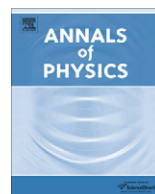




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# Adiabatic Berry phase in an atom–molecule conversion system

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## ABSTRACT

We investigate the Berry phase of adiabatic quantum evolution in the atom–molecule conversion system that is governed by a nonlinear Schrödinger equation. We find that the Berry phase consists of two parts: the usual Berry connection term and a novel term from the nonlinearity brought forth by the atom–molecule coupling. The total geometric phase can be still viewed as the flux of the magnetic field of a monopole through the surface enclosed by a closed path in parameter space. The charge of the monopole, however, is found to be one third of the elementary charge of the usual quantized monopole. We also derive the classical Hannay angle of a geometric nature associated with the adiabatic evolution. It exactly equals minus Berry phase, indicating a novel connection between Berry phase and Hannay angle in contrast to the usual derivative form.

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## 1. Introduction

Berry phase [1], which reveals the gauge structure associated with a phase shift in adiabatic processes in quantum mechanics, has attracted great interest in physics [2]. This quantal phase is connected with a classical angle, namely, the Hannay angle [3], by a simple and elegant expression in the semiclassical limit [4]. A vast amount of literature has been devoted to the generalization and application of the geometric structures and their relationship in various physical systems [5–10].

Association of ultracold atoms into molecules is currently a topic of much experimental and theoretical interest [11] with important applications ranging from the search for the permanent electric dipole moment [12] to BCS-BEC (Bose–Einstein condensate) crossover physics [13]. Through Feshbach

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resonance [14] or photoassociation [15], a pair of atoms can bond into a molecule. The atom–molecule conversion under mean field treatment is governed by a nonlinear Schrödinger equation, in which the nonlinearity is from the fact that two or more atoms are needed to form one molecule [16]. Since the adiabatic manipulation is an optimal way to yield high conversion efficiency, great efforts and big progress have been made towards the adiabatic condition [17] and adiabaticity [18] of the nonlinear quantum evolution. Nevertheless, the knowledge of the Berry phase for the adiabatic evolution in such nonlinear system is very limited. This system not only lacks superposition principle due to the presence of nonlinearity [19] but also has no  $U(1)$ -invariance because the chemical potentials of atomic component and molecular component are not identical [20].

In this paper, we study the adiabatic geometric phase in the atom–molecule conversion systems and derive the explicit expression of the Berry phase analytically. We find strikingly that the circuit integral of Berry connection of the instantaneous eigenstate alone cannot account for the geometric phase, while a novel term due to the nonlinearity brought forth by the atom–molecule coupling emerges. The above analytical finding has been verified by our numerical simulation. On the other hand, we recognize that the although above system admits the quantal equations of motion, it appears formally to have classical structure if we regard the total phase and total particle number as a pair of canonical conjugate variables. We thus could exploit this particular feature to construct a canonical transformation to action-angle variables and derive the Hannay angle analytically. We find the Hannay angle in the system exactly equals minus Berry phase. This result indicates a novel connection between Berry phase and Hannay angle in contrast to the usual derivative form [4]. The geometric phase can be interpreted as a flux of a magnetic field of a monopole through the surface enclosed by the closed path in parameter space. The charge of the monopole is found to be one third of the elementary charge of the usual quantized monopole.

Our paper is organized as follows. In Section 2, we present our atom–molecule conversion model and derive the explicit expression of the Berry phase associated with the adiabatic evolution of eigenstates. In Section 3, we give an interpretation of geometric phase as a flux of a magnetic field of a fractional monopole. In Section 4, we investigate the Hannay angle of the adiabatic evolution. Section 5 is our conclusion.

## 2. Berry phase in an atom–molecule conversion system

For simplicity, we consider the following two-mode model, i.e., atom–diatomic molecule conversion system, as an example to demonstrate our theory. The following deduction, in principle, can be extended to the case of multiple modes and multi-atomic molecule formation. The energy of the system reads

$$\mathcal{H} = \frac{R \cos \theta}{2} (\hat{\psi}_1^\dagger \hat{\psi}_1 - \hat{\psi}_2^\dagger \hat{\psi}_2) + \sqrt{\frac{3}{8}} \frac{R \sin \theta}{2} (e^{i\varphi} \hat{\psi}_1^\dagger \hat{\psi}_1^\dagger \hat{\psi}_2 + h.c.), \quad (1)$$

where  $\hat{\psi} = (\hat{\psi}_1, \hat{\psi}_2)$  and  $\hat{\psi}^\dagger = (\hat{\psi}_1^\dagger, \hat{\psi}_2^\dagger)$  are the annihilation and creation operators for atom and molecule, respectively. They obey the commutation relations  $[\hat{\psi}_i, \hat{\psi}_i^\dagger] = \delta_{ij}$  for bosons.  $\mathbf{R} = (R \sin \theta \cos \varphi, R \sin \theta \sin \varphi, R \cos \theta)$  is a vector in 3D parameter space. The terms  $\hat{\psi}_1^\dagger \hat{\psi}_1^\dagger \hat{\psi}_2 + h.c.$  describe the coupling between atom pairs and diatomic molecules, which brings a new gauge structure to the system. With these terms, the system is invariant under the transformation

$$U(\eta) = e^{i\Theta(\eta)}, \quad \Theta(\eta) = \begin{pmatrix} \eta & 0 \\ 0 & 2\eta \end{pmatrix}. \quad (2)$$

