Entanglement, Berry phases, and level crossings for the atomic Breit-Rabi Hamiltonian

Sangchul Oh,[1,*] Zhen Huang,[2] Uri Peskin,[3] and Sabre Kais[1,2,†]
[1]*Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, D-01187 Dresden, Germany*
[2]*Purdue University, Department of Chemistry, West Lafayette, Indiana 47906 USA*
[3]*Technion Israel Institute of Technology, Schulich Faculty of Chemistry, IL-32000 Haifa, Israel*
(Received 16 October 2008; published 9 December 2008)

The relation between level crossings, entanglement, and Berry phases is investigated for the Breit-Rabi Hamiltonian of hydrogen and sodium atoms, describing a hyperfine interaction of electron and nuclear spins in a magnetic field. It is shown that the entanglement between nuclear and electron spins is maximum at avoided crossings. An entangled state encircling avoided crossings acquires a marginal Berry phase of a subsystem like an instantaneous eigenstate moving around real crossings accumulates a Berry phase. Especially, the nodal points of a marginal Berry phase correspond to the avoided crossing points.

DOI: 10.1103/PhysRevA.78.062106 PACS number(s): 03.65.Ud, 03.65.Vf, 32.60.+i

I. INTRODUCTION

Energy levels, eigenvalues of a Hamiltonian, play the most primary role in determining the properties of a quantum system. When energy levels cross or almost cross as parameters of a Hamiltonian vary, various interesting phenomena happen. For example, if two instantaneous energy levels of a time-dependent Hamiltonian undergo an avoided crossing, nonadiabatic tunneling, called Landau-Zener tunneling, between them takes place [1]. Closely related to this, the run time of adiabatic quantum computation is inversely proportional to the square of the energy gap between the ground and first excited levels [2]. An eigenstate encircling adiabatically degeneracy points accumulates a Berry phase in addition to a dynamical phase [3,4]. In quantum chemistry, a conical intersection of electronic energy surfaces of molecules plays a key role in understanding ultrafast radiationless reactions [5,6]. A quantum phase transition, a dramatic change in a ground state as parameters of a system vary, is related to crossings or avoided crossings of two lowest-energy levels [7]. Kais and co-workers have shown that the finite-size scaling method can be used for studying the critical behavior—i.e., the level degeneracy or absorption—of a few-body quantum Hamiltonian $H(\lambda_1,\ldots,\lambda_k)$ as a function of a set of parameters $\{\lambda_i\}$ [8,9]. These parameters could be the external fields, interatomic distances, nuclear charges for stability of negative ions, cluster size, and optical lattice parameters such as the potential depth [10]. Thus, it is important to develop a way of finding level crossings and to understand how eigenstates or relevant physical quantities change at crossing or avoided crossings.

Recently Bhattacharya and Raman presented a powerful algebraic method for finding level crossings without solving an eigenvalue problem directly [11]. Along with this mathematical way, it is necessary to understand what physical quantities can be used to detect or characterize crossings or avoided crossings. First of all, the measurement of a Berry phase could be a good way to detect level crossings because it is due to level crossings. It is well known that avoided crossings or glancing intersections are not the source of Berry phases [5]. Is there any way that Berry phases can detect *avoided level crossings*? Here we show that the marginal Berry phase of an entangled state could be an indicator of avoided level crossings.

The entropy is an another indicator of level crossings. Since level crossings or avoided crossings are accompanied by a drastic change in eigenstates, any contents of information on relevant eigenstates may also vary. The Shannon entropy of the electron density measures the delocalization or the lack of structure in the respective distribution. Thus the Shannon entropy is maximal for a uniform distribution—that is, for an unbound system—and is minimal when the uncertainty about the structure of the distribution is minimal [12]. González-Férez and Dehesa showed that the Shannon entropy could be used as an indicator of avoided crossings [13]. The level crossings or avoided crossings of a single particle are well known. Here we focus on the level crossing of a system with two or more particles and its relation to entanglement. The von Neumann entropy, the quantum version of the Shannon entropy, is a good entanglement measure for a bipartite pure state. In quantum information, much attention has been paid to the relation between entanglement and quantum phase transitions [14,15]. Recently one of the authors investigated the relation between entanglement, Berry phases, and level crossings for two qubits with an *XY*-type interaction and found that the level crossing is not always accompanied by an abrupt change in entanglement [16].

In this paper, in order to study how entanglement and Berry phases vary at level crossings, we consider the Breit-Rabi Hamiltonian describing a hyperfine interaction of electron and nuclear spins in a uniform magnetic field [17]. It is shown that the von Neumann entropy of the electron (or nuclear) spin is maximum at avoided crossings. It is demonstrated that the significant changes in Berry phases and entanglement are closely related to level crossings. We show that the marginal Berry phase of the electron (or nuclear) spin could be a good indicator of avoided level crossings. The marginal Berry phase has nodal points at the avoided crossing points.

The paper is organized as follows. In Sec. II, the Breit-Rabi Hamiltonian is introduced. In Sec. III, as a specific application of the Breit-Rabi Hamiltonian, we consider a hyperfine interaction between a nuclear spin 1/2 and an elec-

*scoh@pks.mpg.de
†Corresponding author: kais@purdue.edu

tron spin 1/2 of a hydrogen atom in a magnetic field. We analyze the close relation between entanglement, Berry phases, and level crossings. In Sec. IV, we make an similar analysis for a sodium atom with a nuclear spin 3/2 and an electron spin 1/2. In Sec. V, we summarize the main results.

