the nonlinear Schrödinger equation is often termed classical [12], although the linear Schrödinger equation has not been called so.

However, our original system is quantum mechanical, which should impose additional structures in the corresponding canonical dynamics. Specifically, the system has the gauge symmetry that $\mathcal{H}$ is invariant under shifts in the overall phase of the wave function. This implies that the total probability must be conserved and the dynamics of the overall phase can be separated from the rest of the degrees of freedom. For example, in a finite dimensional problem, with $j = 1, 2, \ldots, N$, we can choose a new set of canonical variables: $p_j = |\psi_j|^2$, $q_j = \arg\psi_j - \arg\psi_N$, $j = 1, 2, \ldots, N-1$, and $p_N = \sum_{j=1}^{N} |\psi_j|^2$, $q_N = \arg\psi_N$. Because the Hamiltonian is independent of q_N, so that p_N is conserved and can be set to unity, the other variables form a closed set of Hamiltonian dynamics,

$$\frac{dq_j}{dt} = \frac{\partial \mathcal{H}}{\partial p_j}, \quad \frac{dp_j}{dt} = -\frac{\partial \mathcal{H}}{\partial q_j}, \quad (j = 1, \ldots, N-1). \tag{2}$$

The gauge symmetry also allows the introduction of a geometric phase for the quantum state. Let λ be the overall phase of the wave function; we took it to be

$\arg\psi_N$ in the above discussion. We split off this overall phase by writing $\psi_j = e^{i\lambda}\phi_j$; then ϕ_j belongs to the so-called projective Hilbert space. For many physical problems, the new wave function varies cyclically in time, for which one can introduce a geometric phase in generalization of Berry's phase. From Eq. (1), we obtain

$$\frac{d\lambda(t)}{dt} = \sum_{j=1}^{N} \phi_j^* i \frac{\partial}{\partial t}\phi_j - \sum_{j=1}^{N} \phi_j^* \frac{\partial}{\partial \phi_j^*}\mathcal{H}. \tag{3}$$

For a linear quantum system, the second term is the same as the energy [11], whose time integral gives the so-called dynamical phase. The time integral of the first term, $\int_0^\tau dt \sum_{j=1}^N \phi_j^* i \frac{\partial}{\partial t}\phi_j$, gives an additional contribution to the overall phase and is called the Aharonov-Anandan phase [9]. For the nonlinear case, we continue to call it the Aharonov-Anandan phase [13]. We show that this geometric phase plays the role of classical action in the canonical dynamics and is thus an adiabatic invariant.

Eigenstates.—We first consider adiabatic evolution of eigenstates, which is defined by $\frac{\partial}{\partial \psi_j^*}\mathcal{H}(\psi, \psi^*, \boldsymbol{R}) = E(\boldsymbol{R})\psi_j$ $(j = 1, \ldots, N)$. Besides the ground state which has obvious physical significance, higher eigenstates (also called nonlinear coherent modes) can be prepared experimentally [14]. The eigenstates correspond to extremum energy or fixed points of the classical dynamics (2) at a given $\boldsymbol{R}$ [15]. For an elliptic fixed point, we expect it to be able to follow adiabatically the control parameter provided the latter changes slowly compared with the fundamental frequencies of periodic orbits around the fixed point. These frequencies can be evaluated by linearizing Eq. (2) about the fixed point [10] and are identical to the Bogoliubov excitation spectrum of the corresponding eigenstate. In linear quantum mechanics, these frequencies are just the level spacings, so that breakdown of adiabaticity occurs by level crossing. In the nonlinear quantum problem, the fundamental frequencies are generally different from the level spacings, so that adiabaticity can often be maintained even if the energy levels cross as demonstrated below with a two-level model.

Nonlinearity in our quantum problem not only makes different eigenstates nonorthogonal but also can produce more eigenstates than the dimension N of the Hilbert space. Some of these additional eigenstates correspond to hyperbolic points in the classical dynamics, characterized by complex fundamental frequencies and strong sensitivity to small perturbations. We thus expect that such eigenstates are not able to follow adiabatically the control parameter. The complex fundamental frequencies correspond to a complex Bogoliubov spectrum on top of the mean field solution, signifying spontaneous production of quasiparticles. In practice, we need to traverse the dynamical instability regime fast enough to avoid the quasiparticle production and slow enough to avoid nonadiabatic excitations [16].

