Berry Phase of Nonlinear Correction

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We investigate the geometric phase or Berry phase of adiabatic quantum evolution in the Bose-Einstein condensate (BEC) systems governed by nonlinear Gross-Pitaevskii (GP) equations. We study how this phase is modified by the nonlinearity and find that the Bogoliubov fluctuations around the eigenstates are accumulated during the nonlinear adiabatic evolution and contribute a finite phase of geometric nature. A two-mode BEC model is used to illustrate our theory. Our theory is applicable to other nonlinear systems such as paraxial wave equation for nonlinear optics and Ginzburg-Landau equations for complex order parameters in condensed-matter physics.

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Adiabatic theory, as a fundamental issue of quantum mechanics, involves two aspects: i) when the Hamiltonian changes slowly compared to the level spacings, an initial nondegenerate eigenstate remains to be an instantaneous eigenstate\cite{1}; ii) the phase acquired by the eigenstate is the sum of the time integral of the eigenenergy (dynamical phase) and a quantity independent of the time duration and related to the geometric property of the closed path in parameter space (geometric phase or Berry phase)\cite{2,3}. The adiabatic theory has been playing a crucial role in preparation and control of quantum states\cite{4}. Recently, the Berry phase and related geometric phases\cite{5,6} has received renewed interest due to its important use in implementation of quantum computing gates\cite{7} and applications in condensed matter physics\cite{8}.

For a nonlinear quantum system, such as that described by the nonlinear Schrödinger equations, how the adiabatic theory gets modified. Nonlinear quantum systems have become increasingly important in physics. They often arise in the mean field treatment of many-body quantum systems, such as Bose-Einstein condensates (BECs) of dilute atomic gases\cite{9}. Recently, extending the first aspect of adiabatic theory to the nonlinear systems, i.e., investigating the adiabatic condition and adiabaticity for the nonlinear quantum evolution has been done\cite{10,11}, interestingly it was found that the adiabaticity of an eigenstate only requires that the control parameters vary slowly with respect to the Bogoliubov excitation frequencies and has nothing to do with the level spacings. Nevertheless, Berry phase issue in such nonlinear system is far from well understand, while some superficial observations suggest that Berry’s formula without any correction is applicable to nonlinear system suppose the system is invariant under gauge transformation of the first kind\cite{12}.

In this letter, we make a thorough analysis on geometric phase associated with the adiabatic evolution of an eigenstate, and strikingly we find that the Berry phase is dramatically modified by the nonlinearity. This finding is completely contrary to previous superficial observations. The underlying mechanism has been revealed: for a nonlinear system because the Hamiltonian is a functional of the instantaneous wavefunctions, the Bogoliubov fluctuations around the eigenstate caused by the slow change of the system are allowed to feedback to the Hamiltonian. They are accumulated during an adiabatic evolution and eventually contribute a finite phase of geometric nature. A two-mode BEC model is used to illustrate our theory.

Let us consider the BEC trapped in a potential $V(R; r)$, the evolution of its wavefunction is governed by following nonlinear Gross-Pitaevskii (GP) equation ($\hbar = m = 1$)\cite{13},

$$\frac{i}{\hbar} \frac{\partial \psi}{\partial t} = H_0 \psi + g|\psi|^2 \psi, \quad (1)$$

with $H_0 = -\frac{1}{2} \nabla^2 + V(R; r)$, where $R$ is the parameter vector, $g$ is the nonlinear parameter representing the interaction between the coherent atoms. The total energy of the system $E_T = \int dr E(\psi^*, \psi)$, where the energy density $E(\psi, \psi^*) = \psi^* H_0 \psi + \frac{1}{2} g|\psi|^4$. The above system is invariant under gauge transforms of the first kind, $\psi(r, t) \rightarrow \exp(i\eta)\psi(r, t)$ with constant $\eta$. The gauge symmetry implies that the total atom number is conserved, i.e., $\int |\psi|^2 = 1$.