II. BREIT-RABI HAMILTONIAN

Let us consider an atom with a single valence electron in the ground state with orbital angular momentum $L=0$. In the presence of a uniform magnetic field B in the z direction, its atomic spectrum is described by the Breit-Rabi Hamiltonian [17], which is given by the sum of the hyperfine interaction between a nuclear spin $\mathbf{I}$ and an electron spin $\mathbf{S}$ and their Zeeman couplings to the magnetic field

$$H = A\mathbf{I}\cdot\mathbf{S} + (aS_z + bI_z)B, \tag{1}$$

where A is the hyperfine coupling constant, $a=\gamma_e\hbar$, and $b=\gamma_n\hbar$. Here γ_e and γ_n are the electron and nuclear gyromagnetic ratios, respectively. The electron spin operator $\mathbf{S}$ and the nuclear spin operator $\mathbf{I}$ are measured in the unit of $\hbar$.

The Breit-Rabi Hamiltonian (1) is well studied to describe double resonance in nuclear magnetic resonance [18] and muon spin rotation in semiconductors [19]. Although simple and well understood, it still continues to provide new insights. Recently Bhattacharya and Raman found a new class of invariants of the Breit-Rabi Hamiltonian [11]. As will be shown here, it is a prime example for showing the close relation between level crossings, entanglement, and geometric phases. Also it is related to a Hamiltonian of electron spin qubits in quantum dots [20] where the Heisenberg interaction between two electron spins can be turned on and off to implement the controlled-NOT gate.

Before applying the Hamiltonian (1) to specific systems, let us look at its general properties. If $B=0$, then H commutes with both the square of the total spin operator, $\mathbf{J}^2$, and J_z, where the total spin operator is defined by $\mathbf{J}\equiv\mathbf{I}+\mathbf{S}$. However, for $B\neq 0$, due to the fact that $a\neq b$, the Hamiltonian (1) no longer commutes with $\mathbf{J}^2$, but still commutes with J_z. So the eigenvalue m of J_z is a good quantum number for the Breit-Rabi Hamiltonian. With ladder operators $S_\pm=S_x\pm iS_y$ and $I_\pm=I_x\pm iI_y$, the Hamiltonian (1) can be rewritten as

$$H = AI_zS_z + \frac{A}{2}(S_+I_- + S_-I_+) + B(aS_z + bI_z). \tag{2}$$

Let us use a simple notation $|m_S,m_I\rangle$ to represent the product state $|S,m_S\rangle\otimes|I,m_I\rangle$, where $|S,m_S\rangle$ is an eigenstate of $\mathbf{S}^2$ and S_z, and $|I,m_I\rangle$ is an eigenstate of $\mathbf{I}^2$ and I_z. The first and third terms in Eq. (2) give the diagonal matrix elements

$$\langle m_Sm_I|H|m_Sm_I\rangle = f(m_S,m_I) = Am_Sm_I + m_SaB + m_IbB. \tag{3a}$$

The second term in Eq. (2) corresponds to the off-diagonal matrix elements

$$\langle m_S'm_I'|S_+I_-|m_Sm_I\rangle = \sqrt{(S-m_S)(S+m_s+1)}\times\sqrt{(I+m_I)(I-m_I+1)}\,\delta_{m_S',m_S+1}\delta_{m_I',m_I-1}. \tag{3b}$$

Since $m_S'-m_S=1$ and $m_I'-m_I=-1$ (or vice versa), one has the selection rule $\Delta m=(m_S'+m_I')-(m_S+m_I)=0$; that is, the magnetic quantum number $m=m_S+m_I$ is conserved. This implies that the Hamiltonian (1) is block diagonal in the basis set $\{|m_S,m_I\rangle\}$ ordered by m.

III. HYDROGEN ATOM IN A UNIFORM MAGNETIC FIELD

A. Eigenvalues and eigenstates

As a simple but real system described by the Hamiltonian (1), let us consider the interaction between the nuclear spin $I=1/2$ and the electron spin $S=1/2$ of a hydrogen atom in a uniform magnetic field. Since H commutes with the z component of the total spin operator, $J_z=S_z+I_z$, it is convenient to arrange the product basis $\{|m_S,m_I\rangle\}$ in decreasing order of the magnetic quantum number m of J_z as $\{|\frac{1}{2},\frac{1}{2}\rangle,|\frac{1}{2},-\frac{1}{2}\rangle,|-\frac{1}{2},\frac{1}{2}\rangle,|-\frac{1}{2},-\frac{1}{2}\rangle\}$. By means of Eqs. (3a) and (3b), the Breit-Rabi Hamiltonian for a hydrogen atom can be written in the ordered basis

$$H = \frac{1}{4}\begin{pmatrix} A+2(a+b)B & 0 & 0 & 0 \\ 0 & -A+2(a-b)B & 2A & 0 \\ 0 & 2A & -A-2(a-b)B & 0 \\ 0 & 0 & 0 & A-2(a+b)B \end{pmatrix}. \tag{4}$$

The Hamiltonian (4) is block diagonal, so it is straightforward to obtain its eigenvalues and eigenvectors. The subspace of $m=\pm 1$ is spanned by $\{|\frac{1}{2},\frac{1}{2}\rangle,|-\frac{1}{2},-\frac{1}{2}\rangle\}$. The block Hamiltonian on this subspace is already diagonal and has its eigenvalues and eigenvectors

$$E_{\pm 1} = \frac{A}{4} \pm \frac{1}{2}(a+b)B, \tag{5a}$$

$$|E_{\pm 1}\rangle = \left|\pm\frac{1}{2},\pm\frac{1}{2}\right\rangle, \tag{5b}$$

where the subscripts ± 1 in $E_{\pm 1}$ denote the magnetic quantum number $m=\pm 1$. The block Hamiltonian with $m=0$ is defined on the subspace of $\{|\frac{1}{2},-\frac{1}{2}\rangle,|\frac{1}{2},-\frac{1}{2}\rangle\}$ and is written as

$$H_{m=0} = \frac{1}{4}\begin{pmatrix} -A + 2(a-b)B & 2A \\ 2A & -A - 2(a-b)B \end{pmatrix}. \quad (6)$$