As an illustration, we consider a nonlinear two-level model,

$$\begin{aligned} i\frac{\partial\psi_1}{\partial t} &= \left(\frac{R}{2} + \frac{c}{2}(\psi_2^*\psi_2 - \psi_1^*\psi_1)\right)\psi_1 + \frac{v}{2}\psi_2, \\ i\frac{\partial\psi_2}{\partial t} &= \frac{v}{2}\psi_1 - \left(\frac{R}{2} + \frac{c}{2}(\psi_2^*\psi_2 - \psi_1^*\psi_1)\right)\psi_2. \end{aligned} \tag{4}$$

This model was proposed to describe the tunneling of BEC in an optical lattice [17] or in a double-well potential [18]. The parameter c characterizes the interaction strength between atoms; v is the coupling strength between the two modes. The parameter R can be the Bloch wave number or energy difference between the two wells. We are interested in the tunneling between the energy levels shown in the top panels of Fig. 1 when R is increased slowly from the far negative end to the far positive end.

Following our general formalism, we choose the total phase as $\lambda = \arg\psi_2$ and introduce a pair of canonical variables, $q = \arg\psi_1 - \arg\psi_2$ and $p = |\psi_1|^2$. The total energy of the system is $\mathcal{H} = \frac{v}{2}(\psi_1^*\psi_2 + \psi_1\psi_2^*) + \frac{R}{2}(\psi_1^*\psi_1 - \psi_2^*\psi_2) - \frac{c}{4}(\psi_1^*\psi_1 - \psi_2^*\psi_2)^2$. The wave function without the total phase takes the form $\phi_1 = \sqrt{p}e^{iq}$, $\phi_2 = \sqrt{1-p}$. Then we have the equivalent classical Hamiltonian as in Eq. (2),

$$\mathcal{H} = v\sqrt{p(1-p)}\cos q + \frac{R}{2}(2p-1) - \frac{c}{4}(2p-1)^2. \tag{5}$$

In Fig. 1, the structure of eigenenergy levels of Eq. (4) is shown in the top panels while the phase space orbits of the corresponding classical system (5) are shown in the bottom panels. When $c < v$, there are only two eigenstates and two fixed points. Since both f_1 and f_2 are elliptic with finite fundamental frequencies, the corresponding quantum states are expected to be able to follow adiabatically with R. This has been corroborated by our numerical simulations.

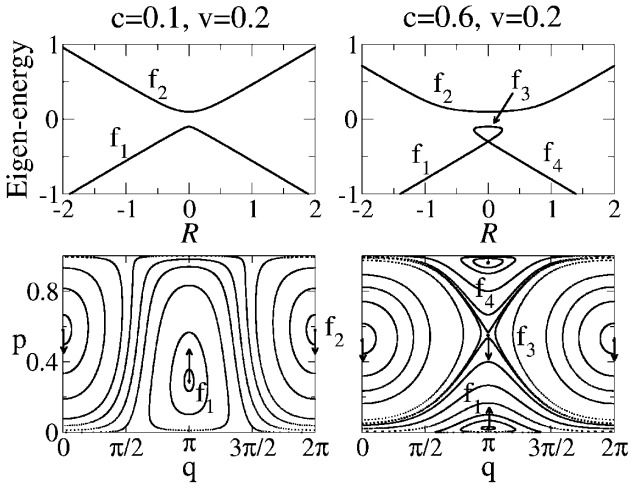

FIG. 1. The two top panels show eigenenergies as a function of R for two typical cases $c < v$ and $c > v$. The two bottom panels show the corresponding phase space portraits at a given value of R ($= -0.05$). The arrows on the fixed points indicate the directions of their movements as R increases.

