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# Effect of many-body quantum fluctuations on matrix Berry phases of a two-dimensional n-type semiconductor quantum dot

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**Abstract**

In the presence of spin–orbit coupling and inversion symmetry of the lateral confinement potential a single electron does not exhibit matrix Berry phases in quasi-two-dimensional semiconductor quantum dots. In such a system we investigate whether many-body correlation effects can lead to finite matrix Berry phases. We find that the transformation properties of many-electron wavefunctions under two-dimensional inversion operation do not allow finite matrix Berry phases. This effect is exact and is independent of the form of electron–electron interactions. On the other hand, quasi-two-dimensional semiconductor quantum dots with lateral confinement potential without inversion symmetry can have finite matrix Berry phases. We find that many-body quantum fluctuations can change matrix Berry phases significantly in such systems.

## 1. Introduction

Electron spins in two-dimensional semiconductors may be manipulated electrically [1–9]. It is more challenging to control single or a few spins coherently in confined nanoquantum dots [10–16]. One way to perform such a coherent control electrically is based on matrix Berry phases [17–19]. There are several semiconductor nanosystems with spin–orbit coupling terms [20, 21] that exhibit matrix Berry phases: they include excitons [22], CdSe nanocrystals [23], acceptor states of p-type semiconductors [24] and ring spin filters [25]. Recently it has been demonstrated theoretically that it is possible to control electrically electron spins of II–VI and III–V n-type semiconductor quantum dots [26] and rings [27] by exploiting matrix Berry phases. In these systems spin–orbit terms are invariant under time reversal operation [28] and the discrete energy levels are doubly degenerate, and these properties are responsible for the generation of matrix Berry phases [29][4].

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[4] The relation between molecular Kramers degeneracy and non-Abelian phase factors is investigated in [29].

Coherent manipulation can be achieved by changing external parameters adiabatically in time. According to the theory of the matrix Berry phase [18] the ground state of a doubly degenerate Hilbert subspace of these II–VI and III–V n-type semiconductor quantum dots changes adiabatically in time as

$$\Psi(t) = C_1(t)\Phi(t) + C_2(t)\overline{\Phi}(t), \tag{1}$$

where $\Phi(t)$ and $\overline{\Phi}(t)$ are the instantaneous *degenerate* single-electron or many-body eigenstates (the overbar in $\overline{\Phi}(t)$ means time reversal state of $\Phi(t)$). The time-dependent Schrödinger equation for the expansion coefficients $C_1$ and $C_2$ of equation (1) can be written as

$$\mathrm{i}\hbar\dot{C}_v = -\sum_w A_{vw}C_w \qquad v = 1, 2, \tag{2}$$

where $A_{vw} = \hbar\sum_k (A_k)_{v,w}\frac{\mathrm{d}\lambda_k}{\mathrm{d}t}$ and $\lambda_k$ are the adiabatic parameters labeled by $k$. The time evolution of the ground state is governed by the $2 \times 2$ non-Abelian vector potentials

 

(NAVPs) between the degenerate eigenstates

$$(A_k)_{v,w} = \mathrm{i}\langle\Phi_v|\frac{\partial}{\partial\lambda_k}|\Phi_w\rangle, \tag{3}$$

where $\Phi_1 = \Phi(t)$ and $\Phi_2 = \overline{\Phi}(t)$.

II–VI and III–V semiconductor quantum dots usually contain several electrons and many-body effects may affect the matrix Berry phase. Formal expressions for many-body NAVPs can be derived including many-body exchange and correlation effects [30]. Correlation effects are taken into account by writing many-body eigenstates as a linear combination of single Slater determinant wavefunctions. When odd numbers of electrons are present the ground states are doubly degenerate. At each time instant $t$ they can be written as linear combinations of Slater determinant states $|\Psi_i\rangle$:

$$|\Phi\rangle = \sum_i^M c_i|\Psi_i\rangle, \qquad |\overline{\Phi}\rangle = \hat{T}\Phi = \sum_i^M d_i|\Psi_i\rangle, \tag{4}$$