Under the mean field limit, i.e., replacing  $\hat{\psi}$  and  $\hat{\psi}^\dagger$  by complex numbers  $\psi$  and  $\psi^*$  that correspond to coherent states of those operators, we rewrite  $\mathcal{H}(\psi, \psi^*; \mathbf{R}) = \sum_{ij} \psi_i^* T_{ij}(\psi, \psi^*; \mathbf{R}) \psi_j$ , where the matrix elements  $T_{11} = -T_{22} = \frac{R \cos \theta}{2}$ ,  $T_{12} = T_{21}^* = \sqrt{\frac{3}{8}} \frac{R \sin \theta}{2} e^{-i\varphi} \psi_1$ , and get the nonlinear Schrödinger equation as follows ( $\hbar = 1$ )

$$i \frac{d}{dt} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = H(\psi, \psi^*; \mathbf{R}) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad (3)$$

with

$$H(\psi, \psi^*; \mathbf{R}) = \begin{pmatrix} \frac{R \cos \theta}{2} & \sqrt{\frac{3}{8}} e^{i\varphi} R \sin \theta \psi_1^* \\ \sqrt{\frac{3}{8}} e^{-i\varphi} R \sin \theta \psi_1 / 2 & -\frac{R \cos \theta}{2} \end{pmatrix}. \tag{4}$$

The projective Hilbert space is spanned by the vector  $\mathbf{n}_a = (2\sqrt{2} \operatorname{Re}[(\psi_1^*)^2 \psi_2], 2\sqrt{2} \operatorname{Im}[(\psi_1^*)^2 \psi_2], |\psi_1|^2 - 2|\psi_2|^2)$ . Obviously, every point in this space corresponds to a class of quantum states among which the states are only different in co-diagonal total phases (see Eq. (2)). With the normalization condition  $|\bar{\psi}_1|^2 + 2|\bar{\psi}_2|^2 = 1$ , one can find that the projection space is a ‘tear-drop’ shaped surface [21].

We notice that even though the matrix in (4) is not conjugate symmetric, the original system represented by Eq. (1) is hermitian and the total system energy is bound. The analogous nonlinear Schrödinger equations have been widely applied in Feshbach molecular formation [17,22].

The eigenstates of the above system  $\bar{\phi}(\mathbf{R}) = (\bar{\phi}_1, \bar{\phi}_2)$  satisfies the following eigenequations

$$H(\bar{\phi}, \bar{\phi}^*; \mathbf{R}) \begin{pmatrix} \bar{\phi}_1 \\ \bar{\phi}_2 \end{pmatrix} = \begin{pmatrix} \mu & 0 \\ 0 & 2\mu \end{pmatrix} \begin{pmatrix} \bar{\phi}_1 \\ \bar{\phi}_2 \end{pmatrix}. \tag{5}$$

The above eigenequations define the eigenfunction  $\bar{\phi}$  and the eigenvalue (or chemical potential)  $\mu$  that are functions of the adiabatic parameter  $\mathbf{R}$ . The eigenequations are solved and the eigenfunctions are obtained as follows,

$$\bar{\phi}_2^\pm = \frac{(-\cos \theta \pm 1)}{\sqrt{6} \sin \theta}, \quad \bar{\phi}_1^\pm = e^{i\varphi/2} \sqrt{1 - 2|\bar{\phi}_2^\pm|^2}, \tag{6}$$

with the eigenvalue (or chemical potential for atom)  $\mu_\pm = \frac{R}{4}(\cos \theta \pm 1)$ .

Now, let us suppose the parameter vector  $\mathbf{R}(t)$  varies slowly in a time interval  $t \in [0, T]$ . For simplicity, we fix  $R, \theta$  and change  $\varphi$  slowly from 0 to  $2\pi$ , forming a loop in the parameter space, i.e.,  $\mathbf{R}(0) = \mathbf{R}(T)$ . The sweep rate  $\alpha = \frac{2\pi}{T}$  measures how slow the system evolves, and  $\alpha \rightarrow 0$  indicates the adiabatic limit. Initially the system populates in an eigenstate, i.e.,  $\psi(0) = \bar{\phi}(\mathbf{R}(0))$ , and it will keep close to the eigenstate during an adiabatic process, guaranteed by the adiabatic theory [17,23]. That is,  $\|\psi(t) - \bar{\phi}(\mathbf{R}(t))\| \equiv 1 - |\langle \psi(t) | \bar{\phi}(\mathbf{R}(t)) \rangle|^2 \sim \alpha^2$ . It indicates that  $|\langle \psi(T) | \psi(0) \rangle|^2 = 1$  in the adiabatic limit  $\alpha \rightarrow 0$ . Moreover, a total phase is acquired over the course of the cycle. As we show below, the total phase (for the atomic component)  $\arg(\langle \psi_1(T) | \psi_1(0) \rangle)$  can be decomposed into two parts in the adiabatic limit, i.e.,  $\lim_{\alpha \rightarrow 0} \arg(\langle \psi_1(T) | \psi_1(0) \rangle) = -(\gamma_a + \gamma_g)$ . The former has dynamical property and can be expressed as the time integral of the chemical potential for atom; the latter is of geometric property and its explicit expression will be derived analytically and shown to be dramatically different from the usual Berry phase formula.