One can interpret the Hamiltonian $H_{m=0}$ as that of a spin in an effective magnetic field in the x-z plane, $\mathbf{B}_{\text{eff}} \equiv (A/2, 0, (a-b)B/2)$. The eigenvalues and eigenvectors of $H_{m=0}$ can be written easily as

$$E_0^{\pm} = -\frac{A}{4} \pm \frac{1}{2}\sqrt{(a-b)^2B^2 + A^2}, \quad (7a)$$

$$|E_0^+\rangle = \cos\frac{\alpha}{2}\left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \sin\frac{\alpha}{2}\left|-\frac{1}{2}, \frac{1}{2}\right\rangle, \quad (7b)$$

$$|E_0^-\rangle = -\sin\frac{\alpha}{2}\left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \cos\frac{\alpha}{2}\left|-\frac{1}{2}, \frac{1}{2}\right\rangle, \quad (7c)$$

where $\tan\alpha \equiv \frac{A}{(a-b)B}$. In a weak-magnetic-field limit (so called the Zeeman region), the Zeeman energy is smaller than the hyperfine coupling. At $B=0$—i.e., $\alpha=\pi/2$—the ground eigenstate $|E_0^-\rangle$ becomes the singlet state, $|E_0^-\rangle = \frac{1}{\sqrt{2}}(|-\frac{1}{2}, \frac{1}{2}\rangle - |\frac{1}{2}, -\frac{1}{2}\rangle)$. In a strong magnetic field called the Paschen-Back region, the Zeeman couplings are dominant. That is, in the limit of $B \to \infty$, one has $\alpha \to 0$ and $|E_0^-\rangle \to |-\frac{1}{2}, \frac{1}{2}\rangle$.

The eigenvalues and eigenstates of the Breit-Rabi Hamiltonian for a hydrogen atom, Eqs. (5) and (7), depend on two parameters: the hyperfine constant A and the magnetic field B. The hyperfine constant A of the hydrogen atom in vacuum is positive. However, if a hydrogen atom is in an inert gas, the hyperfine constant A could be negative [21], resembling the spin-spin coupling constant in a Heisenberg model. We assume that A as well as B varies and can be negative. To this end, A in Eqs. (5) and (7) is replaced by $f\,A$ with $-1 \leqslant f \leqslant 1$, so A is still kept as a positive constant in vacuum. If f is negative, so is the hyperfine constant.

Depending on f and B, the ground state of the Hamiltonian (4) is given either by $|E_{\pm 1}\rangle$ or by $|E_0^-\rangle$. It is convenient to plot the energy levels normalized by A. Then, Eqs. (5) and (7) become $E_{\pm 1}/A = \frac{f}{4} \pm \frac{1}{2}(a'+b')B$ and $E_0^{\pm}/A = -\frac{f}{4} \pm \frac{1}{2}\sqrt{(a'-b')^2B^2+f^2}$, where $a' \equiv a/A \approx 19.767\ \text{T}^{-1}$ and $b' \equiv b/A \approx -0.03\ \text{T}^{-1}$ are taken from Ref. [22], and B is measured in units of tesla. The energy levels E_m/A are plotted as functions of B for $f=1$ in Fig. 1(a) and for $f=-0.5$ in Fig. 1(b). For $f \geqslant 0$, the ground level is E_0^-. For $f<0$, two levels $E_0^{\pm}$ and $E_{\pm 1}$ with different magnetic quantum numbers cross at $f = \frac{2a'b'}{a'-b'}|B|$. Figure 2(a) shows the energy gap Δ/A between the ground and first excited states as a function of f and B, where we take $a'=0.1\ \text{T}^{-1}$ and $b'=-0.01\ \text{T}^{-1}$ to see clearly the phase diagram of the ground state of the Hamiltonian (4) determined by the magnetic quantum number m. As shown in Fig. 2(a), the energy gap Δ/A vanishes along the lines defined by $f = \frac{2a'b'}{a'-b'}|B|$ and the negative f axis. In the region of $f < \frac{2a'b'}{a'-b'}|B|$, the ground state becomes either $|E_{+1}\rangle$ or $|E_{-1}\rangle$ with magnetic quantum number $m=1$ or $m=-1$, respectively. On the other hand, the ground state in the region defined by $f > \frac{2a'b'}{a'-b'}|B|$ is given by $|E_0^-\rangle$ with magnetic quantum number $m=0$. One can see that the magnetic quantum number m of the ground state changes abruptly at the level crossing points.

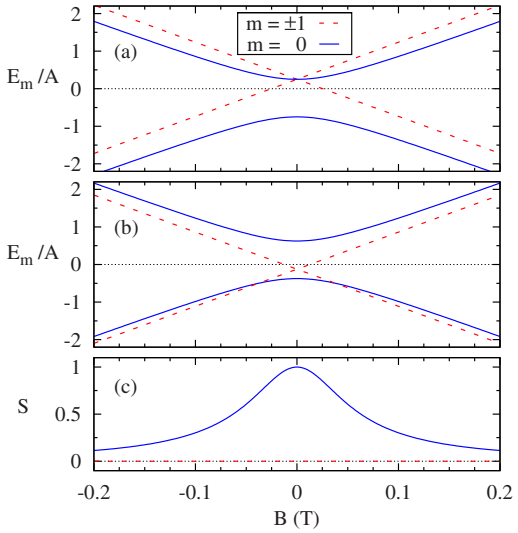

FIG. 1. (Color online) Energy levels E_m/A of the Breit-Rabi Hamiltonian for a hydrogen atom as functions of the magnetic field B with (a) $f=1$ and (b) $f=-0.5$. (c) The von Neumann entropy S of the electron (or nuclear) spin for each eigenstate. Here $a' = 19.767\ \text{T}^{-1}$ and $b' = -0.03\ \text{T}^{-1}$ are taken from Ref. [22].

