Control of many electron states in semiconductor quantum dots by non-Abelian vector potentials

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Adiabatic time evolution of degenerate eigenstates of a quantum system provides a means for controlling electronic states since mixing between degenerate levels generates a matrix Berry phase. In the presence of spin-orbit coupling in n-type semiconductor quantum dots the electron Hamiltonian is invariant under time reversal operation and the many body groundstate may be doubly degenerate. This double degeneracy can generate non-Abelian vector potentials when odd number of electrons are present. We find that the antisymmetry of many electron wavefunction has no effect on the matrix Berry phase. We have derived equations that allow one to investigate the effect of electron correlations by expressing the non-Abelian vector potentials for many electron system in terms of single electron non-Abelian vector potentials.

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I. INTRODUCTION

Single electron control in semiconductor quantum dots would be valuable for spintronics, quantum information, and spin qubits[1, 2]. Adiabatic time evolution of degenerate eigenstates of a quantum system provides a means for controlling individual electrons since mixing between degenerate levels generates a matrix Berry phase[3, 4]. It has been shown that universal quantum computation is possible by means of non-Abelian unitary operations[5, 6]. Recently several proposals on how to generate matrix Berry phases have been made in semiconductor systems[7, 8, 9, 10, 11]. In one of these proposals it has been suggested that a single electron in a n-type semiconductor quantum dot with spin-orbit terms can have matrix Berry phases[11]. All the discrete energy levels of quantum dots possess a double degeneracy because the Rashba and/or Dresselhaus spin orbit coupling terms have time reversal symmetry[12]. In Ref.[11] it was suggested that the adiabatic transformation can be performed electrically by changing the confinement potentials of the quantum dot. It was shown that matrix Berry phases can be produced only when the parity symmetry of two-dimensional harmonic potentials is broken. A degenerate pair of states also exists in quantum rings[13]. The relevant symmetry of this system is the combined operation of time reversal and large gauge transformations. However, it is often not easy to populate a quantum dot or ring with just one electron and usually there are several electrons in it[14, 15]. It is not certain that many body groundstates are doubly degenerate in the presence of time reversal symmetry. Moreover, it is unclear how the effects of exchange and correlation many body physics change the non-Abelian vector potentials. These issues are investigated in the present paper.

Before we give a summary of the main points of the present paper let us give a brief introduction of the basic ideas behind matrix Berry phases. Consider a degenerate pair of states |Ψ1⟩ and |Ψ2⟩, which may be single particle or many body states. If the system is in a superposition state |Ψ(0)⟩ = c1(0)|Ψ1(0)⟩ + c2(0)|Ψ2(0)⟩ at time t=0 an adiabatic evolution of the parameters λp can transform this state into another state |Ψ(t)⟩ = c1(t)|Ψ1(t)⟩ + c2(t)|Ψ2(t)⟩ after some time t. Here the orthonormal basis states |Ψi(t)⟩ are the instantaneous eigenstates of the Hamiltonian. For a cyclic change with the period T, represented by a closed contour C in the parameter space, the states |Ψ1(T)⟩ and |Ψ2(T)⟩ return to the initial states |Ψ1(0)⟩ and |Ψ2(0)⟩, but the coefficients c1(T) and c2(T) may not return the initial values. In such a case a 2 × 2 matrix Berry phase (non-Abelian Berry phase) ΦC is generated

\[
\left( \begin{array}{c} c_1(T) \\ c_2(T) \end{array} \right) = \Phi_C \left( \begin{array}{c} c_1(0) \\ c_2(0) \end{array} \right).
\] (1)

The expansion coefficients c1(t) and c2(t) satisfy the time-dependent Schrödinger equation

\[
i\hbar \dot{c}_i = - \sum_j A_{ij} c_j \quad i = 1, 2.
\] (2)

The matrix elements Aij are given by Aij = ℏ \sum p (Ap)ij \frac{\partial \lambda_p}{\partial t}, where the sum over p in Aij is meant to be the sum over λp. The non-Abelian vector potentials Aq are 2 × 2 matrices

\[
(A_p)_{ij} = i \langle \Psi_i | \frac{\partial \Psi_j}{\partial \lambda_p} \rangle.
\] (3)

Note that the wavefunctions Ψi and Ψj are degenerate. The role of the non-Abelian vector potentials is to keep the energy degeneracy intact while the system parameters change.

Our investigation shows that when even number of electrons are present the many body groundstate may not be doubly degenerate. However, when odd number
of electrons are present the groundstate may be doubly degenerate. In the simplest possible approximation the antisymmetry of many body wavefunctions can be ignored. Then the degenerate groundstates for three electrons are given by $|\Psi_1\rangle = \phi_1(r_1)\phi_2(r_2)\phi_3(r_3)$ and $|\Psi_2\rangle = \phi_1(r_1)\phi_2(r_2)\phi_3(r_3)$, where $\phi_i$ are single electron wavefunctions, see Fig. 1. In this case one can show that the solutions of the time dependent Schrödinger equation, Eq. (2), have the form

$$
\begin{pmatrix}
  c_1(t) \\
  c_2(t)
\end{pmatrix} = e^{i\mathbf{f}(t)}
\begin{pmatrix}
  B_1(t) \\
  B_2(t)
\end{pmatrix}.
$$

(4)

The function $f(t)$ depends on the single electron non-Abelian vector potentials of the first shell, and the functions $B_1(t)$ and $B_2(t)$ depend on the single electron non-Abelian vector potentials of the second shell, see Fig. 1. (The function $f(t)$ is periodic with the period $T$.) The probability to find an electron in the state $|\phi_3\rangle$ is $|c_1(T)|^2 = |B_1(T)|^2$, $|c_2(T)|^2 = |B_2(T)|^2$. So these probabilities are independent of the phase factor $e^{i\mathbf{f}(t)}$, i.e., of the non-Abelian vector potentials of the first shell.