The Eq. (3) and its conjugate construct a canonical structure of classical dynamics with the energy  $\mathcal{H}(\psi, \psi^*; \mathbf{R})$  as classical Hamiltonian and  $(\psi, i\psi^*)$  as a canonical variable pair. The gauge symmetry of  $\mathcal{H}$  given by (2) implies that the total atom number is conserved  $|\bar{\psi}_1|^2 + 2|\bar{\psi}_2|^2 = 1$  and the dynamics of the overall phase can be separated from the rest of the degrees of freedom [24]. For simplicity and without losing generality, we denote  $\lambda = \arg \psi_1$  and set total phase as  $\lambda$  for atomic components and  $2\lambda$  for molecular components, respectively. The other variables form a close set of Hamiltonian dynamics with the canonical pair defined as  $q = -\arg \psi_2 + 2\arg \psi_1$  and  $p = |\psi_2|^2$ . From (3) and its complex conjugate, we get

$$\frac{d\lambda}{dt} = p \frac{dq}{dt} - \mathcal{H}(p, q) - \Lambda(p, q), \tag{7}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q}, \quad \dot{q} = \frac{\partial \mathcal{H}}{\partial p}, \tag{8}$$

in which  $\mathcal{H}(p, q) = \frac{R \cos \theta}{2}(1 - 3p) + \sqrt{\frac{3}{8}} R \sin \theta (1 - 2p) \sqrt{p} \cos(q - \varphi)$  and  $\Lambda(p, q) = \operatorname{Re} \left( \sum_{i,j,k} \sqrt{p_i} \left( p_j \frac{\partial \tilde{T}_{ik}}{\partial p_j} - i \frac{\partial \tilde{T}_{ik}}{\partial q_j} \right) \sqrt{p_k} \right)$  and  $\tilde{T}_{ik}(p, q) = e^{i(\arg(\psi_k) - \arg(\psi_i))} T_{ik}$ . After some calculations, we get  $\Lambda(p, q) = \sqrt{\frac{3}{8}} \frac{R \sin \theta}{2} (1 - 2p) \sqrt{p} \cos(q - \varphi)$ .

The fixed point of the above Hamiltonian can be derived by setting the right-hand functions equal to zero in Eq. (8). We readily obtain  $\bar{p} = |\bar{\phi}_z^\pm|^2$  and  $\bar{q} = \varphi$ . These fixed points are local energy minima of system and therefore correspond to the eigenstates defined by (5).

For a linear quantum case, both matrix  $\{H_{ij}\}$  and  $\{T_{ij}\}$  are the functions of the parameter  $\mathbf{R}$  only, so that the last term in Eq. (7) vanishes, i.e.,  $\Lambda(p, q) = 0$ . The second term in the right-hand of Eq. (7) is the energy, whose time integral gives so-called dynamical phase. The time integral of the first term is the Aharonov–Anandan phase for a cyclic quantum evolution [25]. The above observation is readily extended to the adiabatic evolution of a quantum eigenstate, because the adiabatic theorem of quantum mechanics dictates that an initial nondegenerate eigenstate remains to be an instantaneous eigenstate and the evolution will be cyclic when the parameters move slowly in a circuit. In this case, the second term is the eigenenergy and the first term is just the Berry connection, i.e.,  $i \langle \bar{\phi}(\mathbf{R}) | \nabla | \bar{\phi}(\mathbf{R}) \rangle$ . Then the Berry phase equals the circuit integral of the Berry connection.

However, for our atom–molecule system, the contribution of the last term in (7) should be taken into account. Notice that the chemical potential is usually not identical to the energy while the dynamic phase should be the time integral of the chemical potential, and we need to evaluate the following quantity in adiabatic limit,

$$\Xi(p, q; \mathbf{R}) = \mathcal{H}(p, q) + \Lambda(p, q) - \mu(\mathbf{R}). \tag{9}$$

We denote  $p = \bar{p}(\mathbf{R}) + \delta p$  and  $q = \bar{q}(\mathbf{R}) + \delta q$ . Here  $\bar{p}(\mathbf{R})$  and  $\bar{q}(\mathbf{R})$  are the fixed points corresponding to the eigenstates defined by (5). The vector  $(\delta p, \delta q)$  represents the correction to the adiabatic eigenstates in the order of  $\alpha$  [26]. As will be shown,  $(\delta p, \delta q)$  contains some secular terms in addition to the rapid oscillations. These secular terms will be accumulated in the nonlinear adiabatic evolution and contribute to the geometric phase.

We expand the quantity  $\Xi(p, q; \mathbf{R})$  around the fixed point,

$$\Xi(p, q; \mathbf{R}) = \sqrt{\frac{3}{8}} \frac{R \sin \theta}{2} \frac{(1 - 6\bar{p})}{2\sqrt{\bar{p}}} \delta p + o(\delta q^2, \delta p^2). \tag{10}$$

Here we use the relations:  $\mathcal{H}(\bar{p}, \bar{q}) + \Lambda(\bar{p}, \bar{q}) = \mu(\mathbf{R})$ ,  $\partial \mathcal{H}(p, q) / \partial p|_{\bar{p}, \bar{q}} = \partial \mathcal{H}(p, q) / \partial q|_{\bar{p}, \bar{q}} = 0$ , and  $\frac{\partial \Lambda}{\partial q}|_{(\bar{p}, \bar{q})} = 0$ .