B. Entanglement

Let us discuss the relation between level crossings and entanglement. Entanglement refers to the quantum correla-

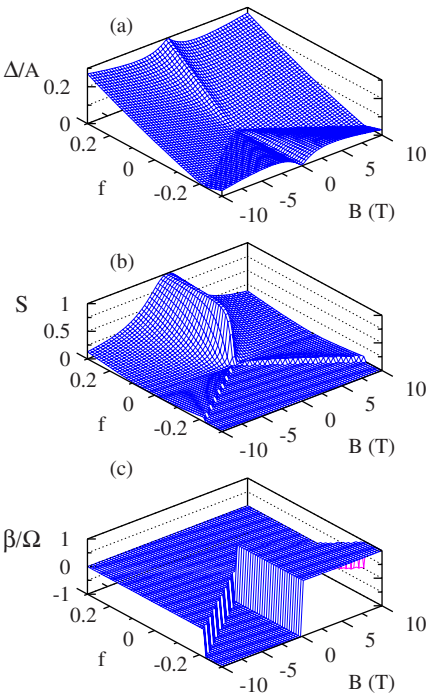

FIG. 2. (Color online) (a) Energy gap Δ/A between the ground and first excited states, (b) the von Neumann entropy S of the electron (or nuclear) spin, and (c) the Berry phase β/Ω of the ground state for a hydrogen atom as a function of f and B. Here $a' = 0.01\ \text{T}^{-1}$ and $b' = -0.1\ \text{T}^{-1}$ are taken to see the jumps clearly at the level crossings.

tion between subsystems and has no classical analog [23,24]. When level crossing happens as the parameter of the Hamiltonian varies, the ground state changes drastically. Entanglement as a physical quantity may also undergo a significant change. However, entanglement is not always a good indicator of level crossing as shown in Ref. [16].

First, let us examine the relation between entanglement and level crossings for each eigenstate. The von Neumann entropy S of a subsystem is a good entanglement measure for a pure bipartite system. If $|\psi_{AB}\rangle$ is a quantum state of a system composed of two subsystems A and B, the entanglement between A and B is measured by the von Neumann entropy of the subsystem, $S(\rho_A)=-\mathrm{tr}(\rho_A \log \rho_A)=S(\rho_B)=-\mathrm{tr}(\rho_B \log_2 \rho_B)$, where the reduced density matrix ρ_A of the subsystem A is obtained by tracing out the degrees of freedom of B as $\rho_A=\mathrm{tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|)$. If the ground state is given by $|E_{\pm 1}\rangle$—i.e., a product state—then the von Neumann entropy S of the electron (or nuclear) spin is zero. On the other hand, for the quantum state $|E_0^{\pm}\rangle$ of the electron and nuclear spins, the von Neumann entropy of the electron (or nuclear) spin can be written as

$$S(\rho_A) = -\frac{1+\cos\alpha}{2}\log_2\frac{1+\cos\alpha}{2} - \frac{1-\cos\alpha}{2}\log_2\frac{1-\cos\alpha}{2}. \tag{8}$$

Figure 1(c) shows the von Neumann entropy of the electron (or nuclear) spin for each eigenstate as a function of B. For the eigenstates $|E_0^{\pm}\rangle$, it is maximum at $B=0$—i.e., at the avoided crossing point. This is analogous to the sharp change in Shannon entropy at the avoided crossing in Ref. [13].

Now, let us look at how entanglement changes at level crossings as the parameters of the Hamiltonian vary. Figure 2(b) plots the von Neumann entropy S of the electron (or nuclear) spin for the ground state as a function of f and B. Across the level crossing line $f=\frac{2a'b'}{a'-b'}|B|$, the von Neumann entropy changes abruptly. For $f>0$, S becomes 1 as B goes to 0. Along the line of $f=0$, the von Neumann entropy S vanishes even though there is no level crossing. It will be interesting to investigate the more general case that entanglement does not work as an indicator to level crossings.

C. Berry phase

An instantaneous eigenstate encircling the energy level crossing points acquires the Berry phase in addition to the dynamical phase. The information on the level crossings is encoded in the Berry phase. At $B=0$ and $f=1$, the two levels $E_{\pm 1}$ cross and the other two levels $E_0^{\pm}$ avoid crossing. Also $E_{\pm 1}$ and E_0^{-} cross at $f=\frac{2a'b'}{a'-b'}|B|$. Here we focus on the Berry phase due to the level crossing or avoided crossing at $B=0$.

Due to the fact that $a \gg |b|$, an electron spin rotates much faster than a nuclear spin. We assume that the magnetic field $\mathbf{B}$ is rotated slowly enough for both the electron and nuclear spins to evolve adiabatically. The magnetic field $\mathbf{B}=B\hat{\mathbf{n}}$ in the direction of $\hat{\mathbf{n}}=(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is constructed starting from $\mathbf{B}=B\hat{\mathbf{z}}$. First, it is rotated about the y axis by an angle θ. And it is subsequently rotated about the z axis by an angle ϕ. The SO(3) rotation of the magnetic field described above corresponds to the $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$ transformation on the Hamiltonian (1); thus, one obtains the Breit-Rabi Hamiltonian in the magnetic field $\mathbf{B}=B\hat{\mathbf{n}}$:

$$H(\theta,\phi) = A\mathbf{I}\cdot\mathbf{S} + a\mathbf{B}\cdot\mathbf{S} + b\mathbf{B}\cdot\mathbf{I}. \tag{9}$$

