Berry connection in atom-molecule systems

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In the mean-field theory of atom-molecule systems, where bosonic atoms combine to form molecules, there is no usual U(1) symmetry, presenting an apparent hurdle for defining the Berry phase and Berry curvature for these systems. We define a Berry connection for this system, with which the Berry phase and Berry curvature can be naturally computed. We use a three-level atom-molecule system to illustrate our results. In particular, we have computed the mean-field Berry curvature of this system analytically, and compared it to the Berry curvature computed with the second-quantized model of the same system. An excellent agreement is found, indicating the validity of our definition.

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I. INTRODUCTION

In 1984, Berry discovered that in the adiabatic evolution of a quantum system, besides the dynamics phase, there exists an additional phase accompanying the evolution and this phase depends only on the geometric path in the parameter space [1]. This geometric phase, now called the Berry phase, along with the corresponding Berry curvature, has found wide applications in condensed matter physics [2,3] and important uses in the implementation of quantum computing gates [4,5]. Recently, the Berry phase has been generalized to nonlinear quantum system, such as the Bose-Einstein condensates described by the nonlinear Schrödinger equations [6]. This generalization is possible because of the well-known fact that quantum systems mathematically have a classical Hamiltonian structure [7,8].

A recent development in the field of ultracold atoms is to use Feshbach resonances [9] or a stimulated optical Raman transition [10,11] to convert two atoms into a molecule. This kind of atom-molecule systems can be well described by a mean-field theory and can become nonlinear systems when both the atoms and the molecules are bosons and the number of particles in this system is large. As nonlinearity can cause the breakdown of the adiabatic process, there has been great interest in the adiabatic evolution of the atom-molecule systems [12–17]. Naturally, there are also efforts to try to study the Berry phase in this type of systems [18]. It is not trivial to define the Berry phase in these atom-molecule systems: the mean-field Hamiltonian of these systems contains terms of the form $\psi_e^*\psi_a\psi_a$, which obviously does not have U(1) gauge invariance; this lack of U(1) invariance poses a difficulty in defining the Berry phase. In Ref. [18], the authors managed to circumvent the difficulty and defined Berry phase for these atom-molecule systems. However, it is not clear how the Berry connection and, therefore, the Berry curvature can be defined with their approach. It is also not clear how the mean-field Berry phase defined in Ref. [18] is related to the Berry phase for the second-quantized model of the system, which can be defined without any ambiguity.

In this paper, we show a Berry connection can be defined in the mean-field theory of the atom-molecule systems. With this Berry connection, the Berry phase and Berry curvature can be computed in the usual way. In particular, to show the validity of our definition, the Berry curvatures computed as such are compared to the Berry curvatures for the second-quantized model. This is done both analytically and numerically. Although our approach is general, we choose to use a three-level atom-molecule system [19,20] as an example to illustrate our results.

The paper is organized as follows. In Sec. II, we shall briefly introduce our theoretical model. In Sec. III, we define a Berry connection for this system. In Sec. IV, we compute the Berry curvatures for certain mean-field eigenstates, and compare them to the results obtained with the second-quantized model. Excellent agreement is found. Finally, in Sec. V, we discuss the results and conclude.

II. THREE-LEVEL ATOM-MOLECULE SYSTEM

We consider an atom-molecule Λ system shown in Fig. 1. With the atomic energy level set to be zero, the Hamiltonian of this atom-molecule system under the rotating-wave approximation can be written as

$$\hat{H}_N = \hbar\omega_e\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar\omega_g\hat{\psi}_g^\dagger\hat{\psi}_g + \hbar\Omega_d e^{i\nu_d t}\hat{\psi}_e^\dagger\hat{\psi}_g + \hbar\frac{\Omega_p e^{-i\nu_p t}}{\sqrt{N}}\hat{\psi}_e^\dagger\hat{\psi}_a\hat{\psi}_a + \text{H.c.}, \quad (1)$$

where ν_d and ν_p are the frequencies of laser pulse Ω_d and laser pulse Ω_p, respectively; the bosonic annihilation and creation operators $\hat{\psi}_\alpha$ and $\hat{\psi}_\alpha^\dagger$ are for state $|\alpha\rangle$ with α being a, g, or e; and N is the total number of atoms.