On the other hand, the  $(\delta p, \delta q)$  can be evaluated from the following Hamiltonian equations,

$$\dot{q} = \left. \frac{\partial^2 \mathcal{H}}{\partial p \partial p} \right|_{(\bar{p}, \bar{q})} \delta p + \left. \frac{\partial^2 \mathcal{H}}{\partial p \partial q} \right|_{(\bar{p}, \bar{q})} \delta q + o(\delta q^2, \delta p^2), \tag{11}$$

$$\dot{p} = - \left. \frac{\partial^2 \mathcal{H}}{\partial q \partial p} \right|_{(\bar{p}, \bar{q})} \delta p - \left. \frac{\partial^2 \mathcal{H}}{\partial q \partial q} \right|_{(\bar{p}, \bar{q})} \delta q + o(\delta q^2, \delta p^2). \tag{12}$$

Omitting the higher order terms and, keeping the secular terms by average over the fast oscillations, we obtain  $\langle (\delta p), \langle \delta q \rangle \rangle^T = \Omega^{-1} \left( \frac{d\bar{p}}{d\mathbf{R}} \dot{\mathbf{R}}, \frac{d\bar{q}}{d\mathbf{R}} \dot{\mathbf{R}} \right)^T$  with the matrix  $\Omega = \frac{\sqrt{8}}{\sqrt{3}R \sin \theta} \begin{pmatrix} 0 & -\frac{2p\sqrt{\bar{p}}}{(1+6\bar{p})} \\ \frac{1}{(1-2p)\sqrt{\bar{p}}} & 0 \end{pmatrix}$ . Then,

we get  $\delta p = -\frac{\sqrt{8}}{\sqrt{3}R \sin \theta} \frac{2p\sqrt{\bar{p}}}{(1+6\bar{p})} \dot{\mathbf{R}}$ . Therefore, by substituting the result into (10), and from (7), we get the total phase acquired by the eigenstate in adiabatic limit,  $\lambda = -(\gamma_d + \gamma_g)$ , with  $\gamma_d = \int \mu dt$  and the geometric phase,

$$\gamma_g = \oint \bar{p} d\varphi + \oint \frac{(1 - 6\bar{p})\bar{p}}{1 + 6\bar{p}} d\varphi, \tag{13}$$

$$= \frac{1}{6} \oint (1 \mp \cos \theta) d\varphi. \tag{14}$$

In contrast to previous works [27], the adiabatic geometric phase in the atom–molecule system is dramatically modified. The first term in the right-hand of Eq. (13) is the usual expression of the Berry phase that can be rewritten as the circuit integral of the Berry connection  $i \langle \bar{\phi}(\mathbf{R}) | \nabla | \bar{\phi}(\mathbf{R}) \rangle$ . The sec-

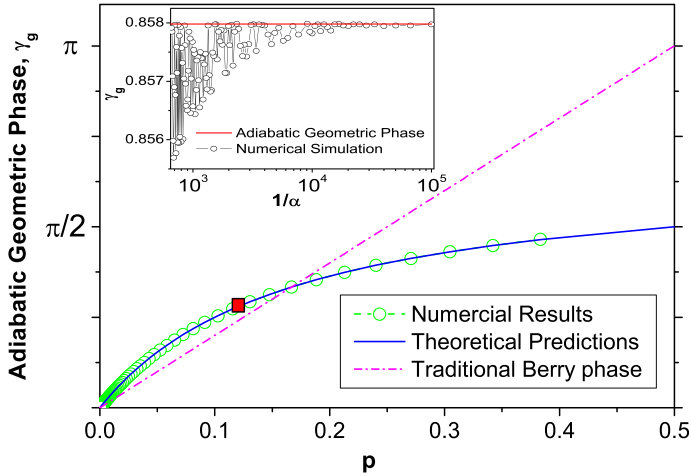


Fig. 1. The numerical results and comparison with theoretical predictions for the adiabatic geometric phase of eigenstate of  $\mu_+$ , in which the sweeping rate is  $\alpha = 0.0001$ . The insert figure shows convergence of geometric phase with sweeping rate.

ond novel term indicates that, the high-order correction to adiabatic approximate solution that is negligible in linear case, could be accumulated in the nonlinear adiabatic evolution with an infinite time duration in adiabatic limit and contributes a finite phase with geometric nature.

The above theoretical formulation on the Berry phase has been verified numerically by directly integrating the Schrödinger equation along the circle path in parameter space with  $R$  and  $\theta$  fixed, and  $\varphi$  varying with a very small sweeping rate  $\alpha$ , i.e.,  $\varphi = \alpha t$ . In Fig. 1, we show the numerical results and compare them with theoretical predictions for the adiabatic geometric phase of eigenstate of  $\mu_+$ , in which the sweeping rate is  $\alpha = 0.0001$ . The insert figure shows the convergence of the adiabatic geometric phase with the sweeping rates.