The hyperfine interaction $A\mathbf{I}\cdot\mathbf{S}$ is spherical symmetric, so the eigenvalues and eigenvectors of the Hamiltonian (9) are identical to those of the Hamiltonian (4) except replacing $|\pm\frac{1}{2}\rangle$ by $|\hat{\mathbf{n}};\pm\frac{1}{2}\rangle$. Here $|\hat{\mathbf{n}};\pm\frac{1}{2}\rangle$ are eigenstates of $\hat{\mathbf{n}}\cdot\mathbf{S}$ or $\hat{\mathbf{n}}\cdot\mathbf{I}$. If the magnetic field $\mathbf{B}$ is rotated slowly about the z axis by 2π to make a cone with a solid angle $\Omega=2\pi(1-\cos\theta)$, then the instantaneous eigenstate $|\hat{\mathbf{n}};\pm\frac{1}{2}\rangle$ follows it and accumulates the Berry phase $\beta_{\pm}=\mp\frac{1}{2}\Omega$. The total Berry phase β of electron and nuclear spins is the sum of two phases acquired by each one. It depends on the magnetic quantum number m:

$$\beta = \begin{cases} \mp\Omega & \text{for } m = \pm 1, \\ 0 & \text{for } m = 0. \end{cases} \tag{10}$$

As expected, the Berry phase is nonzero only for real crossings—i.e., $m=\pm 1$. Figure 2(c) plots the total Berry phase as a function of B and f and shows that the total Berry phase jumps at the level crossings. The zero Berry phase of the eigenstates $|E_0^{\pm}(\theta,\phi)\rangle$ can be understood in two ways. First, two levels $E_0^{\pm}$ avoid crossing at $B=0$, so it is zero. Another view is as follows. Since $|E_0^{\pm}\rangle$ is a superposition of $|\frac{1}{2},-\frac{1}{2}\rangle$ and $|-\frac{1}{2},\frac{1}{2}\rangle$, the Berry phase of the electron spin is opposite to that of the nuclear spin and they cancel each other.

Although the entangled states $|E_0^{\pm}\rangle$ of electron and nuclear spins accumulate no Berry phase, each subsystem (electron spin or nuclear spin) can get nonzero marginal Berry phases of mixed states. Following studies on the geometric phase of mixed states [25,26] and the relation between entanglement and marginal Berry phases [26–28], we investigate the relation between avoided level crossings, marginal Berry phases, and entanglement. For an adiabatic cyclic evolution parametrized by $\mathbf{x}$, an instantaneous eigenstate of a bipartite system AB can be expressed in a Schmidt decomposition $|\psi(\mathbf{x})\rangle=\sum_{i=1}^{M}\sqrt{p_i}|e_i(\mathbf{x})\rangle\otimes|f_i(\mathbf{x})\rangle$, where $\{|e_i(\mathbf{x})\rangle\}_{i=1}^{N_A}$ is an orthonormal basis for a subsystem A, $\{|f_i(\mathbf{x})\rangle\}_{i=1}^{N_B}$ for a subsystem B, $M\leqslant\min\{N_A,N_B\}$, and $\sum_{i=1}^{M}p_i=1$. Here our attention is restricted to the case that the Schmidt coefficients $\sqrt{p_i}$ are independent of $\mathbf{x}$. After an adiabatic cyclic evolution implemented by $\mathbf{x}(0)=\mathbf{x}(T)$, the total Berry phase of the bipartite system AB is given by

$$\beta = \sum_{i=1}^{M} p_i(\beta_i^A + \beta_i^B), \tag{11}$$

where $\beta_i^A=i\oint_C d\mathbf{x}\cdot\langle e_i(\mathbf{x})|\nabla_{\mathbf{x}}|e_i(\mathbf{x})\rangle$. Then the marginal mixed-state Berry phase Γ_A of a subsystem A is defined by

$$\Gamma_A = \arg\sum_i p_i \exp(i\beta_i^A). \tag{12}$$

With Eqs. (11) and (12), let us analyze how the total Berry phase and the marginal Berry phase of $|E_0^{-}\rangle$ depend on B. The

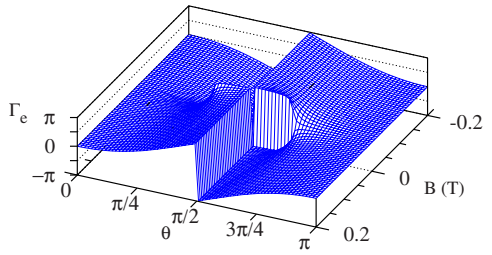

FIG. 3. (Color online) Marginal Berry phase Γ_e of the electron spin for the entangled eigenstate $|E_0^-\rangle$ of a hydrogen atom as a function of B and the azimuthal angle θ. Here we take $f=1$, $a'=19.767\ \mathrm{T}^{-1}$, and $b'=-0.03\ \mathrm{T}^{-1}$.

two Schmidt coefficients are given by $p_1=\sin^2\frac{\alpha}{2}$ and $p_2=\cos^2\frac{\alpha}{2}$. It is easy to obtain the marginal Berry phase of the electron spin, $\Gamma_e=\arctan(\cos\alpha\tan\frac{\Omega}{2})$, and the average Berry phase of the electron spin, $\beta_e\equiv p_1\beta_1^e+p_2\beta_2^e=\frac{\Omega}{2}\cos\alpha$. In the limit of $B\gg 1$—i.e., $\alpha\to 0$—one has $|E_0^-\rangle\to|-\frac{1}{2},\frac{1}{2}\rangle$ and $\beta_e=\Omega/2$. Also the marginal Berry phase of the electron spin is given by $\Gamma_e=\Omega/2$ for $0\leqslant\theta<\frac{\pi}{2}$. Figure 3 plots Γ_e as a function of B and the azimuthal angle θ. The marginal Berry phase of the electron spin jumps at $\theta=\pi/2$ and $B=0$. The node at $B=0$ corresponds to the avoided crossing.