We note that Ω_p can be made complex. One way to achieve this is to split the laser pulse ν_p into two beams 1 and 2 and then recombine and focus them on the system. This will lead to a complex Ω_p as $\Omega_p = \varepsilon_1 + \varepsilon_2 e^{-i\varphi}$, where the phase φ is determined by the optical path difference between the two beams.

We split the Schrödinger picture Hamiltonian into two parts, $\hat{H}_N = \hat{H}_{N0} + \hat{H}_{N1}$, where

$$\hat{H}_{N0} = \hbar\nu_p\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar(\nu_p - \nu_d)\hat{\psi}_g^\dagger\hat{\psi}_g, \quad (2)$$

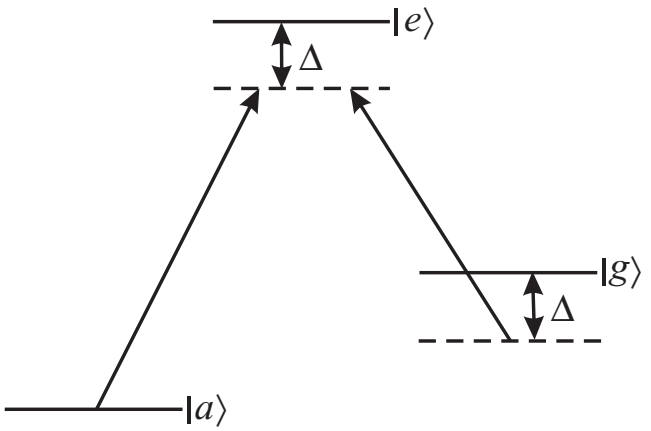

FIG. 1. Schematic level diagram of an atom-molecule Λ system. is the atomic energy level, $|g\rangle$ is the molecular ground state, and $|e\rangle$ is the excited molecular energy level. Ω_d and Ω_p are the two Rabi frequencies of the laser pulses. Δ is the detuning of the pump field with respect to the transition from $|a\rangle$ to $|e\rangle$.

$$\hat{H}_{N1} = \hbar(\omega_e - \nu_p)\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar(\omega_g - \nu_p + \nu_d)\hat{\psi}_g^\dagger\hat{\psi}_g + \hbar\Omega_d e^{-i\nu_d t}\hat{\psi}_e^\dagger\hat{\psi}_g + \hbar\frac{\Omega_p e^{-i\nu_p t}}{\sqrt{N}}\hat{\psi}_e^\dagger\hat{\psi}_a\hat{\psi}_a + \text{H.c.} \quad (3)$$

After choosing $\omega_e = \omega_g + \nu_d$ and using the the interaction picture Hamiltonian $\hat{H}_{NI} = e^{i\hat{H}_{N0}t/\hbar}\hat{H}_{N1}e^{-i\hat{H}_{N0}t/\hbar}$, we obtain

$$\hat{H}_{NI} = \hbar\Delta\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar\Delta\hat{\psi}_g^\dagger\hat{\psi}_g + \hbar Z\hat{\psi}_e^\dagger\hat{\psi}_g + \hbar\frac{(X - iY)}{\sqrt{N}}\hat{\psi}_e^\dagger\hat{\psi}_a\hat{\psi}_a + \text{H.c.}, \quad (4)$$

where $\Delta = \omega_e - \nu_p$, $Z = \Omega_d$, and $X - iY = \Omega_p$. The three parameters, X, Y, and Z, characterize the influences of the laser beams.