In the next simplest possible approximation the antisymmetry of many body wavefunctions can be included. In this case the doubly degenerate many body groundstates may be taken to be two Slater determinant wavefunctions, $\Psi_1$ and $\Psi_2$, that are time reversed states of each other, see Fig. 2. It will be shown below that the antisymmetry of these Slater determinant wavefunctions does not change the results obtained above for the matrix Berry phase. In addition to the antisymmetry one can include correlation effects. This can be done by including four basis vectors $\Psi_1$, $\Psi_2$, $\Psi_3$ and $\Psi_4$, see Fig. 2. In this case the groundstates are given by linear combinations of these four states and are thus correlated. It can be shown that the non-Abelian gauge potentials for a correlated electron system are related to non-Abelian gauge potentials for single electrons, provided that the definition of single electron non-Abelian gauge potentials is extended to

$$
(a_{\lambda})_{k,p} = i\langle\phi_k|\partial_{\lambda}\phi_p\rangle
$$

(5)

when $\phi_k$ and $\phi_p$ belong to different single electron energy shells. We will call these inter shell non-Abelian gauge potentials.

FIG. 1: Single electron eigenstates form degenerate energy shells. In each shell electron wavefunctions form a time reversed pair.

FIG. 2: Four many body basis states in the three electron Hilbert space. The basis pair $(\Psi_1, \Psi_2)$ or $(\Psi_1, \Psi_3)$ is a time reversed pair and has the same total single electron energy. So do $\Psi_2$ and $\Psi_3$. Black dots represent electrons.

In Sec. II we describe the Hamiltonian of the system in detail, and in Sec. III we discuss why matrix Berry phases can be produced only when the parity symmetry of two-dimensional harmonic potentials is broken. A computational scheme to include systematically many electron physics is explained in Sec. IV. The absence of a matrix Berry phase for the two-electron case is shown in Sec. V. In Sec. VI we show that a matrix Berry phase is present in the three-electron case. Correlation effects are discussed in VII and conclusions are given in Sec. VIII.

II. MODEL HAMILTONIAN

An electric field $E$ is along the $z$-axis and electrons are confined in a triangular potential $V(z)$. When the width of the quantum well along the $z$-axis is sufficiently small we may include only the lowest subband state along the $z$-axis. We denote this wavefunction by $f(z)$. From the expectation value $\langle f(z)|k^2|f(z)\rangle = 0.8(2m^*eE/\hbar^2)^{2/3}$ we estimate the characteristic length scale along the $z$-axis: $R_z = 1/\sqrt{0.8(2m^*eE/\hbar^2)^{2/3}}$. The Hamiltonian in the absence of the spin orbit coupling is

$$
H_K = -\frac{\hbar^2\nabla^2}{2m^*} + U(x, y) + V(z).
$$

(6)

We take the two-dimensional potential to be $U(x, y) = \frac{1}{2}m^*\omega_x^2x^2 + \frac{1}{2}m^*\omega_y^2y^2 + V_p(x, y)$. The strengths of the harmonic potentials are denoted by $\omega_x$ and $\omega_y$. They may be varied by changing gate potentials of the quantum dot system. The characteristic length scales along $x$- and
y-axis are \( R_{x,y} = \sqrt{\frac{j}{\alpha^2 \omega_{x,y}}} \). The potential \( V_p(x,y) \) is chosen in such a way that the parity symmetry of electron wavefunctions is broken. We can choose it to be \( V_p(x,y) = e^r y \). It represents an electric field along the y-axis and its strength \( e^r \) may be varied electrically.

In a periodic crystal potential of a semiconductor the spin orbit interaction has two contributions. The Rashba term is

\[
H_R = c_R (\sigma_z k_y - \sigma_y k_x). \tag{7}
\]

Here \( \sigma_{x,y} \) are Pauli spin matrices and \( k_{x,y} \) are momentum operators \( (k_x = \frac{ie}{\hbar} \partial_x \text{ and similarly with } k_y) \). The constant \( c_R \) depends on the external electric field \( E \) applied along the z-axis. The Dresselhaus spin orbit term \( H_D \) is

\[
H_D = c_D ((\sigma_x k_x (k_y^2 - k_z^2)) + (\sigma_y k_y (k_x^2 - k_z^2))). \tag{8}
\]

There is another term of the form \( \sigma_z (k_z^2) (k_z^2 - k_y^2) \) in the Dresselhaus spin orbit term but it vanishes since the expectation value \( \langle k_z \rangle = (f(z)k_z \bar{f}(z) = 0 \rangle \) for the first subband along z-axis. The constant \( c_D \) represents breaking of inversion symmetry by the crystal in zinc blende structures. The total single electron Hamiltonian of semiconductor quantum dot is \( H_S = H_K + H_R + H_D \).

When several electrons are present in the dot the total Hamiltonian consists of single particle Hamiltonians and two-particle interaction terms \( H = H_0 + V_{\text{int}} \), where \( H_0 = \sum_i H_i \) and \( V_{\text{int}} = \frac{1}{2} \sum_{i \neq j} V(r_i - r_j) \) with \( V(r_i - r_j) = \frac{e^2}{\epsilon r_i r_j} \). (\( H_i \) is the single particle Hamiltonian for the ith electron and \( \epsilon \) is the background dielectric constant). The total many electron Hamiltonian is invariant under time reversal symmetry.