IV. SODIUM ATOM IN A UNIFORM MAGNETIC FIELD

A. Energy spectrum

Now we consider an ^{23}Na atom in its $3S_{1/2}$ ground state in the presence of a uniform magnetic field B along the z axis. The nuclear and electron spins of an ^{23}Na atom are $I=2/3$ and $S=1/2$, respectively. Although the Breit-Rabi Hamiltonian of an ^{23}Na atom is similar to that of a hydrogen atom in Sec. III, the former shows different features from the latter. The ground state of the Breit-Rabi Hamiltonian of an ^{23}Na atom has both real crossing at $B=0$ and avoided crossing at $B\neq 0$ as will be shown. As in Sec. III, it is convenient to arrange the product basis $\{|m_S,m_I\rangle\}$ in decreasing order of the magnetic quantum number m of J_z as follows: $\{|\frac{1}{2},\frac{3}{2}\rangle\}$, $\{|\frac{1}{2},\frac{1}{2}\rangle,|-\frac{1}{2},\frac{3}{2}\rangle\}$, $\{|\frac{1}{2},-\frac{1}{2}\rangle,|-\frac{1}{2},\frac{1}{2}\rangle\}$, $\{|\frac{1}{2},-\frac{3}{2}\rangle,|-\frac{1}{2},-\frac{1}{2}\rangle\}$, and $\{|-\frac{1}{2},-\frac{3}{2}\rangle\}$. For example, $\{|\frac{1}{2},\frac{1}{2}\rangle,|-\frac{1}{2},\frac{3}{2}\rangle\}$ spans the subspace of $m=1$. In this ordered basis set, the Hamiltonian (1) for the sodium atom can be represented by a block-diagonal matrix

$$H=\begin{pmatrix}
f\left(\frac{1}{2},\frac{3}{2}\right) & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & f\left(\frac{1}{2},\frac{1}{2}\right) & \frac{\sqrt{3}}{2}A & 0 & 0 & 0 & 0 & 0\\
0 & \frac{\sqrt{3}}{2}A & f\left(\frac{-1}{2},\frac{3}{2}\right) & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & f\left(\frac{1}{2},\frac{-1}{2}\right) & \frac{A}{2} & 0 & 0 & 0\\
0 & 0 & 0 & \frac{A}{2} & f\left(\frac{-1}{2},\frac{1}{2}\right) & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & f\left(\frac{1}{2},\frac{-3}{2}\right) & \frac{\sqrt{3}}{2}A & 0\\
0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2}A & f\left(\frac{-1}{2},\frac{-1}{2}\right) & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & f\left(\frac{-1}{2},\frac{-3}{2}\right)
\end{pmatrix}, \tag{13}$$

where $f(m_S,m_I)\equiv Am_Sm_I+m_SaB+m_IbB$. Each block is at most a 2×2 matrix and can be easily diagonalized. First, consider the subspace of $m=\pm 2$. The corresponding eigenvalues and eigenvectors can be written as

$$E_{\pm 2}=\frac{3}{4}A\pm\frac{1}{2}(a+3b)B, \tag{14a}$$

$$|E_{\pm 2}\rangle=\left|\pm\frac{1}{2},\pm\frac{3}{2}\right\rangle. \tag{14b}$$

Notice that Eqs. (14) are comparable to Eqs. (5). Second, in the subspace with $m=1$ spanned by $\{|\frac{1}{2},-\frac{1}{2}\rangle,|-\frac{1}{2},\frac{1}{2}\rangle\}$, one obtains the eigenvalues and eigenvectors

$$E_{+1}^{\pm}=-\frac{A}{4}+bB\pm\frac{1}{2}\sqrt{[A+(a-b)B]^2+3A^2}, \tag{15a}$$

$$|E_{+1}^{+}\rangle = \cos\frac{\alpha_1}{2}\left|\frac{1}{2},\frac{1}{2}\right\rangle + \sin\frac{\alpha_1}{2}\left|-\frac{1}{2},\frac{3}{2}\right\rangle, \quad (15b)$$

$$|E_{+1}^{-}\rangle = -\sin\frac{\alpha_1}{2}\left|\frac{1}{2},\frac{1}{2}\right\rangle + \cos\frac{\alpha_1}{2}\left|-\frac{1}{2},\frac{3}{2}\right\rangle, \quad (15c)$$

where $\tan\alpha_1 \equiv \frac{\sqrt{3}A}{A+(a-b)B}$. Third, the Hamiltonian of $m=-1$ is defined on the subspace spanned by $\{|\frac{1}{2},-\frac{3}{2}\rangle,|-\frac{1}{2},-\frac{1}{2}\rangle\}$. Its eigenvalues and eigenstates are given by

$$E_{-1}^{\pm} = -\frac{A}{4} - bB \pm \frac{1}{2}\sqrt{[A-(a-b)B]^2+3A^2}, \quad (16a)$$

$$|E_{-1}^{+}\rangle = \cos\frac{\alpha_2}{2}\left|-\frac{1}{2},-\frac{1}{2}\right\rangle + \sin\frac{\alpha_2}{2}\left|\frac{1}{2},-\frac{3}{2}\right\rangle, \quad (16b)$$

$$|E_{-1}^{-}\rangle = -\sin\frac{\alpha_2}{2}\left|-\frac{1}{2},-\frac{1}{2}\right\rangle + \cos\frac{\alpha_2}{2}\left|\frac{1}{2},-\frac{3}{2}\right\rangle, \quad (16c)$$