In the limit $N \to \infty$, this atom-molecule system becomes classical and can be described by the following mean-field Hamiltonian

$$H_s = \lim_{N\to\infty}\frac{\langle\hat{H}_{NI}\rangle}{N} = \hbar\Delta\psi_e^*\psi_e + \hbar\Delta\psi_g^*\psi_g + \hbar Z\psi_e^*\psi_g + \hbar(X - iY)\psi_e^*\psi_a\psi_a + \text{H.c.}, \quad (5)$$

where ψ_α is complex amplitude for the state $|\alpha\rangle$. The normalization is $2|\psi_e|^2 + 2|\psi_g|^2 + |\psi_a|^2 = 1$.

III. MEAN-FIELD BERRY CONNECTION

A particularly interesting point of this atom-molecule system is that its mean-field Hamiltonian H_s has no U(1) system. Instead, the Hamiltonian is invariant under the following transformation:

$$\begin{pmatrix}\psi_e\\ \psi_g\\ \psi_a\end{pmatrix} \to \mathrm{U}_s(1)\begin{pmatrix}\psi_e\\ \psi_g\\ \psi_a\end{pmatrix} = \begin{pmatrix}e^{2i\phi} & 0 & 0\\ 0 & e^{2i\phi} & 0\\ 0 & 0 & e^{i\phi}\end{pmatrix}\begin{pmatrix}\psi_e\\ \psi_g\\ \psi_a\end{pmatrix}. \quad (6)$$

Following Ref. [18], we shall call $\mathrm{U}_s(1)$ a skewed gauge transformation. This lack of U(1) gauge transformation presents an apparent difficulty in defining the Berry phase (or Berry connection) in this mean-field model. However, we notice that the mean-field Hamiltonian in Eq. (5) has a classical Hamiltonian structure. Namely, we can define three pairs of conjugate variables, $p_e = \sqrt{i\hbar}\psi_e^*, q_e = \sqrt{i\hbar}\psi_e$, $p_g = \sqrt{i\hbar}\psi_g^*, q_g = \sqrt{i\hbar}\psi_g$, and $p_a = \sqrt{i\hbar}\psi_a^*, q_a = \sqrt{i\hbar}\psi_a$, for this Hamiltonian. As the nonlinear Berry phase introduced in Ref. [6] applies in any system which has a classical Hamiltonian structure, it should also apply in this atom-molecule system. If we focus on the integrable regions, the system can be described by a set of action and angle variables. This means that we can define the Berry connection for this system as [6]

$$\vec{A} = i\overline{\langle\psi|\vec{\nabla}|\psi\rangle}, \quad (7)$$

where $\vec{\nabla} = (\partial/\partial X, \partial/\partial Y, \partial/\partial Z)$, and the bar indicates an average over all initial angles with the same actions. According to the quantum adiabatic theorem, in a linear quantum system the occupation probabilities of different eigenstates $|a_n|^2$ are adiabatic constants. In fact, they are actions $I_n = |a_n|^2$ when the system is regarded mathematically as a classical Hamiltonian system; their corresponding angle variables θ_n's are the phases of the a_n's. Therefore, for an instantaneous eigenstate, the averaging over the angles is no longer needed, and the Berry connection becomes

$$\vec{A}_n = i\langle\psi_n|\vec{\nabla}|\psi_n\rangle, \quad (8)$$

where $|\psi_n\rangle$ is an instantaneous eigenstate of the system. Let us now analyze the general properties of this connection.

Under the skewed gauge transformation $\mathrm{U}_s(1)$, we have

$$\vec{A} = i\langle\psi|\vec{\nabla}|\psi\rangle \longrightarrow \vec{A}' = \langle\psi|'i\frac{d}{dR}|\psi\rangle' = \vec{A} + (2|\psi_e|^2 + 2|\psi_g|^2 + |\psi_a|^2)\vec{\nabla}\phi, \quad (9)$$

where the last term is a trivial total derivative due to the conservation of the number of particles in the system. This indicates that the Berry connection defined in Eq. (7) is "gauge" invariant under $\mathrm{U}_s(1)$.