### III. BREAKING OF PARITY SYMMETRY OF WAVEFUNCTIONS

The eigenenergies of the single electron Hamiltonian is depicted in Fig.1. Each energy is doubly degenerate. An eigenstate of the Hamiltonian is a linear combination of the eigenstates of the single particle Hamiltonian depicted in Fig.1. Each energy is doubly degenerate. An eigenenergy of the single electron Hamiltonian is

\[
\langle \phi \rangle = \sum_{m} c_{mn\uparrow} |mn\uparrow\rangle + \sum_{m} c_{mn\downarrow} |mn\downarrow\rangle. \tag{9}
\]

In the basis states \( |mn\sigma\rangle \) the quantum number \( m(n) \) and \( \sigma \) label the harmonic oscillator levels along the \( x \)-axis (\( y \)-axis) and the component of electron spin. The subband wavefunction \( f(z) \) is suppressed in the notation \( |mn\sigma\rangle \). The wavefunction \( |\phi\rangle \) can also be written as a column vector \( |\phi\rangle = \left( \begin{array}{c} F_\uparrow \\ F_\downarrow \end{array} \right) \), where \( F_\uparrow = \sum_{mn} c_{mn\uparrow} |mn\rangle \) and \( F_\downarrow = \sum_{mn} c_{mn\downarrow} |mn\rangle \). The expansion coefficients satisfy a matrix equation

\[
\sum_{m'n'n'} \langle m'n'\sigma' |H|m'n\sigma\rangle c_{m'n'n'} = Ec_{m'n\sigma}. \tag{10}
\]

The single electron wavefunctions used in this section are self-consistent Hartree-Fock single electron states if \( H_S \) is replaced by the HF single electron Hamiltonian. In the absence of the Zeeman term the single particle Hamiltonian is invariant under time reversal symmetry: \( \vec{k} \rightarrow -\vec{k} \) and \( \vec{\sigma} \rightarrow -\vec{\sigma} \). The time reversal operator is \( T = -i\alpha y C \), where the operator \( C \) stands for complex conjugation. The time reversed state of \(|\phi\rangle\) is

\[
\langle \tilde{\phi}_1 \rangle = T|\phi\rangle = -\sum_{mn} c_{mn\uparrow} |mn\uparrow\rangle + \sum_{mn} c_{mn\downarrow} |mn\downarrow\rangle. \tag{11}
\]

This can also be written as a column vector \(|\phi_1\rangle = \left( \begin{array}{c} -F_\downarrow^* \\ F_\uparrow^* \end{array} \right) \). Note that \( T^2|\phi\rangle = -|\phi\rangle \). These two states are degenerate and orthonormal. We have suppressed the Bloch wavefunction of the conduction band in applying the time reversal operator since it is unaffected by the operator \( T \). Our wavefunctions are all effective mass wavefunctions and only the conduction band Bloch wavefunction at \( \vec{k} = 0 \) is relevant.

Even in the presence of doubly degenerate states a matrix Berry phase may not always exist. It was shown numerically that only distorted two-dimensional harmonic potentials breaking the parity symmetry generate matrix Berry phases. Here reasons for this effect for the single electron case is given in detail. In this argument only one electron is assumed to be present in the dot, \( c_D = 0 \), and \( V_p(x,y) = 0 \). The adiabatic parameters are \( \lambda_1 = c_R \) and \( \lambda_2 = \omega_x \). Let us consider \( H_R \) as a perturbation and apply a perturbation theory to \( |00\uparrow\rangle \)

\[
|\phi\rangle \approx |00\uparrow\rangle + \sum_{mn} \frac{|mn\downarrow\rangle \langle mn\downarrow| H_R |00\uparrow\rangle}{E_{00} - E_{mn}} |mn\downarrow\rangle \quad + \quad \sum_{mn'} \frac{|mn\uparrow\rangle \langle mn\uparrow| H_R |mn'\downarrow\rangle}{E_{00} - E_{mn}} |mn'\downarrow\rangle \quad + \quad \ldots, \tag{12}
\]

where \( E_{mn} = (m + 1/2)\hbar \omega_x + (n + 1/2)\hbar \omega_y \). The wavefunction of \(|00\uparrow\rangle\) has even parity. The matrix element \( \langle mn\downarrow| H_R |00\uparrow\rangle \) couples \(|00\uparrow\rangle\) to only odd parity states \(|mn\downarrow\rangle \). Therefore the wavefunction corresponding to the second term in Eq.(12) has odd parity with spin down. The wavefunction of the third term in Eq.(12) has even parity with spin up. This perturbation series indicates that the exact lowest energy state has the form \(|\phi_1\rangle = \left( \begin{array}{c} F_e \\ F_o \end{array} \right) \), where \( F_e \) and \( F_o \) even and odd functions.

The time reversed wavefunction is \( \tilde{\phi}_1 = \left( \begin{array}{c} -F_o^* \\ F_e^* \end{array} \right) \). For this particular pair of degenerate states the off-diagonal elements of non-Abelian vector potentials are zero:

\[
\langle \tilde{\phi}_1 | \frac{\partial}{\partial \lambda_k} \phi_1 \rangle = -\langle F_e | \frac{\partial}{\partial \lambda_k} | F_o \rangle + \langle F_o | \frac{\partial}{\partial \lambda_k} | F_e \rangle = -\sum_{q,p} \alpha_k \frac{\partial}{\partial \lambda_k} \langle \phi_q | \phi_p \rangle + \sum_{q,p} \beta_k \frac{\partial}{\partial \lambda_k} \langle \phi_p | \phi_q \rangle = 0. \tag{13}
\]
Here \( F_q = \sum a_q \varphi_q \) with \( q = (m, n) \) such that the two-dimensional harmonic wavefunctions \( \varphi_q \) are even functions. The function \( F_p = \sum b_p \varphi_p \) with \( p = (m', n') \) are such that \( \varphi_p \) are odd functions (Note that one can show \( \langle \varphi_p | \frac{\partial}{\partial x} | \varphi_p \rangle = 0 \)). Since the off-diagonal non-Abelian vector potentials are zero the matrix Berry phase is absent. In what follows a distorted two-dimensional harmonic potential is assumed. The adiabatic parameters are \( c_R \) and \( c' \).