### 3. Geometric meaning of the nonlinear Berry phase: fractional monopole

For the linear systems, the Berry phase has been interpreted as the flux of a magnetic field of a quantized monopole through the surface enclosed by the loop in parameter space. This is demonstrated by the spin-half system, i.e.,  $H = -\frac{1}{2}\mathbf{R} \cdot \boldsymbol{\sigma}$  where  $\boldsymbol{\sigma}$  denotes pauli matrices and  $\mathbf{R} = (R \sin \theta \cos \phi, R \sin \theta \sin \phi, R \cos \theta)$  is a vector in the 3-D parameter space. The eigenvalues of the system are  $E_{\pm} = \pm \frac{R}{2}$ , and their eigenstates are  $|\psi_{\pm}\rangle = (\pm\sqrt{(1 \pm \cos \theta)/2}e^{-i\varphi/2}, \sqrt{(1 \mp \cos \theta)/2}e^{i\varphi/2})^T$ , respectively. The Berry phase equals the circuit integral of the Berry connection  $i\langle\psi(\mathbf{R})|\nabla|\psi(\mathbf{R})\rangle$ , can be interpreted as the flux of the magnetic field of a virtual monopole with the charge  $g_0 = \frac{1}{2}$ . In general, the degeneracies of the spectrum in parameter space are the singularities of the virtual magnetic field, and therefore play an important role in connexion with the geometric phase. Each degeneracy can be seen as a charge distribution located at the contact point between energy surfaces. Because the eigenstates are smooth and single valued outside the degeneracies, the total charge of the distribution, i.e., the monopole charge, is necessarily an integer multiple of the elementary charge  $g_0 = 1/2$ . The non-elementary monopoles with integer multiples of  $g_0$  have been found in case of light propagating and in condensed matter physics [28,29]. The mechanism for the production of monopole charges larger than the elementary  $g_0$  is due to constraints that act on the system [30].

For our nonlinear system, when parameters  $\mathbf{R} = (R, \theta, \varphi)$  are considered as spherical coordinates of a vector in a 3-D space, and then from (14) we get the vector potential,

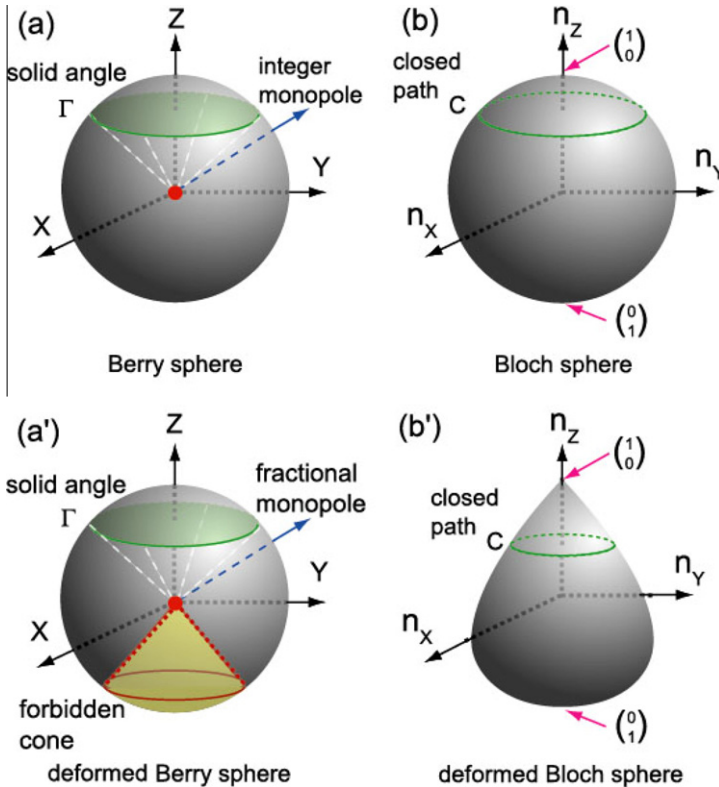
$$\mathbf{A} = \frac{1}{6} \frac{(1 - \cos \theta)}{R \sin \theta} \hat{e}_{\varphi}. \tag{15}$$

Here, for convenience we only consider the case for  $\mu_{\pm}$ . Hence, the Berry phase of atom–molecule conversion system can be interpreted as the flux of a magnetic field of a virtual monopole through the surface enclosed by the closed path in parameter space (see in Fig. 2(a')),  $\mathbf{B} = \nabla \times \mathbf{A}_{spin} = g \frac{\mathbf{R}}{R^3}$ . Here, the monopole charge  $g = \frac{1}{3}g_0$ , the fractional of the elementary charge of quantized monopole.

The fractional charge of monopole of this system is due to the symmetry breaking of the parameter space by the boundary. From (6), we find that  $|\bar{\psi}_2|$  increases with  $\theta$  monotonously. When  $\theta = 2\pi/3$ ,  $|\bar{\psi}_2| = 1/\sqrt{2}$  reaches its extreme value (since  $|\bar{\psi}_1|^2 + 2|\bar{\psi}_2|^2 = 1$ ). It implies that there is no eigenstate in the regime  $\theta > 2\pi/3$ , i.e., the Berry sphere of this system is a deformed sphere with a forbidden cone bounded by  $\theta = 2\pi/3$ . We illustrate this structure in Fig. 2(a'). The strange string lies on the negative Z-axis i.e.,  $\theta = \pi$ .