Let $\lambda$ be the overall phase of the wave function; we may take it to be the phase of the wavefunction at a fixed position $r_0$, for example, $\lambda = -\arg(\psi(r_0, t))$. We split off this overall phase by writing $\psi = e^{-i\lambda} \phi$, then $\phi$ belongs to the so called projective Hilbert space. From (1) we obtain

$$\frac{d\lambda}{dt} = -i\phi^* \frac{\partial}{\partial t} \phi + \int dr E(\phi^*, \phi) + \frac{g}{2} \phi^* |\phi|^2 \phi. \quad (2)$$

The eigenequation of the system is

$$H_0 \overline{\psi} + g|\psi|^2 \psi = \mu \overline{\psi}.$$  

where $\overline{\psi}$ is the eigenfunction and $\mu$ is the eigenvalue (or chemical potential).

Now we consider the parameter vector $R$ varies slowly in time, and introduce the dimensionless adiabatic parameter of $\varepsilon \sim |\frac{dR}{dt}|$ as the measure how slow the parameters change. The adiabatic parameter tends to zero, i.e., $\varepsilon \rightarrow 0$, indicating the adiabatic limit.
Consequently, the expression of the total phase can be expanded in a perturbation series in the adiabatic parameter, i.e.,

$$\frac{d\lambda}{dt} = \alpha_0(\varepsilon^0) + \alpha_1(\varepsilon^1) + o(\varepsilon^2).$$

(4)

When the parameters move in a circuit, the eigenstates evolve for an infinite long time duration in the adiabatic limit. The time integral of the zero-order term gives so-called dynamic phase because it is closely related to the temporal process of the evolution. The time integral of the first-order term gives an additional contribution to the overall phase, which will be shown later is of a geometric nature, that is, only depends on the geometry of the close path in the parameter space. The contribution of the higher-order term vanishes in the adiabatic limit.

In the quantum evolution with slowly-changing parameters, we assume $\phi = \overline{\phi}(R) + \delta\phi(R)$, where $\overline{\phi}(R)$ is the wavefunction of the instantaneous eigenstate corresponding to the local minimum energy. $\delta\phi$ denotes the secular part of the Bogoliubov fluctuations induced by the system’s slow change while the rapid oscillations in the fluctuations are ignored because they vanish after a long-term average. $\delta\phi$ depends on the adiabatic parameter and is of order $\varepsilon$, then from Eq.(2) and with the help of relation Eq.(3), we have the explicit expressions as follows,

$$\alpha_0(\varepsilon^0) = \mu(R),$$

(5)

$$\alpha_1(\varepsilon^1) = -i\langle \partial(R) + g(\overline{\phi}(R), \overline{\phi}(R))\rangle \langle \delta\phi, \delta\phi^* \rangle,$$

(6)

where we denote $\langle a|b \rangle = \int dr(a^*b), \langle a, b \rangle |c, d \rangle = \int dr(a^*c + b^*d),$ and the second order term like $\frac{\delta\phi}{\delta t}$ has been ignored.

From the above expressions we see that the dynamical phase has been modified to be the time integral of the chemical potential rather than the energy. This is because the instantaneous eigenstates are feedback to the Hamiltonian. More interestingly, the first-order term, i.e., the Berry phase term has been modified due to the feedback of the Bogoliubov fluctuations to the Hamiltonian. To evaluate it qualitatively and express the modified geometric phase explicitly, let us introduce a set of orthogonal basis $|k\rangle$ and the variable $\psi_j$ is the j-th component, i.e., $\psi_j = \langle j|\psi\rangle$. Without losing generality, the projective Hilbert space is set to be of a specific gauge so that the phase of the N-th component is zero. In the projective Hilbert space, the new variables $(n_j, \theta_j)$ are introduced through $\phi_j = \sqrt{n_j}e^{i\theta_j}$. Substituting the expression of $\phi_j = \sqrt{n_j}e^{i\theta_j}e^{-i\int \beta d\nu}$ into the GP equation, and separating real and imaginary parts, we have following differential equations for the density $\delta n_j$ and phase $\delta \theta_j$, respectively,

$$\frac{d\delta n_j}{dt} = f_j, \quad \frac{d\delta \theta_j}{dt} = h_j, \quad j = 1, 2, \ldots N - 1$$