When $c > v$, there are two more eigenstates, forming a loop structure; in the phase space portrait, there appear two more fixed points with one of them, f_3, being hyperbolic. Because of this structure change, the adiabatic evolution becomes very different here. First, the eigenstate corresponding to f_3 will not be able to follow the adiabatic change of R since f_3 is hyperbolic. This has been checked by our numerical integration of Eq. (4). Second, the fixed point f_1 can annihilate itself by colliding with f_3 as R changes slowly, leading to the breakdown of adiabaticity of the tunneling as reported numerically in Ref. [17]. Finally we notice that there is a level crossing between f_1 and f_4 at $R = 0$; however, our calculation shows that their fundamental frequencies are $v[(\frac{c}{v})^2 - 1]^{1/2} \neq 0$. This clearly illustrates our statement in the general formalism that the fundamental frequencies are not related to the level spacing in the nonlinear case.

Cyclic and quasicyclic states.—Compared with eigenstates, adiabatic evolution of noneigenstates is in general very complicated as the motions given by Eq. (2) may be chaotic [15]. We choose to focus on the states around an elliptic point, where the classical orbits are regular. Here the motions are confined on the $(N-1)$-dimensional torus, and we may introduce a set of action-angle variables, $\boldsymbol{I} = (I_1, I_2, \ldots, I_{N-1}), \boldsymbol{\Theta} = (\Theta_1, \Theta_2, \ldots, \Theta_{N-1})$ [10]. The angular variables change with time at frequencies $\boldsymbol{\omega} = (\omega_1, \omega_2, \ldots, \omega_{N-1})$ while the actions $\boldsymbol{I}$ are constants. More importantly, according to the classical adiabatic theorem [10], the actions $\boldsymbol{I}$ are adiabatic invariants in the sense that they remain constant even if the control parameter $\boldsymbol{R}$ changes (slowly) in time. The existence of these adiabatic invariants presents strong constraint on the motion and guarantees a state initially close to an eigenstate (elliptic point) to stay near it as the system is changed slowly.

Furthermore, we can attach a physical meaning to these adiabatic invariants in the effective classical description by making connection to the Aharonov-Anandan phase of the states. The AA phase is defined as the time integral of the first term in Eq. (3) for a periodic orbit or a quasiperiodic state [19],

$$\gamma_{\mathrm{AA}}(\boldsymbol{R}) = \int_0^\tau dt \sum_{j=1}^{N} \phi_j^* i \frac{\partial}{\partial t} \phi_j. \tag{6}$$

We can rewrite it with the canonical variables (q_j, p_j) and further with the action-angle variables,

$$\gamma_{\mathrm{AA}} = \sum_{j=1}^{N-1} \int_0^\tau p_j dq_j = \boldsymbol{I} \cdot \boldsymbol{\Omega}, \tag{7}$$

where $\boldsymbol{\Omega} = (\omega_1 \tau, \omega_2 \tau, \ldots, \omega_{N-1}\tau)$ and τ is a time period. Therefore, the actions are related to the AA phase γ_{AA}, which is an observable physical quantity [20]. In the special case of $N = 2$, there is only one independent action, so the AA phase is simply $\gamma_{\mathrm{AA}} = 2\pi I$. This simple connection can be expanded to the general case of $N > 2$, where one can single out a particular cyclic state that involves only one action I_j. For this cyclic state, we again have the simple relation $\gamma_{\mathrm{AA}} = 2\pi I_j$.

How do the above adiabatic invariants connect to the familiar notions in the standard linear quantum mechanics? Consider the time evolution of a general state in a linear quantum system for a given $\boldsymbol{R}$, $\psi_j(t) = \psi_j(0)e^{-iE_j t}$, $j = 1, \ldots, N$, where E_j's are the eigenenergies. This is a (quasi-)cyclic state with the projective wave functions given by $\Phi_j(t) = \psi_j(0)e^{-i(E_j - E_N)t}$, $j = 1, \ldots, (N-1)$ and $\Phi_N(t) = \psi_N(0)$. Its AA phase can be computed with Eq. (6); after comparing with Eq. (7), we immediately find that $I_j = |\psi_j(0)|^2$. Therefore, in linear quantum mechanics, these adiabatically invariant actions I_j are nothing but the probabilities on the energy levels. In this way, we have rederived the adiabatic theorem of linear quantum mechanics [21].