where $\hat{T}$ is the time reversal operator and $M$ is the number of instantaneous Slater determinant states in the linear combinations. These states are time reversal states of each other. (We have suppressed $t$ in the quantities appearing in equation (4), and from now on we will do so unless explicitly written.) The diagonal elements of the NAVPs are

$$(A_k)_{1,1} = \mathrm{i}\langle\Phi|\frac{\partial}{\partial\lambda_k}|\Phi\rangle = \mathrm{i}\sum_i c_i^*\frac{\partial c_i}{\partial\lambda_k} + \sum_{i,j} c_i^* c_j (B_k)_{i,j}, \tag{5}$$

where the elements of the NAVP between Slater determinant states are

$$(B_k)_{i,j} = \mathrm{i}\langle\Psi_i|\frac{\partial}{\partial\lambda_k}|\Psi_j\rangle. \tag{6}$$

(The Slater determinant states in this expression can have different total confinement energies.) It can be shown that if $(B_k)_{i,j}$ is non-zero one can find single-electron wavefunctions $\phi_p$ and $\phi_q$ so that

$$(B_k)_{i,j} = (a_k)_{p,q} = \mathrm{i}\langle\phi_p|\frac{\partial}{\partial\lambda_k}|\phi_q\rangle. \tag{7}$$

When the single-electron eigenstates $\phi_p$ and $\phi_q$ belong to different energy shells $(a_k)_{p,q}$ are called single-electron *inter-shell* NAVPs [30]. The other diagonal elements $(A_k)_{2,2}$ are given by equation (5) except that $\Phi$ is replaced by $\overline{\Phi}$. The off-diagonal elements are

$$(A_k)_{1,2} = \mathrm{i}\langle\Phi|\frac{\partial}{\partial\lambda_k}|\overline{\Phi}\rangle = \mathrm{i}\sum_i c_i^*\frac{\partial d_i}{\partial\lambda_k} + \sum_{i,j} c_i^* d_j (B_k)_{i,j}, \tag{8}$$

with $(A_k)_{2,1} = (A_k)_{1,2}^*$. Within this approach one can use a Hartree–Fock approximation based on single Slater determinant ground states, and show that fermion antisymmetry does not change the value of the matrix Berry phase.

These formal results have not been applied to investigate the interplay between matrix Berry phase and many-body correlations of II–VI and III–V semiconductor quantum dots. For example, not much is known about how the effects beyond the Hartree–Fock approximation, i.e. correlation effects, change the matrix Berry phase. The total many-electron Hamiltonian consists of four terms: the kinetic part $H_\mathrm{K}$, confinement potential $V_\mathrm{C}$, spin–orbit terms $H_\mathrm{so}$ and electron–electron interactions $V$:

$$H = H_\mathrm{K} + V_\mathrm{C} + H_\mathrm{so} + V. \tag{9}$$

Note that $V_\mathrm{C}$ *may or may not* be invariant under two-dimensional inversion operation. However, $H_\mathrm{so}$ is *not* invariant under two-dimensional inversion operation and, consequently, the total Hamiltonian $H$ is not invariant under two-dimensional inversion operation, irrespective of the invariance of $V_\mathrm{C}$. This implies that eigenstates of the total Hamiltonian $H$ are not eigenstates of the two-dimensional inversion operator. In the absence of many-body effects it can be shown that, when the lateral electric confinement potential has inversion symmetry, i.e. $V_\mathrm{C}$ is invariant under two-dimensional inversion operation, the matrix Berry phase is absent [26]. This is because off-diagonal elements of single-electron *intra-shell* NAVPs, equation (3), may vanish. However, in the many-electron case the NAVPs may take finite values since they are related to the single-electron *inter-shell* NAVPs, which can be non-zero, as can be seen from equation (7). It is thus unclear whether the matrix Berry phase remains zero or not. In addition, it is not understood how many-body correlation effects change quantitatively the matrix Berry phase when a distortion potential breaks inversion symmetry of the lateral electric confinement potential. Such a quantitative estimate should be valuable in understanding experimental results of matrix Berry phases.