(7)

where

$$f_j = 2 \sum_{k=1}^{N} n_k \sqrt{n_k n_m} \text{Im} \left[ C_{jk}(R)e^{i(\theta_k - \theta_j)} \right]$$

$$+ 2g \sum_{k,l,m=1}^{N} \sqrt{n_i n_j n_k} n_m \text{Im}[D_{jk,kl,m}] e^{i(\theta_i + \theta_m - \theta_j - \theta_k)],} \quad (8)$$

$$h_j = -\sum_{k=1}^{N} \sqrt{n_k} \text{Re} \left[ C_{jk}(R)e^{i(\theta_k - \theta_j)} \right]$$

$$g \sum_{k,l,m=1}^{N} \sqrt{n_k n_l n_m} \text{Re}[D_{jk,kl,m}] e^{i(\theta_i + \theta_m - \theta_j - \theta_k)] + \beta,} \quad (9)$$

with $C_{jk}(R) = \langle j|H_0(R)|k\rangle, D_{jk,kl,m} = \langle j|k|l\rangle|m\rangle$.

The last equation is from the fact that in the projective Hilbert space the phase of wavefunction of the N-th component is set to be zero. The norm conversation condition $n_N = 1 - \sum_{k=1}^{N-1} n_k$ could be used to remove the variable $n_N$ in the above equations. In the representation of new variables, $(\vec{n}, \vec{\theta})$ satisfy equations of the equilibrium state, i.e., $(\frac{\partial n_k}{\partial t}, \frac{\partial \theta_k}{\partial t}) |_{[\vec{n}, \vec{\theta}]} = 0$.

$(\vec{n}, \vec{\theta})$ are function of the parameter $R$ corresponding to the eigenstates of GP equation. Let us make perturbation expansion around the eigenstate with $n_1 = n_j(R) + \delta n_j(R), \theta_j = \theta_j(R) + \delta \theta_j(R)$. Here, $\overline{\phi}(R) = \sqrt{\overline{n}_j} e^{i \overline{\theta}_j(R)}, (\overline{n}_j(R), \overline{\theta}_j(R))$ are the fluctuations depending on the adiabatic parameter and of order $\varepsilon$. Then inserting the above expansion into the equations (7) and ignoring the higher order terms such as $\frac{\delta\phi}{\delta t}$, with denoting $\nu = (n_1, \theta_1; \ldots; n_{N-1}, \theta_{N-1})$ we obtain that

$$\frac{d\vec{\nu}}{dR} \frac{dR}{dt} = \mathcal{L} \delta\nu,$$

(11)

where the matrix takes the form,

$$\mathcal{L} = \{ L_{jk} \}_{N-1, N-1}, \quad \dot{L}_{jk} = \frac{\partial L_{jk}}{\partial \theta_k} \frac{\partial L_{jk}}{\partial n_j} \bigg|_{\nu = \overline{\nu}}.$$}

then, inversely we have

$$\delta\nu = \mathcal{L}^{-1} \frac{d\vec{\nu}}{dR} \frac{dR}{dt}.$$
in which

$$\Pi_j = \left( \frac{1}{2} \rho_j^{-1/2} e^{i \tilde{\sigma}_j}, i \sqrt{\rho_j} e^{-i \tilde{\sigma}_j}, -i \sqrt{\rho_j} e^{-i \tilde{\sigma}_j}, \frac{1}{2} \rho_j^{-1/2} e^{-i \tilde{\sigma}_j} \right).$$  \hspace{1cm} (15)

Substituting (13) and (14) into (6), we finally obtain the explicit expression of adiabatic geometric phase that contains two terms,

$$\gamma_g = \gamma_B + \gamma_{NL}$$ \hspace{1cm} (16)

where the first term is the usual Berry phase formula,

$$\gamma_B = -i \oint \langle \Phi | \nabla_R | \Phi \rangle dR = \oint \sum_{j=1}^{N-1} \rho_j \frac{\partial \rho_j}{\partial R} dR.$$ \hspace{1cm} (17)

and additional term is from the nonlinearity, taking the form,

$$\gamma_{NL} = g \oint \left( \Lambda |\Pi \circ \mathcal{L}|^{-1} \frac{d \tau}{dR} \right) dR.$$ \hspace{1cm} (18)