**4. Hannay angle in atom–molecule conversion system**

Extending to consider the classical counterpart, i.e., Hannay angle, of the above new form of Berry phase is of interest. Note that although the above system admits the quantal equations of motion, it appears formally to have classical structure if we regard the total phase and total particle number as a pair of canonical conjugate variables. We thus could exploit this particular feature to construct a canonical transformation to action-angle variables and derive the Hannay angle, i.e., the geometric



**Fig. 2.** The parameter space (a) and Bloch sphere (b) for a spin-half particle in magnetic field. (a') and (b') are the parameter space and Bloch sphere for the atom–molecule conversion system, respectively. The parameters change adiabatically along a close path shown as the green circles in the parameter spaces or Berry spheres. Accordingly, the eigenstate will evolve and form a close path schematically plotted as green circles on the Bloch spheres. The gray cone in (a') is the boundary for which  $\theta = 2\pi/3$ , inside which, i.e.,  $\theta > 2\pi/3$ , no eigenstate exists. See text for details. (For interpretation of color mentioned in this figure the reader is referred to the web version of the article.)

part involved in the angular evolution analytically. The dynamics of quantum system governed by Eq. (3) can be formally described by a classical system with the total energy as its classical Hamiltonian. For the two-mode model, it reads

$$\mathcal{H} = A(|\psi_1|^2 - |\psi_2|^2) + B|\psi_1|^2|\psi_2| \cos(\zeta_2 - 2\zeta_1 - \varphi), \tag{16}$$

in which  $\zeta_j = \arg(\psi_j)$ ,  $A = \frac{R \cos \theta}{2}$  and  $B = \sqrt{\frac{3}{8}}R \sin \theta$ . By introducing new canonical variables  $p_1 = |\psi_1|^2 + 2|\psi_2|^2$ ,  $q_1 = \zeta_1$ ,  $p_2 = |\psi_2|^2$ , and  $q_2 = \zeta_2 - 2\zeta_1$ , we obtain

$$\mathcal{H}(p_1; p_2, q_2) = A(p_1 - 3p_2) + B(p_1 - 2p_2)\sqrt{p_2} \cos(q_2 - \varphi). \tag{17}$$

To calculate the Hannay angle one needs to find the canonical transformation to the action-angle variables, and rewrite the Hamiltonian in terms of them. It is much difficult to do this directly from the above Hamiltonian. Here, we only focus on the Hannay angle of eigenstate, therefore we can simplify the Hamiltonian by expanding it around the eigenstate.

By denoting eigenstates with new variables as  $(\bar{p}_2, \bar{q}_2)$  and  $p_1 = 1$ , it satisfies

$$\left. \frac{\partial \mathcal{H}(1; p_2, q_2)}{\partial p_2} \right|_{\bar{p}_2, \bar{q}_2} = \left. \frac{\partial \mathcal{H}(1; p_2, q_2)}{\partial q_2} \right|_{\bar{p}_2, \bar{q}_2} = 0. \tag{18}$$

We then expand the Hamiltonian around  $(\bar{p}_2, \bar{q}_2)$ , and only keep the second orders

$$\mathcal{H}^d(p_1; p_2, q_2) = \mathcal{H}_0(p_1) + T(p_1)\delta p + G(p_1)\delta p^2 + F(p_1)\delta q^2, \tag{19}$$

where  $\delta p = p_2 - \bar{p}_2$ ,  $\delta p = q_2 - \varphi$  (here we have used the relation  $\bar{q}_2 = \varphi$ ),  $\mathcal{H}_0(p_1) = \mathcal{H}(p_1; \bar{p}_2, \varphi) = A(p_1 - 3\bar{p}_2) + B(p_1 - 2\bar{p}_2)\sqrt{\bar{p}_2}$ ,

$$T(p_1) = \left. \frac{\partial \mathcal{H}(p_1; p_2, q_2)}{\partial p_2} \right|_{\bar{p}_2, \bar{q}_2} = B(p_1 - 1)/2\sqrt{\bar{p}_2}, \tag{20}$$

$$G(p_1) = \left. \frac{\partial^2 \mathcal{H}(p_1; p_2, q_2)}{\partial p_2^2} \right|_{\bar{p}_2, \bar{q}_2} = -B(p_1 + 6\bar{p}_2)/8(\bar{p}_2)^{3/2}, \tag{21}$$

and

$$F(p_1) = \left. \frac{\partial^2 \mathcal{H}(p_1; p_2, q_2)}{\partial q_2^2} \right|_{\bar{p}_2, \bar{q}_2} = -B(p_1 - 2\bar{p}_2)/2\sqrt{\bar{p}_2}. \tag{22}$$

Considering  $E = \mathcal{H}^d(p_1; p_2, q_2)$  to be a constant, we have

$$p_1 = \Upsilon(\delta p, \delta q; E) = l, \tag{23}$$

where  $\Upsilon(\delta p, \delta q; E) = \frac{3A\sqrt{\bar{p}_2}\delta p + A\delta p^2/\sqrt{\bar{p}_2} + 2A\sqrt{\bar{p}_2}\bar{p}_2 + E}{B + A\sqrt{\bar{p}_2} + A\delta p/\sqrt{\bar{p}_2} - A\delta p^2/\sqrt{\bar{p}_2^3}}$ . Because  $p_1$  and  $(\delta p, \delta q)$  are independent variables, the above equation implies  $l$  should be a constant. Then from (23), we have

$$E = \mathcal{H}_0(l) - \frac{T^2(l)}{4G(l)} + G(l)\left(\delta p + \frac{T(l)}{2G(l)}\right)^2 + F(l)\delta q^2. \tag{24}$$