In order to investigate these issues we use the formal results of equations (4)–(8). We have investigated the effect of many-body correlations and have found that they do not induce a finite matrix Berry phase when the lateral confinement potential is invariant under two-dimensional inversion operation. This is an *exact* result. The main physics is that, although there is coupling between different single-electron energy levels, many-body correlation effects cancel this coupling. On the other hand, for lateral confinement potentials without inversion symmetry we find that many-body quantum fluctuations change the matrix Berry phase. In this case it is difficult to investigate exactly correlation effects. We have treated them in an approximation that includes a finite number $M$ of many-body basis vectors, and have performed a numerical computation to estimate the effect of quantum fluctuations on the matrix Berry phase. Our approximate calculation shows that the effect of quantum fluctuations on the matrix Berry phase becomes more significant as the ratio between the Coulomb strength and the single-electron energy spacing increases. The main results of our investigation may be tested experimentally in semiconductor dots, as we discuss in section 4.

Our paper is organized as follows. In section 2 we describe our model Hamiltonian. In section 3 we compute the matrix Berry phase when the lateral confinement potential is not invariant under two-dimensional inversion operation. Discussions are given in section 4.

## 2. Model Hamiltonian

The total single-electron Hamiltonian of a II–VI or III–V n-type semiconductor quantum dot contains an electric confinement potential and spin–orbit coupling terms. An electron with the effective mass $m^*$ of such a system can be described by the Hamiltonian [26]

$$\begin{aligned} h_{\mathrm{S}} &= h_{\mathrm{K}} + h_{\mathrm{R}}, \\ h_{\mathrm{K}} &= -\frac{\hbar^2\nabla^2}{2m^*} + U(\vec{r}) + V(z), \\ h_{\mathrm{R}} &= c_{\mathrm{R}}\left(\sigma_x k_y - \sigma_y k_x\right), \end{aligned} \tag{10}$$

where the two-dimensional lateral confinement potential is

$$U(\vec{r}) = \tfrac{1}{2}m^*\omega_x^2 x^2 + \tfrac{1}{2}m^*\omega_y^2 y^2 + V_p(x, y), \tag{11}$$

and the vertical confinement potential is $V(z)$ (here the two-dimensional coordinate is $\vec{r} = (x, y)$). An electric field $E$ is applied along the $z$ axis and electrons are confined in a triangular potential $V(z)$, and it is assumed that only the lowest subband along the $z$ axis is occupied. Thus in our model quantum dots are effectively quasi-two-dimensional. The Rashba constant $c_{\mathrm{R}}$ changes when the electric field $E$ is varied. The potential $V_p(\vec{r}) = \epsilon' y$ perturbs the two-dimensional harmonic potential with the strengths $\omega_x$ and $\omega_y$. This potential can be realized by applying a constant electric field along the $y$ axis and its strength $\epsilon'$ is controlled by the magnitude of the applied electric field along the $y$ axis. The crucial point about $U(\vec{r})$ and $V(z)$ is that they can be changed *electrically*, which provides a means to control coherently electron spins. The Rashba spin–orbit term [20] is $h_{\mathrm{R}}$ with Pauli spin matrices $\sigma_{x,y}$ and a momentum operator $k_x = \frac{1}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}$ (similarly with $k_y$). The Dresselhaus term can also be included, but since it does not change results qualitatively we *omit* it here. The Hamiltonian, equation (10), represents a simple model of the physical system, but it has all the correct symmetries. It is invariant under time reversal operation and each eigenenergy is doubly degenerate. The Hamiltonian is not invariant under two-dimensional inversion operation $\vec{r} \to -\vec{r}$ since the Rashba spin–orbit term breaks inversion symmetry. In order to build up many-body wavefunctions we need to first construct single-electron eigenstates. Each of these wavefunctions consists of the spin-up and-down components:

$$|\phi\rangle = \begin{pmatrix} F_\uparrow(\vec{r}) \\ F_\downarrow(\vec{r}) \end{pmatrix} = \begin{pmatrix} \sum_{mn} c_{mn\uparrow}\langle\vec{r}|mn\uparrow\rangle \\ \sum_{m'n'} c_{m'n'\downarrow}\langle\vec{r}|m'n'\downarrow\rangle \end{pmatrix}, \tag{12}$$

where $|mn\rangle$ are eigenstates of two-dimensional harmonic oscillators.

## 3. Breaking of inversion symmetry, correlations and matrix Berry phase

When the lateral potential has two-dimensional inversion symmetry the effect of many-body correlations will not produce a finite value of the matrix Berry phase. This can be shown to be an exact result. (See appendix B.) It follows from the transformation properties of the wavefunctions under inversion operation. It should be stressed that, although the lateral potential has inversion symmetry, the total Hamiltonian does not. When the inversion symmetry of $U(\vec{r})$ is broken many-body correlations will induce a finite value of the matrix Berry phase. It is not possible to compute this effect exactly unlike the case when $U(\vec{r})$ has inversion symmetry. In a previous work a truncated single-electron $4 \times 4$ Hamiltonian matrix was used [26]. However, many-body states built from these approximate single-electron wavefunctions do not adequately describe many-body correlation effects. In this paper we find improved single-electron wavefunctions, and use them to build many-body wavefunctions. Here we will compute the degenerate ground states approximately by using a finite number of Slater determinant basis states, i.e. using $M = 4$ in equation (4). This approximation should be valid as long as the single-electron energy spacing is larger than or comparable to the characteristic Coulomb energy scale.

### 3.1. Single-electron Hamiltonian matrix

We employ an improved approximation of a $6 \times 6$ truncated single-electron Hamiltonian matrix, whose eigenvectors can be written, according to equation (12), as

$$\begin{aligned} |\phi\rangle \cong\ & c_{0,0,\uparrow}|00\uparrow\rangle + c_{0,1,\uparrow}|0,1,\uparrow\rangle + c_{0,2,\uparrow}|0,2,\uparrow\rangle \\ & + c_{0,0,\downarrow}|0,0,\downarrow\rangle + c_{0,1,\downarrow}|0,1,\downarrow\rangle + c_{0,2,\downarrow}|0,2,\downarrow\rangle. \end{aligned} \tag{13}$$

These expansion coefficients $c_{mn\sigma}$ of the basis states $|mn\sigma\rangle$ are eigenvectors of the $6 \times 6$ Hamiltonian matrix

$$H_{\mathrm{single}} = \begin{pmatrix} E_0 & E_{\mathrm{P}} & 0 & 0 & -\mathrm{i}E_{\mathrm{R}} & 0 \\ E_{\mathrm{P}} & E_1 & \sqrt{2}E_{\mathrm{P}} & \mathrm{i}E_{\mathrm{R}} & 0 & -\sqrt{2}\mathrm{i}E_{\mathrm{R}} \\ 0 & \sqrt{2}E_{\mathrm{P}} & E_2 & 0 & \sqrt{2}\mathrm{i}E_{\mathrm{R}} & 0 \\ 0 & -\mathrm{i}E_{\mathrm{R}} & 0 & E_0 & E_{\mathrm{P}} & 0 \\ \mathrm{i}E_{\mathrm{R}} & 0 & -\sqrt{2}\mathrm{i}E_{\mathrm{R}} & E_{\mathrm{P}} & E_1 & \sqrt{2}E_{\mathrm{P}} \\ 0 & \sqrt{2}\mathrm{i}E_{\mathrm{R}} & 0 & 0 & \sqrt{2}E_{\mathrm{P}} & E_2 \end{pmatrix}. \tag{14}$$