Here, $\Lambda = (\rho_1 + \sum_{j=1}^{N-1} \rho_j - 1)\rho_1^{1/2} e^{-i \tilde{\sigma}_1}, \rho_1 + \sum_{j=1}^{N-1} \rho_j - 1)\rho_1^{1/2} e^{-i \tilde{\sigma}_1}, \ldots, (\rho_{N-1} + \sum_{j=1}^{N-1} \rho_j - 1)\rho_{N-1}^{1/2} e^{-i \tilde{\sigma}_{N-1}}),$ and diagonal matrix

$$\Pi = \text{diag}(\Pi_1, \Pi_2, \ldots, \Pi_{N-1}).$$

Notice that to simplify the expression of $\Lambda$, we use the approximation that the overlap integral $D_{j,k,l,m} \approx 0$ when the subscripts are not all identical.

Both $\gamma_B$ and $\gamma_{NL}$ have the geometric property of parameter space. The novel second term indicates that, the Bogoliubov fluctuations induced by the slow change of the system that is negligible in linear case, however, could be accumulated in the nonlinear adiabatic evolution and contribute the finite phase of a geometric nature. This is because the Hamiltonian in the nonlinear system contains the instantaneous wavefunction and as a result the Bogoliubov fluctuations around the eigenstate are allowed to feedback to the Hamiltonian.

As an illustration of our theoretical formulism, we consider the two-mode BEC model as example, which is described by the following GP equation (14),

$$i \frac{d}{dt} \left( \begin{array}{c} \Psi_1 \\ \Psi_2 \end{array} \right) = H(\Psi_1, \Psi_2) \left( \begin{array}{c} \Psi_1 \\ \Psi_2 \end{array} \right),$$ \hspace{1cm} (19)

with

$$H(\Psi_1, \Psi_2) = \left( \begin{array}{cc} Z|\Psi_1|^2 + \frac{\rho}{2} e^{-i \varphi} & \frac{\rho}{2} e^{i \varphi} \\ \frac{\rho}{2} e^{i \varphi} & Z|\Psi_2|^2 \end{array} \right).$$ \hspace{1cm} (20)

The energy of the system $E(\Phi_1, \Phi_2) = \frac{Z}{2}(|\Psi_1|^4 + |\Psi_2|^4) + \frac{\rho}{2} (e^{-i \varphi} |\Psi_1|^4 + e^{i \varphi} |\Psi_2|^4).$ The above system is invariant under gauge transforms of the first kind. The eigenfunctions take the forms of $H \circ \left( \begin{array}{c} \Phi_1 \\ \Phi_2 \end{array} \right) = \mu \left( \begin{array}{c} \Phi_1 \\ \Phi_2 \end{array} \right).$ For the nonlinear system, the number of the eigenstates may be larger than the dimension of the Hilbert space and the eigenstate could be unstable[10]. We have obtained four eigenstates for the case $Z > \rho$ by solving the above eigenquation. Three of them are stable and one is unstable. We choose following stable eigenstate for example to illustrate our theory, i.e., $\Phi_1 = \left[ \frac{1}{2} \left( 1 - \sqrt{1 - \frac{\rho^2}{Z^2}} \right) \right]^{1/2}, \quad \Phi_2 = \left[ \frac{1}{2} \left( 1 + \sqrt{1 - \frac{\rho^2}{Z^2}} \right) \right]^{1/2} e^{i \varphi},$ with eigenvalue of $\mu = Z.$

We choose the overall phase $\lambda = -\arg(\Psi_1),$ from GP equation (19), we have

$$\frac{d\lambda}{dt} = -i(\Phi_1 \Phi_2^* \frac{\partial}{\partial t}(\Phi_1, \Phi_2)) + E(\Phi_1, \Phi_2) + \frac{Z}{2}(|\Phi_1|^4 + |\Phi_2|^4).$$ \hspace{1cm} (21)