where $\tan\alpha_2 \equiv \frac{\sqrt{3}A}{A-(a-b)B}$. Note that Eqs. (16) can be obtained from Eqs. (15) by replacing B with $-B$. Finally, the subspace of $m=0$ is spanned by $\{|\frac{1}{2},-\frac{1}{2}\rangle,|\frac{1}{2},-\frac{1}{2}\rangle\}$. The corresponding eigenvalues and eigenvectors are given by

$$E_0^{\pm} = -\frac{A}{4} \pm \frac{1}{2}\sqrt{(a-b)^2B^2+4A^2}, \quad (17a)$$

$$|E_0^{+}\rangle = \cos\frac{\alpha_0}{2}\left|\frac{1}{2},-\frac{1}{2}\right\rangle + \sin\frac{\alpha_0}{2}\left|-\frac{1}{2},\frac{1}{2}\right\rangle, \quad (17b)$$

$$|E_0^{-}\rangle = -\sin\frac{\alpha_0}{2}\left|\frac{1}{2},-\frac{1}{2}\right\rangle + \cos\frac{\alpha_0}{2}\left|-\frac{1}{2},\frac{1}{2}\right\rangle, \quad (17c)$$

where $\tan\alpha_0 \equiv \frac{A}{(a-b)B}$. As expected, Eqs. (17) is very similar to Eqs. (7) in the case of a hydrogen atom.

B. Entanglement

Let us examine the relation between entanglement and level crossings or avoided crossings for a sodium atom. With the values of the parameters A, a, and b of the ^{23}Na atom in Ref. [22], the energy levels $E_m^{\pm}/A$ are plotted in Fig. 4(a). The von Neumann entropies of the electron (or nuclear) spin for each eigenstates are shown in Fig. 4(b). The ground state is given by $|E_{+1}^{-}\rangle$ for $B>0$ and $|E_{-1}^{-}\rangle$ for $B<0$. Two levels E_{+1}^{+} and E_{+1}^{-} are avoided crossing and maximally entangled at $A-(a-b)B=\sqrt{3}A$. Another two levels E_{-1}^{+} and E_{-1}^{-} are avoided crossing and maximally entangled at $A+(a-b)B=\sqrt{3}A$. Two levels with $m=0$, $E_0^{\pm}$ are avoided crossing and maximally entangled at $B=0$. Two levels $E_{\pm 2}$ show real crossing at $B=0$ and have zero von Neumann entropies. Again one can see that the eigenstate is maximally entangled at the avoided crossing point. This is analogous to the results in Ref. [13], where Shannon entropy is used as an indicator of avoided crossings.

C. Berry phase

As in Sec. III C, let us consider an adiabatic cyclic evolution of nuclear and electron spins of a sodium atom by rotating the magnetic field $B\hat{\mathbf{n}}$ slowly. For an adiabatic rotation keeping the azimuthal angle θ constant and varying the polar angle ϕ from 0 to 2π, the instantaneous eigenstates accumulate the total Berry phases proportional to the magnetic quantum number m, $\beta=\mp m\Omega$. In contrast to a hydrogen atom, the ground state is given either by $|E_{+1}^{-}\rangle$ or by $|E_{-1}^{-}\rangle$ with $m=\pm 1$, so it acquires the total Berry phase $\beta=\mp\Omega$.

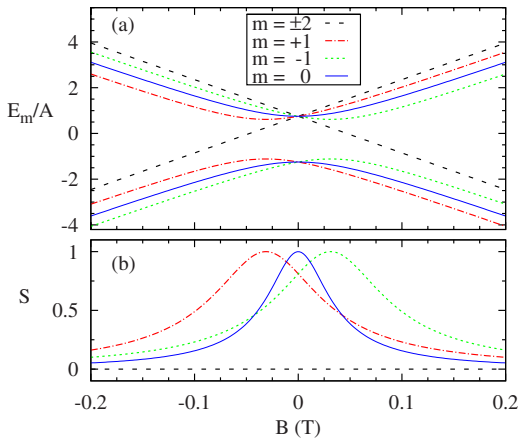

FIG. 4. (Color online) (a) Energy levels E_m/A and (b) the von Neumann entropy S of the electron (or nuclear) spin for the eigenstates of the sodium atom as a function of B. The two parameters of a sodium atom, $a'=32.091$ T^{-1} and $b'=-0.012709$ T^{-1}, are taken from Ref. [22].

Let us analyze how the marginal Berry phase of the entangled state is related to the avoided crossings. We focus on the eigenstate $|E_{+1}^{-}\rangle$. It has two Schmidt coefficients $p_1=\sin^2\frac{\alpha_1}{2}$ and $p_2=\cos^2\frac{\alpha_1}{2}$. With Eq. (11), one obtains the total phase as a sum of the Berry phases acquired by nuclear and electron spins with weights of the Schmidt coefficients:

$$\beta = \sin^2\frac{\alpha_1}{2}\left(-\frac{\Omega}{2}-\frac{\Omega}{2}\right) + \cos^2\frac{\alpha_1}{2}\left(+\frac{\Omega}{2}-\frac{3\Omega}{2}\right) = -\Omega. \quad (18)$$

From Eq. (12), one obtains the marginal Berry phases of an electron spin Γ_e and of nuclear spin Γ_n:

$$\Gamma_n = \arg\left(\sin^2\frac{\alpha_1}{2}e^{-i\Omega/2} + \cos^2\frac{\alpha_1}{2}e^{-i3\Omega/2}\right), \quad (19a)$$

$$\Gamma_e = \arctan\left(\cos\alpha_1\tan\frac{\Omega}{2}\right). \quad (19b)$$

Figure 5 plots the marginal Berry phase of a nuclear spin Γ_n as a function of B and the azimuthal angle θ. In the limit of $B\gg 1$—i.e., $\alpha_1\to 0$—one has $|E_{+1}^{-}\rangle\to|-\frac{1}{2},\frac{3}{2}\rangle$, $\Gamma_e=\Omega/2$, and $\Gamma_n=-3\Omega/2$. It is clearly seen that the node of the marginal Berry phase of a nuclear (or electron) spin corresponds to the avoid crossing at $A+(a-b)B=\sqrt{3}A$. Thus it could be expected that the marginal Berry phase of a subsystem for an entangled state has a node at avoided crossings.