The basis vectors of this Hamiltonian matrix are ordered as $|00\uparrow\rangle$, $|01\uparrow\rangle$, $|02\uparrow\rangle$, etc. To reduce the number of independent external parameters we can set the ratio between the harmonic frequencies to be a constant, for example, $\omega_x = 3\omega_y$. Then the energies of the two-dimensional harmonic oscillators are $E_0 = 2\hbar\omega_y$, $E_1 = 3\hbar\omega_y$ and $E_2 = 4\hbar\omega_y$. The eigenvalues of this matrix are

$$\begin{aligned} X_1 &= \frac{3}{2}E_0 - \frac{1}{3}\varepsilon\cos\left(\frac{\theta}{3}\right), \\ X_2 &= \frac{3}{2}E_0 + \frac{1}{6}\varepsilon\left(\cos\left(\frac{\theta}{3}\right) - \sqrt{3}\sin\left(\frac{\theta}{3}\right)\right), \\ X_3 &= \frac{3}{2}E_0 + \frac{1}{6}\varepsilon\left(\cos\left(\frac{\theta}{3}\right) + \sqrt{3}\sin\left(\frac{\theta}{3}\right)\right), \end{aligned} \tag{15}$$

where

$$\begin{gathered}\varepsilon = \sqrt{3}\sqrt{E_0^2 + 12\delta}, \qquad \delta = E_{\mathrm{P}}^2 + E_{\mathrm{R}}^2, \\ A = -18E_0\left(E_{\mathrm{P}}^2 + E_{\mathrm{R}}^2\right), \\ B = \tfrac{1}{6}\sqrt{108\left(E_0^2 + 12\delta\right)^3 - 11664E_0^2\delta^2}, \\ \cos\theta = \frac{A}{\sqrt{A^2+B^2}}, \qquad \sin\theta = \frac{B}{\sqrt{A^2+B^2}}.\end{gathered} \tag{16}$$

Because of time reversal symmetry each eigenenergy is doubly degenerate. The doubly degenerate wavefunctions of the energy shells with eigenenergies $X_1$, $X_2$ and $X_3$ are denoted by $(\phi_1, \phi_2)$, $(\phi_3, \phi_4)$ and $(\phi_5, \phi_6)$, respectively. There is some arbitrariness in choosing these eigenstates since new eigenstates may be obtained by applying unitary transformations to the old set in each degenerate energy shell [18]. We choose the expansion coefficients of the first, second and third pairs of degenerate eigenstates of equation (14) as

$$\begin{aligned}\vec{c}(1) &= \frac{1}{\sqrt{N_1}}\left(\alpha_1, \beta_1, \gamma_1, \delta_1, 0, 1\right), \\ \vec{c}(2) &= \frac{1}{\sqrt{N_1}}\left(-\delta_1^*, 0, -1, \alpha_1^*, \beta_1^*, \gamma_1^*\right),\end{aligned} \tag{17}$$

$$\begin{aligned}\vec{c}(3) &= \frac{1}{\sqrt{N_2}}\left(\alpha_2, \beta_2, \gamma_2, \delta_2, 0, 1\right), \\ \vec{c}(4) &= \frac{1}{\sqrt{N_2}}\left(-\delta_2^*, 0, -1, \alpha_2^*, \beta_2^*, \gamma_2^*\right),\end{aligned} \tag{18}$$

and

$$\begin{aligned}\vec{c}(5) &= \frac{1}{\sqrt{N_3}}\left(\alpha_3, \beta_3, \gamma_3, \delta_3, 0, 1\right), \\ \vec{c}(6) &= \frac{1}{\sqrt{N_3}}\left(-\delta_3^*, 0, -1, \alpha_3^*, \beta_3^*, \gamma_3^*\right).\end{aligned} \tag{19}$$

Here $\vec{c}(p)$ denotes the expansion coefficients $\{c_{mn\sigma}(p)\}$ of the $p$th eigenstate. The quantities $\alpha_p$, $\beta_p$, $\gamma_p$ and $\delta_p$ are too complicated and lengthy to give here: however, they are all purely real or imaginary. This choice of the eigenstates simplifies the calculation of the many-body NAVPs. When $U(\vec{r})$ has inversion symmetry, i.e. $E_{\mathrm{P}} = 0$, then $\alpha_i$ and $\gamma_i$ are zero.