Usually, the Berry connection $\vec{A}$ defined in Eq. (7) is guaranteed to be real by the U(1) gauge symmetry. Due to the lack of U(1) symmetry in this atom-molecule system, the so-defined $\vec{A}$ is in general complex. However, this complexity does not pose any difficulty. To see this, we decompose it explicitly into the real part and the imaginary part

$$\vec{A} = \frac{i}{2}(\overline{\langle\psi|\vec{\nabla}|\psi\rangle} - \overline{\langle\vec{\nabla}\psi|\psi\rangle}) + \frac{i}{2}\vec{\nabla}(\overline{\langle\psi|\psi\rangle}), \quad (10)$$

which shows clearly that the imaginary part is a total derivative and, therefore, nonessential.

There is another way to justify the definition in Eq. (7), that is, through its semiclassical relation with the quantum Berry connection, which can be defined and computed with respect to the second-quantized Hamiltonian $\hat{H}_{N1}$. We denote it as $\vec{A}_N$, where the subscript N is referred to the number of atoms in the system. One can prove that [21]

$$\lim_{N\longrightarrow\infty}\left(\frac{\vec{B}_N}{N} - \vec{B}\right) = 0, \quad (11)$$

where $\vec{B} = \vec{\nabla}\times\vec{A}$ and $\vec{B}_N = \vec{\nabla}\times\vec{A}_N$ are the mean-field and quantum Berry curvatures, respectively. To prove this relation, one first notices that the mean-field Hamiltonian is in fact the semiclassical limit of $\hat{H}_{N1}$. To see this clearly, we can use the

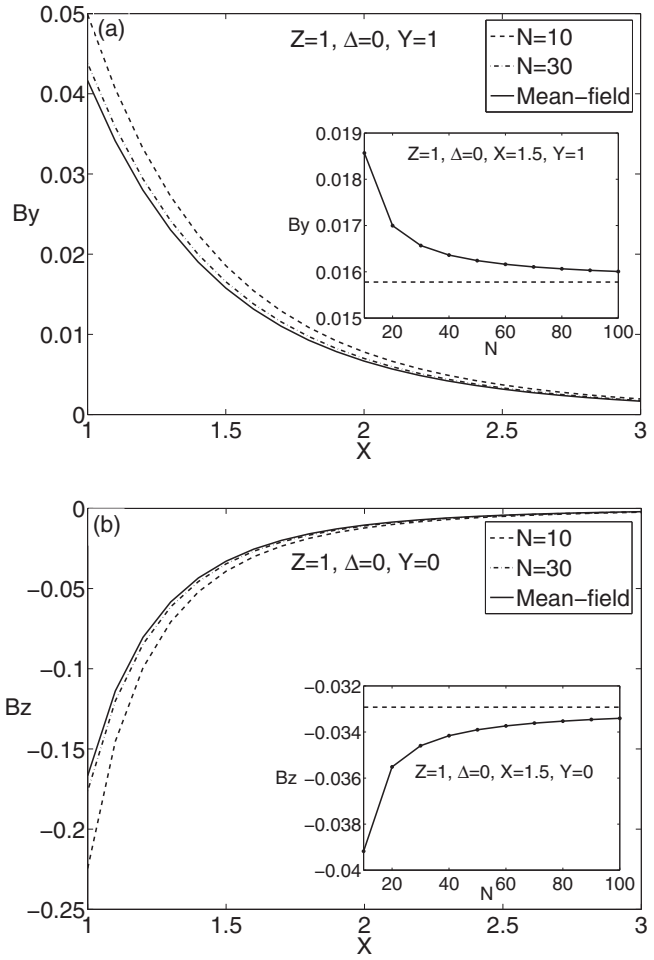

FIG. 2. (a) y component of the Berry curvature as a function of X at $Y = Z = 1$ and $\Delta = 0$. The inset shows how this Berry curvature changes as a function of N, the number of particles, at $X = 1.5$. (b) z component of the Berry curvature as a function of X at $Z = 1$ and $Y = \Delta = 0$. The inset shows how this Berry curvature changes as a function of N at $X = 1.5$. The dotted lines in the insets are for the mean-field values of the Berry curvature.