### IV. COMPUTATIONAL SCHEME TO INCLUDE MANY ELECTRON PHYSICS

![Diagram](image)

**FIG. 3:** Five many body basis states in the two electron Hilbert space. The basis state \( \Psi_1 \) is the time reversed state of itself.

A computational scheme that includes systematically many electron physics is explained here. We find an efficient computational scheme of computing eigenstates and eigenvalues of the many electron Hamiltonian of a semiconductor quantum dots with an arbitrary shape of the confinement potential. We follow the following steps.

Single electron Hamiltonian is first solved in the presence of spin-orbit terms. This can be done by following the steps given in Sec.III. The number of single electron basis states \( |mnr \rangle \) can be truncated to a reasonable number by comparing the relative magnitude of the single particle energy spacing and the strength of the Coulomb interaction.

Using these single electron eigenstates Slater determinant states \( \Psi_i \) and their time reversed states \( \overline{\Psi}_i \) are formed. \( \overline{\Psi}_i \) is obtained from \( \Psi_i \) by replacing the single electron wavefunctions with their time reversed states: \( \phi_i \rightarrow \overline{\phi}_i \). It will be inefficient to use two diagonal harmonic potential wavefunction \( \varphi_{mn} \) to build these Slater determinant states. The following relation hold for two arbitrary states \( \Psi_a \) and \( \Psi_b \): \( \langle T \Psi_a | T \Psi_b \rangle = \langle \Psi_a | \Psi_b \rangle \). From this relation it follows that the Hamiltonian matrix elements have the following properties: \( \langle \Psi_i | H | \Psi_j \rangle = \langle \overline{\Psi}_i | H | \overline{\Psi}_j \rangle \), \( \langle \Psi_i | H | \overline{\Psi}_j \rangle = -\langle \Psi_j | H | \overline{\Psi}_i \rangle \), and \( \langle \Psi_i | H | \overline{\Psi}_j \rangle = \langle \overline{\Psi}_j | H | \overline{\Psi}_i \rangle \).

When there are odd number of electrons the basis vectors of many electron Hamiltonian are chosen to include time reversed pairs: \( \{ \Psi_1, \overline{\Psi}_1, \Psi_2, \overline{\Psi}_2, ... \} \), see Fig. 2. The eigenstates are doubly degenerate in the odd electron case. Let us show this for the three electron case using the following Slater determinant wavefunctions as the basis vectors in the many body Hilbert space \( \{ \Psi_1, \overline{\Psi}_1, \Psi_2, \overline{\Psi}_2 \} \). These states are depicted in Fig. 2. The wavefunctions of the lowest energy degenerate pair are \( \Phi = a \Psi_1 + b \overline{\Psi}_1 + c \Psi_2 + d \overline{\Psi}_2 \) and \( \overline{\Phi} = T \Phi = a^* \Psi_1 - b^* \overline{\Psi}_1 + c^* \Psi_2 - d^* \overline{\Psi}_2 \). Clearly \( \langle \Phi | H | \Phi \rangle = \langle \overline{\Phi} | H | \overline{\Phi} \rangle \). Note \( \Phi \) and \( \overline{\Phi} \) are a time reversed pair, orthogonal, and satisfies \( T^2 \Phi = -\Phi \). The two eigenvalues of \( H \) are each doubly degenerate.

When there are even number of electrons the basis vectors of the many electron Hamiltonian are chosen as \( \{ \Psi_1, \Psi_2, \overline{\Psi}_2, \overline{\Psi}_3, \overline{\Psi}_3, ... \} \). In this scheme the groundstate is non degenerate. This can be shown shown, for example, in an approximation that includes five many body basis vectors in the presence of two electrons, see Fig. 3. The groundstate can then be written as a linear combination \( \Phi = a \Psi_1 + b \Psi_2 + c \overline{\Psi}_2 + d \overline{\Psi}_3 + e \overline{\Psi}_3 \). Its time reversed state is \( \overline{\Phi} = a^* \overline{\Psi}_1 + b^* \Psi_2 - c^* \overline{\Psi}_2 - d^* \Psi_3 - e^* \overline{\Psi}_3 \). Clearly these two states are not orthogonal. Since \( \langle \Phi | H | \Phi \rangle = \langle T^2 \Phi | H | T^2 \Phi \rangle \) and \( T^2 \Phi \neq -\Phi \) one finds that the energy expectation values are non degenerate, \( \langle \Phi | H | \Phi \rangle \neq \langle \Phi | H | \overline{\Phi} \rangle \), i.e., time reversed states are non degenerate. The matrix Berry phase is thus absent. In the simplest possible approximation the groundstate \( \Psi \) of two electron system is given by the single Slater determinant made of the single particles states \( \{ \phi_1, \phi_2 \} \). In this case the initial state should return to itself after the adiabatic cycle. It is instructive to verify this explicitly by transforming each single particles states. The initial state is

\[
|\Psi(0)\rangle = \phi_1(\vec{r}_1)\overline{\phi}_1(\vec{r}_2) - \phi_1(\vec{r}_2)\overline{\phi}_1(\vec{r}_1).
\]