### *3.2. Many-body Hamiltonian matrix*

Using the previous results for single-electron wavefunctions we construct many-body ground states. Let us assume there are three electrons in the dot. In order to calculate the many-electron NAVPs we need to compute the expansion coefficients $c_i$ and $d_i$ of equation (4). We include three single-electron energy shells, each with double degeneracy. In our approximation we truncate the number of Slater determinant wavefunctions to four with the lowest total confinement energies. They are

$$\begin{aligned}|\Psi_1\rangle &= a_3^+ a_2^+ a_1^+|0\rangle, \\ |\overline{\Psi}_1\rangle &= a_4^+ a_2^+ a_1^+|0\rangle = |\Psi_2\rangle, \\ |\Psi_3\rangle &= a_5^+ a_2^+ a_1^+|0\rangle, \\ |\overline{\Psi}_3\rangle &= a_6^+ a_2^+ a_1^+|0\rangle = |\Psi_4\rangle,\end{aligned} \tag{20}$$

where $a_i^+$ creates an electron in the $i$th single-electron eigenstate $|\phi_i\rangle$, given in equations (17)–(19). The vacuum state is $|0\rangle$. The truncated many-body Hamiltonian matrix is

$$H = \begin{pmatrix} E_{\mathrm{A}} & 0 & a & b \\ 0 & E_{\mathrm{A}} & -b^* & a^* \\ a^* & -b & E_{\mathrm{B}} & 0 \\ b^* & a & 0 & E_{\mathrm{B}} \end{pmatrix}, \tag{21}$$

where the matrix elements are

$$\begin{aligned}\langle\Psi_1|H|\Psi_1\rangle &= E_{\mathrm{A}}, \\ \langle\Psi_3|H|\Psi_3\rangle &= E_{\mathrm{B}}, \\ \langle\Psi_1|V|\Psi_3\rangle &= a, \\ \langle\Psi_1|V|\Psi_4\rangle &= b, \\ \langle\Psi_1|V|\Psi_2\rangle &= 0 \\ \langle\Psi_3|V|\Psi_4\rangle &= 0.\end{aligned} \tag{22}$$

The matrix elements $a$ and $b$ contain Hartree and exchange contributions. All the quantities $E_{\mathrm{A}}$, $E_{\mathrm{B}}$, $a$ and $b$ change when the adiabatic parameters change because they depend on the single-electron wavefunctions, equations (17)–(19), that are functions of the adiabatic parameters. The ground-state eigenenergy is doubly degenerate with the value

$$E_{\mathrm{G}} = \tfrac{1}{2}\left(E_{\mathrm{A}} + E_{\mathrm{B}} - D^{\frac{1}{2}}\right), \tag{23}$$

where

$$D = (E_{\mathrm{A}} - E_{\mathrm{B}})^2 + 4(|a|^2 + |b|^2). \tag{24}$$

One of the doubly degenerate ground states has the expansion coefficients

$$(c_1, c_2, c_3, c_4) = \frac{1}{\sqrt{N_1}}\left(-bK, -a^*K, 0, 1\right), \tag{25}$$

where

$$K = \frac{(-E_{\mathrm{A}} + E_{\mathrm{B}} + D^{\frac{1}{2}})}{2\left(|a|^2 + |b|^2\right)}. \tag{26}$$

The other degenerate state is obtained by taking time reversal of this state

$$(d_1, d_2, d_3, d_4) = \frac{1}{\sqrt{N_1}}\left(aK, -b^*K, -1, 0\right). \tag{27}$$

Since $c_{mn\sigma}(p)$ of equations (17)–(19) are purely real or imaginary it follows from the expression for the Coulomb matrix elements, equation (C.1), that $a$ is real and $b$ is imaginary. Then from equation (26) we also see that $K$ is

real. This implies that the expansion coefficients $c_i$ and $d_i$ are always purely real or imaginary.