We thus could exploit this particular feature to construct a canonical transformation to action-angle variables. Assuming the generating function  $S = S_1(E; q_1) + S_2(E; q_2)$  where  $S_1$  and  $S_2$  have the relations  $p_1 = \frac{\partial S_1(E; q_1)}{\partial q_1}$  and  $p_2 = \frac{\partial S_2(E; q_2)}{\partial q_2}$ , and then from (23) and (24), we obtain

$$\frac{\partial S_1(E; q_1)}{\partial q_1} = l, \tag{25}$$

$$\frac{\partial S_2(E; q_2)}{\partial q_2} = \sqrt{\frac{E}{G} - \frac{F}{G}(q_2 - \varphi)^2} - \frac{T}{2G} + \bar{p}_2, \tag{26}$$

where  $\bar{E} = E - \mathcal{H}_0 + \frac{T^2(l)}{4G(l)}$ . According to the definition of actions, we have

$$J_1 = \frac{1}{2\pi} \oint l dp_1 = l, \tag{27}$$

$$J_2 = \frac{1}{\pi} \int_{\varphi}^{q_2^{\max}} \frac{\partial S_2(E; q_2)}{\partial q_2} dq_2, \tag{28}$$

$$= \frac{E - \mathcal{H}_0 + \frac{T^2(l)}{4G(l)}}{2(FG)^{1/2}}. \tag{29}$$

From (25) and (26), and considering  $(p_2, q_2)$  to be periodic evolution around  $(\bar{p}, \varphi)$ , we will have

$$S_1 = lq_1, \tag{30}$$

$$S_2 = S_g + \left( \bar{p}_2 - \frac{T}{2G} \right) (q_2 - \varphi), \tag{31}$$

in which

$$S_g = \int_{\varphi}^{q_2} \left[ \frac{\bar{E}}{G} - \frac{F}{G} (q_2 - \varphi)^2 \right]^{1/2} dq_2, \tag{32}$$

$$= 2J_2 \int_0^{\Gamma(q_2)} [1 - x^2]^{1/2} dx, \tag{33}$$

where  $\Gamma(q_2) = \frac{\sqrt{\bar{E}}}{\sqrt{(E - \mathcal{H}_0 + \frac{T^2}{4G})}} (q_2 - \varphi)$ .

Then we can obtain the new Hamiltonian with action-angle variables  $(J_1, \theta_1; J_2, \theta_2)$

$$\bar{\mathcal{H}}(J_1, \theta_1; J_2, \theta_2) = \mathcal{H}(J_1, J_2) + \frac{\partial S(J_1, J_2, q_1, q_2; \varphi)}{\partial t}, \tag{34}$$

where  $\mathcal{H}(J_1, J_2) = \mathcal{H}^d(p_1; p_2, q_2)$  and has the following form

$$\mathcal{H}(J_1, J_2) = 2[F(J_1)G(J_1)]^{1/2} J_2 + \mathcal{H}_0(J_1) - \frac{T^2(J_1)}{4G(J_1)}. \tag{35}$$

The Hannay angle is then obtained as

$$\theta_x^h = \oint \frac{\partial}{\partial J_x} \left( \frac{\partial S}{\partial \varphi} \right) d\varphi. \tag{36}$$

The Berry phase is shift of total phase, hence it should correspond to the Hannay angle for  $J_1$ . From the expression of generating function, we have  $\frac{\partial}{\partial J_1} \left( \frac{\partial S}{\partial \varphi} \right) = \frac{\partial}{\partial J_1} \left( \frac{\partial S_g}{\partial \varphi} \right) + \frac{\partial}{\partial J_1} \left( \frac{T}{2G} \right)$ . It is easy to find  $\frac{\partial}{\partial J_1} \left( \frac{\partial S_g}{\partial \varphi} \right) \propto J_2$ . By substituting the expressions of (20) and (21) and considering  $J_1 = 1$  and  $J_2 = 0$  for eigenstate, we finally obtain the Hannay angle

$$\theta^h = - \oint \frac{2\bar{p}_2}{1 + 6p_2} d\varphi. \tag{37}$$

Comparing this result with (13), we have  $\gamma_g = -\theta^h$ , i.e., the Hannay angle is found to exactly equal minus Berry phase of Eq. (13).

Now we discuss the novel connection between Berry phase and Hannay angle  $\gamma_g = -\theta^h$ . It is somewhat different from the usual derivative form that is known to exist at the semiclassical level for general Hamiltonian systems [3]. This is because although our above two-mode system admits the quantal equations of motion, it formally has classical structure exactly. That is, for the finite-mode systems, the quantum–classical correspondence could be exact rather than under the semiclassical approximation, and the quantal phase exactly corresponds to the classical angular variable. On the other hand, both the Berry phase and Hannay’s angle reflect the geometric property of the same cyclic



procedure. We thus expect that they should be equivalent. The above argument is applicable to the linear spin-1/2 system and spin-1 system [7,8], where the Hannay angles have been calculated and found to be identical to the Berry phase except for a sign.