After a cycle the single electron wavefunctions transform into

\[
\phi_1 \rightarrow a_1 \phi_1 + b_1 \overline{\phi}_1 \quad \text{and} \quad \overline{\phi}_1 \rightarrow a_2 \phi_1 + b_2 \overline{\phi}_1.
\]

The transformed two electron Slater determinant is

\[
|\Psi(T)\rangle = \langle a_1 b_2 - b_1 a_2 \rangle |\phi_1(\vec{r}_1)\overline{\phi}_1(\vec{r}_2) - \phi_1(\vec{r}_2)\overline{\phi}_1(\vec{r}_1)\rangle,
\]

which is \( \langle a_1 b_2 - b_1 a_2 \rangle |\Psi(0)\rangle \). Since the transformed single electron states are time reversed states of each other \( \langle a_2 b_2 \rangle = (-b_1, a_1) \). So the factor in the transformed wavefunction is \( a_1 b_2 - b_1 a_2 = |a_1|^2 + |b_1|^2 = 1 \).

### V. SIMPLEST POSSIBLE APPROXIMATION WITH ANTISYMMETRY OF WAVEFUNCTIONS

Now consider odd number of electrons, for example, three electrons in a dot. In the simplest possible approximation with fermionic antisymmetry two many body basis states, \( \Psi_1 \) and \( \overline{\Psi}_1 \), can be included. These are Slater determinant states and are depicted in Fig. 2. This approximation is well justified when the typical single electron energy spacing is larger than the characteristic Coulomb energy. Clearly \( \Psi_1 \) and \( \overline{\Psi}_1 \) are orthogonal.
\[ \langle \Psi_1 | \overline{\Psi}_1 \rangle = 0. \] The Hamiltonian matrix is
\[ H = \begin{pmatrix} \langle \Psi_1 | H | \Psi_1 \rangle & \langle \Psi_1 | H | \overline{\Psi}_1 \rangle \\ \langle \overline{\Psi}_1 | H | \Psi_1 \rangle & \langle \overline{\Psi}_1 | H | \overline{\Psi}_1 \rangle \end{pmatrix}. \] (16)

The off-diagonal matrix elements of the Hamiltonian matrix is zero since \( \langle \Psi_1 | H | \overline{\Psi}_1 \rangle = -\langle \overline{\Psi}_1 | H | \Psi_1 \rangle \), which follows from \( \langle T | \Psi_a | T | \Psi_b \rangle = \langle \Psi_b | T | \Psi_a \rangle \). It is instructive to show this explicitly by evaluating the matrix element
\[ \langle \Psi_1 | V_{\text{int}} | \overline{\Psi}_1 \rangle = [(23)|V|24] - [(23)|V|42] + [(13)|V|14] - [(13)|V|41]. \] (17)

Here the first and third terms are direct Coulomb matrix elements while the second and fourth terms are their exchange counter parts. The direct Coulomb matrix elements are zero since \( \phi_3^* (\vec{r}) \phi_4 (\vec{r}) = \phi_5^* (\vec{r}) \overline{\phi}_3 (\vec{r}) = 0 \). So only their exchange counter parts remain, which are given by
\[ (23)|V|42) = \int dr_1 dr_2 \phi_1^*(\vec{r}_1) \phi_5^*(\vec{r}_2) V(\vec{r}_1 - \vec{r}_2) \overline{\phi}_3 (\vec{r}_1) \overline{\phi}_2 (\vec{r}_2). \]
and
\[ (13)|V|41) = \int dr_1 dr_2 \phi_1^*(\vec{r}_1) \phi_5^*(\vec{r}_2) V(\vec{r}_1 - \vec{r}_2) \overline{\phi}_3 (\vec{r}_1) \phi_1 (\vec{r}_2). \]

One can show
\[ \langle \Psi_1 | V_{\text{int}} | \overline{\Psi}_1 \rangle = - (23)|V|42) - (13)|V|41) = 0. \] (20)

This is because
\[ (23)|V|42) = -(13)|V|41), \] (21)
which follows from \( \phi_2^* = \overline{\phi}_1, \phi_4 = \overline{\phi}_3, \) and
\[ \overline{\phi}_1 (\vec{r}) \overline{\phi}_3 (\vec{r}) = F_{11}(\vec{r}) F_{31}(\vec{r}) + F_{13}(\vec{r}) F_{33}(\vec{r}), \]
\[ \phi_5^* (\vec{r}) \overline{\phi}_1 (\vec{r}) = -F^*_{33}(\vec{r}) F_{51}(\vec{r}) + F^*_{31}(\vec{r}) F_{53}(\vec{r}), \]
\[ \phi_5^* (\vec{r}) \overline{\phi}_3 (\vec{r}) = -F^*_{11}(\vec{r}) F_{51}(\vec{r}) + F^*_{13}(\vec{r}) F_{53}(\vec{r}), \]
\[ \phi_5^* (\vec{r}) \phi_1 (\vec{r}) = F^*_{31}(\vec{r}) F_{11}(\vec{r}) + F^*_{33}(\vec{r}) F_{13}(\vec{r}). \] (22)

Note that the second and third terms are equal except for the minus sign. The off-diagonal elements are thus zero, and
\[ H = \begin{pmatrix} \langle \Psi_1 | H | \Psi_1 \rangle & 0 \\ 0 & \langle \overline{\Psi}_1 | H | \overline{\Psi}_1 \rangle \end{pmatrix}. \] (23)

This implies that \( \Psi_1 \) and \( \overline{\Psi}_1 \) are eigenstates and are degenerate in energy.