The conservation of probabilities on the energy levels can be generalized to the case where the system is nonlinear in an intermediate range of the parameter $\boldsymbol{R}$ (Fig. 2). When the actions (AA phases) are conserved during the entire process, the initial and final probabilities on the energy levels must remain the same, $I_j = I_j'$, because the system is linear at the beginning and end of the process so the actions are just the occupation probabilities. In the intermediate range where the nonlinearity is present, the probabilities will change because the conserved actions are not probabilities on the energy levels.

We now illustrate this important result using our two-level model, where, at the two ends with $|R| \gg c$, the nonlinear term can be ignored and the system is effectively linear. For $c < v$, where all the fixed points are elliptic, the fundamental frequency ω for the periodic orbit remains finite and the AA phase (action) is conserved [see lines (a) in the right panels of Fig. 3]. The initial and final probabilities on each level are indeed the same [Fig. 3(a)], although they oscillate in the intermediate range of the parameter where the system is nonlinear. As the nonlinearity gets strong, the occurrence of tunneling begins to depend on the choice of the initial state. In Fig. 3(b), where one starts with probability $I = 0.1$ on level two, tunneling happens; however, in Fig. 3(c) where one starts with probability $I = 0.8$ on level two, there is no tunneling. The difference is whether there is collision

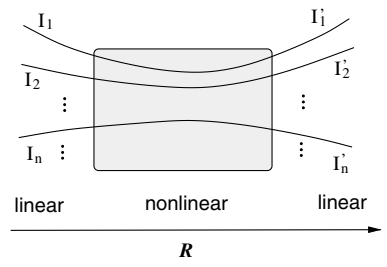

FIG. 2. Nonlinear tunneling of a system that is nonlinear in an intermediate range of the parameter $\boldsymbol{R}$. I's and I''s are the occupation probabilities on different eigenstates, at the beginning and the end of the tunneling process, respectively.

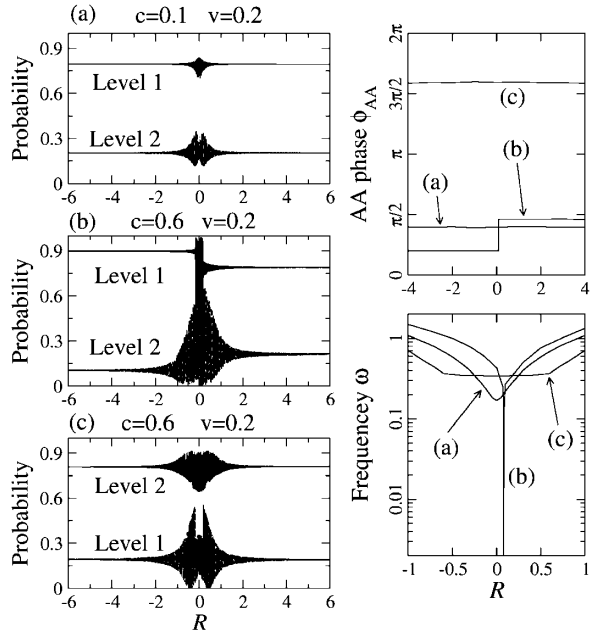

FIG. 3. Left panels: Change of probabilities on the two levels with R, which changes with rate $\alpha = 0.0001$, for three different cases. The right two panels show how the AA phases and the fundamental frequencies change with R in these three cases, respectively.

with the hyperbolic point f_3. In Fig. 3(b), the initial noneigenstate falls on a periodic orbit surrounding the fixed point f_1, which will later collide with the hyperbolic point f_3, where the fundamental frequency drops to zero and the AA phase has a finite jump [see lines (*b*) in the right panels]. The jump height is proportional to the tunneling probability. In Fig. 3(c), the initial state falls on a periodic orbit around the fixed point f_2, which will not collide with f_3.

In summary, we have generalized the quantum adiabatic theorem to systems governed by the nonlinear Schrödinger equation. Adiabaticity of an eigenstate requires that the control parameters vary slowly with respect to the Bogoliubov excitation frequencies. We further show that the Aharonov-Anandan phase can serve as the general adiabatic invariant, in analogy to the canonical actions in classical mechanics. This finding provides an important application of the Aharonov-Anandan phase and is expected to be useful in guiding adiabatic manipulation of the condensated atoms.

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