In the adiabatic evolution, we assume $\Phi_i = \overline{\Phi}_i(\varphi) + \delta \Phi_i(\varphi),$ where $\delta \Phi_i$ is the fluctuation depending on the adiabatic parameter of order $\varepsilon = d\varphi/dt.$ Then we have the explicit expression of the zeroth order,

$$\alpha_0(\varepsilon^0) = Z,$$ \hspace{1cm} (22)

and using conservation of the particle $|\Phi_1|^2 + |\Phi_2|^2 = 1,$ and the fact $\arg(\Phi_1) = 0,$ we have the first-order term,

$$\alpha_1(\varepsilon^1) = -i \overline{\Phi}_2 \frac{\partial}{\partial t} \overline{\Phi}_2$$

$$+ Z \left( (2|\Phi_2|^2 - 1)\overline{\Phi}_2, (2|\overline{\Phi}_2|^2 - 1)\overline{\Phi}_2, (\delta \overline{\Phi}_2, \delta \overline{\Phi}_2) \right) \hspace{1cm} (23)$$

Berry term of the geometric phase is readily deduced,

$$\gamma_B = \pi \left( 1 + \sqrt{1 - \frac{\rho^2}{Z^2}} \right).$$ \hspace{1cm} (24)

Now we are going to derive the additional term which gives the $\gamma_{NL}$ of the geometric phase. Let us introduce the new variables $(n, \theta)$ through $(\Phi_1, \Phi_2) = (\sqrt{1-n}, \sqrt{ne^{i\theta}}).$ Substitute $(\Psi_1, \Psi_2) = e^{-i f^* \beta dt}(\Phi_1, \Phi_2)$ into Eq. (19), and separate the real and imaginary parts, we have four differential equations, in which two of them are identical due to the norm conversation,

$$\frac{dn}{dt} = -\rho \sqrt{1 - n^2} \sin(\theta - \varphi),$$ \hspace{1cm} (25)

$$\frac{d\theta}{dt} = -\rho \sqrt{1 - n^2} \cos(\theta - \varphi) - Z n + \beta,$$ \hspace{1cm} (26)

$$\beta = Z (1 - n) + \frac{\rho}{2} \sqrt{\frac{n}{1 - n}} \cos(\theta - \varphi)$$ \hspace{1cm} (27)
The eigenstate make up the fixed point of equations (25) and (26), i.e., \( \pi = \frac{1}{2} \left( 1 + \sqrt{1 - \frac{\rho^2}{\pi^2}} \right) \theta = \varphi \). Let us make perturbation expansion around the eigenstate with \( n = \pi(\varphi) + \delta n, \theta = \varphi(\varphi) + \delta \theta \). Then inserting the above expansion into the equations (25) and (26), and ignoring the higher order terms of \( \frac{\partial \delta n}{\partial \varphi} \), \( \frac{\partial \delta \theta}{\partial \varphi} \), we obtain that

\[
\left( \frac{\partial \pi}{\partial \varphi} \right) \frac{d \varphi}{dt} = L \left( \frac{\partial \delta n}{\partial \theta} \right),
\]

with

\[
L = \begin{pmatrix}
-2Z + \frac{\rho}{4(\pi - \rho^2)\pi^2} & -\rho \sqrt{\pi - \pi^2} \\
-\rho \sqrt{\pi - \pi^2} & 0
\end{pmatrix}.
\]

Then, we have

\[
\gamma_{NL} = \int_0^{2\pi} \Lambda \Pi L^{-1} \left( \frac{\partial \pi}{\partial \varphi}, \frac{\partial \theta}{\partial \varphi} \right)^T d \varphi.
\]

where \( \Lambda = Z((2\pi - 1)\sqrt{\pi - \varphi}, (2\pi - 1)\sqrt{\varphi}) \). Finally, we get

\[
\gamma_{NL} = \frac{\pi \rho^2}{Z \sqrt{Z^2 - \rho^2}}.
\]

The above new form of geometric phase is verified numerically by directly integrating the Schrödinger Eq.(19) using Runge-Kutta algorithm.

In summary, we show that the Berry phase associated with the adiabatic evolution of BECs has been modified by the nonlinearity. This nonlinear correction is of significance because it could affect the interferences of the matter waves. It is expected to be observed in future's experiments. Our theories, on the other aspect, cover the general nonlinear systems in nonlinear optics and condense matter physics. Since some of the theories covered by our results are meanfield limits of quantum many-body theories, the possibility of generalizing these considerations to quantized field theories from the correspondence principle is of great interest for future study.

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