## 5. Conclusion

We have investigated the issues on adiabatic Berry phase and Hannay angle in the atom–molecule conversion systems. We find that, in the atom–molecule conversion systems, the total phase of an eigenstate acquired in an adiabatic cyclic evolution consists of the dynamic part and the geometric part, while the geometric part cannot be accounted by the usual Berry phase formula due to the non-linearity brought forth by the coupling between atom and molecule. A novel formula of geometric phase is derived and an exotic monopole with fractional elementary charge in the parameter space is found. We also investigate the Hannay angle in the system and find it exactly equal to minus Berry phase. Finally, we make two remarks: (i) Our deduction is towards a simple two-mode nonlinear model in which the nonlinearity is from the fact that two atoms are needed to form one molecule. In principle, our discussions can be extended to multi-mode systems where more than two atoms are needed to form one molecule; (ii) Our above results are mean field limits of quantum many-body theory, and generalizing these considerations to quantized field theories from the correspondence principle is of interest for future study.

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## References

- [1] M.V. Berry, Proc. R. Soc. Lond. A 392 (1984) 45.
- [2] A. Shapere, F. Wilczek (Eds.), *Geometric Phase in Physics*, World Scientific, 1989;  
A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, J. Zwanziger, *The Geometric Phase in Quantum Systems*, Springer, 2003.
- [3] J.H. Hannay, J. Phys. A 18 (1985) 221.
- [4] M.V. Berry, J. Phys. A 18 (1985) 15.
- [5] Y. Aharonov, J. Anandan, Phys. Rev. Lett. 58 (1987) 1593.
- [6] M.V. Berry, J.H. Hannay, J. Phys. A 21 (1988) L325.
- [7] Nilanjana Datta, Gautam Ghosh, Phys. Rev. A 40 (1989) 526.
- [8] S.N. Biswas, S.K. Soni, T.R. Govdindarajan, J. Phys. A 23 (1990) L7.
- [9] Y.C. Ge, M.S. Child, Phys. Rev. Lett. 78 (1997) 2507.
- [10] Jie Liu, Bambi Hu, Baowen Li, Phys. Rev. Lett. 81 (1998) 1749;  
Jie Liu, Bambi Hu, Baowen Li, Phys. Rev. A 58 (1998) 3448.
- [11] T. Köhler, K. Góral, P.S. Julienne, Rev. Mod. Phys. 78 (2006) 1311.
- [12] J.J. Hudson, B.E. Sauer, M.R. Tarbutt, E.A. Hinds, Phys. Rev. Lett. 89 (2002) 023003.
- [13] C.A. Regal, M. Greiner, D.S. Jin, Phys. Rev. Lett. 92 (2004) 040403.
- [14] E.A. Donley et al, Nature London 417 (2002) 529;  
J.L. Roberts et al, Phys. Rev. Lett. 86 (2001) 4211.
- [15] R. Wynar et al, Science 287 (2000) 1016;  
M. Mackie, R. Kowalski, J. Javanainen, Phys. Rev. Lett. 84 (2000) 3803.
- [16] A. Vardi, V.A. Yurovsky, J.R. Anglin, Phys. Rev. A 64 (2001) 063611;  
H.Y. Ling, H. Pu, B. Seanman, Phys. Rev. Lett. 93 (2004) 250403;  
H. Jing, J. Cheng, P. Meystre, Phys. Rev. Lett. 99 (2007) 133002.
- [17] Han Pu et al, Phys. Rev. Lett. 98 (2007) 050406.
- [18] A.P. Itin, S. Watanabe, Phys. Rev. Lett. 99 (2007) 223903.
- [19] Y.S. Kivshar, B.A. Malomed, Rev. Mod. Phys. 61 (1989) 763.
- [20] Shaoying Meng, Li-Bin Fu, Jie Liu, Phys. Rev. A 78 (2008) 053410.
- [21] I. Tikhonenkov et al, Phys. Rev. A 73 (2006) 043605.
- [22] For example J. Li et al, Phys. Rev. A 79 (2009) 025602;  
H. Jing et al, Phys. Rev. Lett. 99 (2007) 133002.
- [23] Jie Liu, Li-Bin Fu, Phys. Lett. A 370 (2007) 17.
- [24] Jie Liu, Biao Wu, Qian Niu, Phys. Rev. Lett. 90 (2003) 170404.
- [25] Y. Aharonov, J.S. Anandan, Phys. Rev. Lett. 58 (1987) 1593.
- [26] Hong Y. Ling et al, Phys. Rev. A 75 (2007) 033615.

- [27] J.C. Garrison, R.Y. Chiao, *Phys. Rev. Lett.* 60 (1988) 165;  
Biao Wu, Jie Liu, Qian Niu, *Phys. Rev. Lett.* 94 (2005) 140402.
- [28] M.V. Berry, The Aharonov–Bohm effect is real physics not ideal physics, in: V. Gorini, A. Frigerio (Eds.), *Fundamental Aspects of Quantum Theory*, vol. 144, Plenum, NATO ASI series, 1986, pp. 319–320.
- [29] B. Simon, *Phys. Rev. Lett.* 51 (1983) 2167.
- [30] P. Leboeuf, A. Mouchet, *J. Phys. A* 36 (2003) 2847.