three pairs of conjugate variables, p_e,q_e, p_g,q_g, and p_a,q_a, and quantize them as follows:

$$[\hat{q}_e, \hat{p}_e] = [\hat{q}_g, \hat{p}_g] = [\hat{q}_a, \hat{p}_a] = \frac{i\hbar}{N}. \tag{12}$$

As can be checked easily, this recovers the second-quantized Hamiltonian $\hat{H}_{NI}$. Since these commutators approach zero as $N \longrightarrow \infty$, we see that the mean-field Hamiltonian H_s is the semiclassical limit of the quantum Hamiltonian H_{NI}. Since $\vec{A}$ defined in Eq. (7) can also be regarded as the connection for Hannay's angle [6], one can then prove the above semiclassical relation by following Berry's argument [22].

IV. EXAMPLE: EIGENSTATES

In this section, we use an example to illustrate the Berry connection that we have introduced in the last section. For simplicity, we focus on the ground state with $\Delta = 0$. When $X^2 + Y^2 > \frac{Z^2}{4}$, the ground state is

$$\psi_e = \tfrac{1}{2}, \psi_g = -\tfrac{1}{2}, \psi_a = 0, \tag{13}$$

with $\mu = -\frac{Z}{2}$. When $X^2 + Y^2 < \frac{Z^2}{4}$, the ground state is

$$\psi_e = -\frac{\sqrt{\frac{2}{3}(X^2+Y^2) + \frac{1}{12}Z^2}}{2(X - iY)}, \tag{14}$$

$$\psi_g = \frac{Z}{4(X - iY)}, \tag{15}$$

$$\psi_a = \sqrt{\frac{2}{3} - \frac{Z^2}{6(X^2+Y^2)}}, \tag{16}$$

with $\mu = -\sqrt{\frac{2}{3}(X^2+Y^2) + \frac{1}{12}Z^2}$.

With the definition of the Berry connection in Eq. (8), we are able to compute the mean-field Berry curvature. We find the Berry curvature is zero when $(X^2 + Y^2) < Z^2/4$. When $(X^2 + Y^2) > Z^2/4$,

$$\{B_x, B_y, B_z\} = \{X, Y, Z\} \frac{Z}{6(X^2+Y^2)^2}. \tag{17}$$

We have also computed the Berry curvature with the second-quantized model $\hat{H}_{NI}$ using the formula

$$B_{N0} = \mathrm{Im} \sum_{m \neq 0} \frac{\langle 0|\vec{\nabla}\hat{H}_{NI}|m\rangle \times \langle m|\vec{\nabla}\hat{H}_{NI}|0\rangle}{(E_m - E_0)^2}, \tag{18}$$

where E_m is the eigenenergy of the eigenstate $|m\rangle$. The second-quantized Berry curvature is compared to the mean-field Berry curvature as shown in Fig. 2. It is clear from the figure that these two sets of results are in very good agreement with the mean field. This further confirms that our definition of the Berry connection in Eq. (7) is valid.

V. CONCLUSION

In the present work, we have given a general definition of a Berry connection for nonlinear systems with a skewed U(1) gauge invariance. We have justified this definition from various aspects, in particular, its relation to a Berry connection for the corresponding quantum systems. We have used a three-level Λ atom-molecular system to illustrate our results. Our result clarifies a mystery surrounding how to define a Berry connection for nonlinear systems with skewed U(1) symmetry.

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