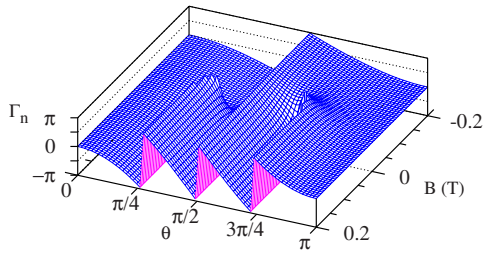

FIG. 5. (Color online) Marginal Berry phase of the nuclear spin Γ_n for the eigenstate $|E_{+1}^{-}\rangle$ as a function of B and θ.

V. CONCLUSIONS

We have considered the Breit-Rabi Hamiltonians for hydrogen and sodium atoms, describing the hyperfine interaction between a nuclear spin and an electron spin in the presence of a magnetic field. We have examined the relation between level crossings, entanglement, and Berry phases. It is shown that entanglement between nuclear and electron spins is maximum at avoided crossing points. The Berry phase and the von Neumann entropy change abruptly at level crossings as the parameters of the Breit-Rabi Hamiltonian for a hydrogen atom vary. An entangled state encircling the avoided crossing acquires the marginal Berry phase of an electron (or nuclear) spin like an eigenstate moving around the real crossing accumulates a Berry phase. We have shown that the nodal points of the marginal Berry phase of an entangled state corresponds to the avoided crossing points.

ACKNOWLEDGMENTS

This work was in part supported by the visitor program of Max Planck Institute for the Physics of Complex Systems. We would like also to thank the Binational Israel-U.S. Foundation (BSF) for financial support.

[1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 2nd ed. (Pergamon Press, Oxford, 1965); C. Zener, Proc. R. Soc. London, Ser. A **137**, 696 (1932).
[2] E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, Science **292**, 472 (2001).
[3] M. V. Berry, Proc. R. Soc. London, Ser. A **392**, 45 (1984).
[4] A. Shapre and F. Wilczek, *Geometric Phases in Physics* (World Scientific, Singapore, 1998).
[5] D. Yarkony, Rev. Mod. Phys. **68**, 985 (1996).
[6] A. Kuppermann, in *Dynamics of Molecules and Chemical Reactions*, edited by R. E. Wyatt and J. Z. H. Zhang (Marcel Dekker, New York, 1996), pp. 411–472.
[7] M. Vojta, Rep. Prog. Phys. **66**, 2069 (2003).
[8] J. P. Neirotti, P. Serra, and S. Kais, Phys. Rev. Lett. **79**, 3142 (1997).
[9] P. Serra, J. P. Neirotti, and S. Kais, Phys. Rev. Lett. **80**, 5293 (1998); Phys. Rev. A **57**, R1481 (1998).
[10] S. Kais and P. Serra, Adv. Chem. Phys. **125**, 1 (2003); Int. Rev. Phys. Chem. **19**, 97 (2000).
[11] M. Bhattacharya and C. Raman, Phys. Rev. Lett. **97**, 140405 (2006); Phys. Rev. A **75**, 033406 (2007).
[12] Q. C. Shi and S. Kais, J. Chem. Phys. **121**, 5611 (2004).
[13] R. González-Férez and J. S. Dehesa, Phys. Rev. Lett. **91**, 113001 (2003).
[14] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
[15] O. Osenda, Z. Huang, and S. Kais, Phys. Rev. A **67**, 062321 (2003).
[16] S. Oh, e-print arXiv:0807.4662v1.
[17] G. Breit and I. I. Rabi, Phys. Rev. **38**, 2082 (1931).
[18] C. P. Slichter, *Principles of Magnetic Resonance* (Springer-Verlag, Berlin, 1990).
[19] B. Patterson, Rev. Mod. Phys. **60**, 69 (1988).
[20] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[21] S. N. Foner, E. L. Cochran, V. A. Bowers, and C. K. Jen, J. Chem. Phys. **32**, 963 (1960).
[22] E. Arimondo, M. Inguscio, and P. Violino, Rev. Mod. Phys. **49**, 31 (1977).
[23] J. Gruska, *Quantum Computing* (McGraw-Hill, London, 1999).
[24] S. Kais, in *Reduced-Density-matrix Mechanics with Applications to Many-electron Atoms and Molecules*, Advances in Chemical Physics, Vol. 134, edited by D. A. Mazziotti (Wiley, New York, 2007).
[25] E. Sjöqvist, A. K. Pati, A. Ekert, J. S. Anandan, M. Ericsson, D. K. L. Oi, and V. Vedral, Phys. Rev. Lett. **85**, 2845 (2000).
[26] E. Sjöqvist, X. X. Yi, and J. Åberg, Phys. Rev. A **72**, 054101 (2005).
[27] X. X. Yi, L. C. Wang, and T. Y. Zheng, Phys. Rev. Lett. **92**, 150406 (2004).
[28] X. X. Yi and E. Sjöqvist, Phys. Rev. A **70**, 042104 (2004).