During the adiabatic change the wavefunction of three electrons evolves as \( |\Psi'(t)\rangle = c_1(t) |\Psi_1(t)\rangle + c_2(t) |\overline{\Psi}_1(t)\rangle \).

The coefficients \( c_1(t) \) and \( c_2(t) \) satisfy the Schroedinger equation Eq.(2) governed by the non-Abelian vector potentials
\[ (A_k)_{11} = i \langle \Psi_1 | \frac{\partial}{\partial \lambda_k} | \Psi_1 \rangle, \]
\[ (A_k)_{12} = i \langle \Psi_1 | \frac{\partial}{\partial \lambda_k} | \overline{\Psi}_1 \rangle, \]
\[ (A_k)_{21} = i \langle \overline{\Psi}_1 | \frac{\partial}{\partial \lambda_k} | \Psi_1 \rangle, \]
\[ (A_k)_{22} = i \langle \overline{\Psi}_1 | \frac{\partial}{\partial \lambda_k} | \overline{\Psi}_1 \rangle. \] (24)

It can be shown using Eqs.(A.3) and (A.4) that these can be written in terms of the non-Abelian vector potentials for single particle states
\[ (A_k)_{11} = (ak)_{11} + (ak)_{22} + (ak)_{33}, \]
\[ (A_k)_{12} = (ak)_{34}, \]
\[ (A_k)_{21} = (ak)_{43}, \]
\[ (A_k)_{22} = (ak)_{11} + (ak)_{22} + (ak)_{44}, \] (25)

where the non-Abelian vector potentials involving the lowest energy single electron states are
\[ (ak)_{11} = i \langle \phi_1 | \frac{\partial}{\partial \lambda_k} | \phi_1 \rangle, \]
\[ (ak)_{22} = i \langle \phi_1 | \frac{\partial}{\partial \lambda_k} | \phi_2 \rangle, \] (26)

and involving the second lowest single electron states are
\[ (ak)_{33} = i \langle \phi_2 | \frac{\partial}{\partial \lambda_k} | \phi_2 \rangle, \]
\[ (ak)_{44} = i \langle \phi_2 | \frac{\partial}{\partial \lambda_k} | \phi_2 \rangle, \]
\[ (ak)_{43} = i \langle \phi_2 | \frac{\partial}{\partial \lambda_k} | \phi_2 \rangle. \] (27)

The solution of the time dependent Schroedinger equation has the form \( \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = A(t) \begin{pmatrix} B_1(t) \\ B_2(t) \end{pmatrix} \). The function \( A(t) \) depends on the electrons in the first shell. It satisfies \( f(t) A(t) = -i \hbar \frac{\partial}{\partial t} A(t) \), where \( f(t) = \sum ((ak)_{11} + (ak)_{22}) \frac{\partial}{\partial \lambda_k} \). The solution of this differential equation is a phase factor
\[ A(t) = e^{\pm i f(t)}. \] (28)

Note that \( (ak)_{11} + (ak)_{22} \) appears in the diagonal elements of the non Abelian vector potentials \( (Ak)_{11} \) and \( (Ak)_{22} \). The functions \( B_1(t) \) and \( B_2(t) \) are the solutions of the time dependent Schroedinger equation
\[ i \hbar \frac{\partial}{\partial t} B_i = - \sum_j \mathcal{M}_{ij} B_j \quad i = 1, 2. \] (29)
with the following non-Abelian gauge potentials.

\[ (\mathcal{A}_k)_{1,1} = (a_k)_{3,3}, \]
\[ (\mathcal{A}_k)_{1,2} = (a_k)_{3,4}, \]
\[ (\mathcal{A}_k)_{2,1} = (a_k)_{4,3}, \]
\[ (\mathcal{A}_k)_{2,2} = (a_k)_{4,4}. \]

(30)

This is precisely the non Abelian vector potentials for the second energy shell. The probability to find an electron in the state \(|\phi_1(T)\rangle = |c_1(T)|^2 = |B_1(T)|^2 = |B_2(T)|^2\). So these probabilities are independent of the non-Abelian vector potentials of the first energy shell. In addition it should be noted that the antisymmetry of the many electron wavefunction does not change the value of the matrix Berry phase obtained from the wavefunctions without the antisymmetry, see Eq.(4). This is the main conclusion of this section.

VI. CORRELATION EFFECTS

Correlation effects can be taken into account by writing many body eigenstates as a linear combination of single Slater determinant wavefunctions \(|\Phi_1, \Phi_2, \Phi_3, \Phi_4, \ldots \rangle = \{\Psi_1, \Psi_1, \Psi_2, \Psi_2, \ldots \rangle\}. These wavefunctions arranged in the increasing order of the total kinetic energy \(E_1 < E_2 < \ldots \). Note that \(|\Phi_i|\Phi_j\rangle = \delta_{i,j}\) for all i and j. If the groundstate is doubly degenerate one of the degenerate groundstates can be written as

\[ \Phi = \sum_{i=1}^{M} c_i |\Phi_i\rangle, \]

(31)

with

\[ \sum_{j=1}^{M} \langle \Phi_i | H | \Phi_j \rangle c_j = E c_i. \]

(32)

Then its time reversed state has the form

\[ \bar{\Phi} = T \Phi = \sum_{i=1}^{M} c_i^* |\bar{\Phi}_i\rangle \]

(33)

since \(T\) is an antiunitary operator. Note that \(|\bar{\Phi}_i\rangle\) are ordered as follows \(|\bar{\Phi}_1, \bar{\Phi}_2, \bar{\Phi}_3, \bar{\Phi}_4, \ldots \rangle = \{\bar{\Psi}_1, \bar{\Psi}_1, \bar{\Psi}_2, \bar{\Psi}_2, \ldots \rangle\). The states \(|\Phi\rangle\) and \(|\bar{\Phi}\rangle\) are eigenstates of the truncated Hamiltonian with the dimension \(M\). (Note that as \(M \rightarrow \infty\) the energy \(E\) will approach the exact eigenvalue.). Some of the Slater determinant states \(|\Psi_i\rangle\) are depicted in Fig.2. Clearly \(|\Phi\rangle\) and \(|\bar{\Phi}\rangle\) are orthogonal. The matrix element between them is zero: \(\langle \Phi | H | \bar{\Phi} \rangle = E \langle \Phi | \bar{\Phi} \rangle = 0\). These two states are degenerate since \(\langle \Phi | H | \Phi \rangle = \langle \bar{\Phi} | H | \bar{\Phi} \rangle\).

The non-Abelian vector potentials are

\[ (A_k)_{1,1} = i \langle \Phi | \frac{\partial}{\partial \lambda_k} | \Phi \rangle, \]
\[ (A_k)_{1,2} = i \langle \Phi | \frac{\partial}{\partial \lambda_k} | \bar{\Phi} \rangle, \]
\[ (A_k)_{2,1} = i \langle \bar{\Phi} | \frac{\partial}{\partial \lambda_k} | \Phi \rangle, \]
\[ (A_k)_{2,2} = i \langle \bar{\Phi} | \frac{\partial}{\partial \lambda_k} | \bar{\Phi} \rangle. \]

(34)

In terms of many body basis states they can be written as

\[ (A_k)_{1,1} = i \sum_{i} c_i^* \frac{\partial c_i}{\partial \lambda_k} + i \sum_{i,j} c_i^* c_j \langle \Phi_i | \frac{\partial}{\partial \lambda_k} | \Phi_j \rangle, \]
\[ (A_k)_{1,2} = i \sum_{i} c_i^* \frac{\partial c_i}{\partial \lambda_k} + i \sum_{i,j} c_i c_j^* \langle \bar{\Phi}_i | \frac{\partial}{\partial \lambda_k} | \bar{\Phi}_j \rangle, \]
\[ (A_k)_{2,1} = i \sum_{i,j} c_i c_j^* \langle \bar{\Phi}_i | \frac{\partial}{\partial \lambda_k} | \Phi_j \rangle, \]
\[ (A_k)_{2,2} = i \sum_{i,j} c_i c_j^* \langle \bar{\Phi}_i | \frac{\partial}{\partial \lambda_k} | \bar{\Phi}_j \rangle. \]

(35)

In the three electron case with the basis vectors given in Fig.2 the diagonal matrix elements \(i \langle \Phi_i | \frac{\partial}{\partial \lambda_k} | \Phi_i \rangle\) and \(i \langle \bar{\Phi}_i | \frac{\partial}{\partial \lambda_k} | \bar{\Phi}_i \rangle\) are given by

\[ i \langle \Psi_1 \frac{\partial}{\partial \lambda_k} | \Psi_1 \rangle = (a_k)_{1,1} + (a_k)_{2,2} + (a_k)_{3,3}, \]
\[ i \langle \bar{\Psi}_1 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_1 \rangle = (a_k)_{1,1} + (a_k)_{2,2} + (a_k)_{3,4}, \]
\[ i \langle \Psi_2 \frac{\partial}{\partial \lambda_k} | \Psi_2 \rangle = (a_k)_{1,1} + (a_k)_{2,2} + (a_k)_{5,5}, \]
\[ i \langle \bar{\Psi}_2 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_2 \rangle = (a_k)_{1,1} + (a_k)_{2,2} + (a_k)_{6,6}. \]

(36)

Similarly one can find off-diagonal matrix elements

\[ i \langle \Psi_1 \frac{\partial}{\partial \lambda_k} | \Psi_2 \rangle = (a_k)_{3,4}, \]
\[ i \langle \bar{\Psi}_1 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_2 \rangle = (a_k)_{5,6}, \]
\[ i \langle \Psi_1 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_2 \rangle = (a_k)_{3,5}, \]
\[ i \langle \bar{\Psi}_1 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_2 \rangle = (a_k)_{3,6}, \]
\[ i \langle \Psi_2 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_2 \rangle = (a_k)_{4,5}, \]
\[ i \langle \bar{\Psi}_2 \frac{\partial}{\partial \lambda_k} | \bar{\Psi}_2 \rangle = (a_k)_{4,6}. \]

(37)

These results follow from Eq.(34). Usually the non Abelian vector potentials are defined between two degenerate states, see Eq.(33). When electron correlations...
are important the matrix elements between two single electron states belonging to different energy shells are relevant (see the last four equations in Eq.(37)). We will call these inter shell non-Abelian vector potentials. Physically the mixing between the second and third shells is facilitated by them. Note that $(a_k)_{j,i} = (a_k)^*_{i,j}$.

VII. DISCUSSIONS AND CONCLUSIONS

We have developed a scheme of computing eigenstates and eigenvalues of the many electron Hamiltonian of a semiconductor quantum dot with an arbitrary shape of the confinement potential. The basis vectors of this many electron Hamiltonian are chosen to include time reversed pairs of Slater determinants. In this scheme the groundstate is non degenerate when an even number of electrons are present while the eigenstates are doubly degenerate when an odd number of electrons are present.

Using this computational scheme we have investigated matrix Berry phases when several electrons are present in a semiconductor quantum dot with spin-orbit coupling terms. When an odd number of electrons is present a matrix Berry phase exists. The effect of the antisymmetry of many electron wavefunctions does not affect the value of the matrix Berry phases. When an odd number of electrons is present a matrix Berry phase exists, the effect of the antisymmetry of many electron wavefunctions does not affect the value of the matrix Berry phases. However, our results in Sec. V give the same values of the matrix Berry phases. We take an elliptic adiabatic path given by $(E_R(t), E_p(t)) = (E_{R,c} + \Delta E_R \cos(\omega t), E_{p,c} + \Delta E_p \sin(\omega t))$. For the parameters $E_{R,c}/E_0 = 2$, $E_{p,c}/E_0 = 1$, $\Delta E_p/E_0 = 0.9$, and $\hbar\omega/E_0 = 0.1$ we find $(|c_1(T)|^2, |c_2(T)|^2) = (0.7971, 0.2036), (0.9138, 0.0867), (0.9810, 0.0191)$, respectively, for different values of the semiaxis of the ellipse $\Delta E_R/E_0 = 1.9, 1.5, 1$. The initial state is $(|c_1(0)|^2, |c_2(0)|^2) = (1, 0)$. Note that the parameter for the semiaxis $\Delta E_R/E_0$ can be varied experimentally either by changing the Dresselhaus field $\Delta E_R$ or the size of the dot through $E_0$. We have verified that two different values of the frequency $\omega$ give the same values of $(|c_1(T)|^2, |c_2(T)|^2)$ as long as the other parameters are unchanged, confirming that the matrix Berry phase is a geometric phase. This should be tested in any experimental investigation of matrix Berry phases. Experimental data of single quantum dots would be less complicated than data of an ensemble of dots with various sizes of dots, and can thus be compared directly with our theoretical results.

APPENDIX A: MATHEMATICAL NOTE

Let $|\Psi_1\rangle$ consists of $\{\phi_1, \phi_2, \phi_3\}$ and let $|\Psi_2\rangle$ consists of $\{\phi_1, \phi_2, \phi_4\}$:
Let us find the off-diagonal non-Abelian vector potential $\phi$ and with
\begin{equation}
\partial_{\lambda_k} |\Psi_1\rangle = \frac{1}{\sqrt{3!}} \{ \phi_1(r_1)\phi_2(r_2)\phi_3(r_3) + \phi_3(r_1)\phi_1(r_2)\phi_2(r_3) + \phi_2(r_1)\phi_3(r_2)\phi_1(r_3) \\
- \phi_3(r_1)\phi_2(r_2)\phi_1(r_3) - \phi_1(r_1)\phi_3(r_2)\phi_2(r_3) - \phi_2(r_1)\phi_1(r_2)\phi_3(r_3) \} (A1)
\end{equation}
and
\begin{equation}
|\Psi_2\rangle = \frac{1}{\sqrt{3!}} \{ \phi_1(r_1)\phi_2(r_2)\phi_4(r_3) + \phi_4(r_1)\phi_1(r_2)\phi_2(r_3) + \phi_2(r_1)\phi_4(r_2)\phi_1(r_3) \\
- \phi_4(r_1)\phi_2(r_2)\phi_1(r_3) - \phi_1(r_1)\phi_4(r_2)\phi_2(r_3) - \phi_2(r_1)\phi_1(r_2)\phi_4(r_3) \}. (A2)
\end{equation}

The diagonal elements of the non-Abelian gauge potential between the Slater determinant wavefunctions are
\begin{equation}
i\langle \Psi_i | \frac{\partial}{\partial \lambda_k} |\Psi_j\rangle = i \sum_p \langle \phi_p(r) | \frac{\partial}{\partial \lambda_k} |\phi_p(r)\rangle. (A3)
\end{equation}

Let us find the off-diagonal non-Abelian vector potential elements $i\langle \Psi_i | \frac{\partial}{\partial \lambda_k} |\Psi_2\rangle$ between the two Slater determinant wavefunctions $|\Psi_1\rangle$ and $|\Psi_2\rangle$. When $\phi_3$ is replaced with $\phi_4$ the state $|\Psi_1\rangle$ transforms into $|\Psi_2\rangle$. We find $\langle \Psi_1 | \frac{\partial}{\partial \lambda_k} |\Psi_2\rangle = \langle \phi_3(\vec{r}) | \frac{\partial}{\partial \lambda_k} |\phi_4(\vec{r})\rangle$. This result may be easily generalized to $N$ particle Slater determinant wavefunctions. In general the non-Abelian vector potential element between two different Slater determinant wavefunctions, $|\Psi_i\rangle$ and $|\Psi_j\rangle$, is non zero when $|\Psi_i\rangle$ can be transformed into $|\Psi_j\rangle$ by replacing one single electron wavefunction in $|\Psi_i\rangle$ with another wavefunction in $|\Psi_j\rangle$. If these single electron wavefunctions are denoted by $\phi_\ell$ with $\phi_p$ then we find
\begin{equation}
\langle \Psi_i | \frac{\partial}{\partial \lambda_k} |\Psi_j\rangle = \langle \phi_\ell(\vec{r}) | \frac{\partial}{\partial \lambda_k} |\phi_p(\vec{r})\rangle. (A4)
\end{equation}

If more than two single electron wavefunctions in $|\Psi_i\rangle$ must be exchanged with those in $|\Psi_j\rangle$ to transform $|\Psi_i\rangle$ into $|\Psi_j\rangle$ then $\langle \Psi_i | \frac{\partial}{\partial \lambda_k} |\Psi_j\rangle = 0$.

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