When inversion symmetry is *present* in $U(\vec{r})$ the results given in equations (25) and (27) simplify since $b = 0$, which follows from

$$b = \langle\Psi_1|H|\Psi_4\rangle = \langle 13|v|16\rangle - \langle 13|v|16\rangle + \langle 23|v|26\rangle - \langle 23|v|62\rangle = 0, \tag{28}$$

where $v$ is the Coulomb interactions between two electrons. (This is because, as can be seen from equations (A.4)–(A.6), $\phi_3(r)^*\phi_6(r)$, $\phi_1(r)^*\phi_6(r)$ and $\phi_3(r)^*\phi_2(r)$ are odd functions of $r$). In this case the expansion coefficients of the doubly degenerate many-body ground states are given by

$$(c_1, c_2, c_3, c_4) = \frac{1}{\sqrt{N_1}}(0, -aK, 0, 1) \tag{29}$$

and

$$(d_1, d_2, d_3, d_4) = \frac{1}{\sqrt{N_1}}(aK, 0, -1, 0)\,. \tag{30}$$

Note that $c_2^* d_3$ may not be zero, but $(B_k)_{2,3} = (a_k)_{4,5} = 0$ from equation (A.8).

### 3.3. Correlation and matrix Berry phase

We are now ready to calculate the matrix Berry phase. The strengths of the distortion potential and Rashba constant are

$$E_{\rm P} = \epsilon' \ell_y/\sqrt{2} \qquad \text{and} \qquad E_{\rm R} = c_{\rm R}/\sqrt{2}\ell_y. \tag{31}$$

We choose these parameters as the adiabatic parameters: $\lambda_1 = E_{\rm P}$ and $\lambda_2 = E_{\rm R}$. (The single-electron Hamiltonian depends on them, see equation (14). As explained in section 2 these parameters can be controlled electrically.) The adiabatic path is elliptic:

$$(\lambda_1(t), \lambda_2(t)) = (E_{\rm R}(t), E_{\rm P}(t)) = (E_{\rm R,c} + \Delta E_{\rm R}\cos(\omega t), E_{P,\rm c} + \Delta E_{\rm P}\sin(\omega t)). \tag{32}$$

We use the parameters $E_{\rm R,c} = 0.5E_0$, $E_{P,\rm c} = 0.3E_0$, $\Delta E_{\rm R} = 0.35E_0$, $\Delta E_{\rm P} = 0.21E_0$ and $\omega = E_0/10$. The following steps are implemented consecutively in computing the matrix Berry phase:

(a) Single-electron eigenvectors are evaluated numerically from equations (17)–(19).
(b) Coulomb matrix elements are computed using equations (C.2).
(c) Many-electron eigenvectors are evaluated from equations (25) and (27).
(d) The many-electron NAVPs, given by equations (5) and (8), are evaluated on the various points on the closed adiabatic path in the parameter space. For this purpose the expansion coefficients $d_i$ are differentiated numerically. Also we use that the diagonal elements of the NAVPs between Slater determinants, equation (6), are zero:

$$(B_k)_{i,i} = \sum_{p\in occ.} (a_k)_{p,p} = 0, \tag{33}$$

where the sum over $p$ indicates a sum over single-electron states that appear in the Slater determinant state $|\Psi_i\rangle$. This follows from the fact that $c_{mn}(p)$ is always purely real or imaginary, see equations (17)–(19). Thus $(a_k)_{p,p} = \frac{\rm i}{2}\frac{\rm d}{{\rm d}\lambda_k}[\sum_{mn} c_{mn}^*(p)c_{mn}(p)] = 0$ for each $p$. (Note that the harmonic oscillator states $|mn\rangle$ do not depend on $\lambda_k$.) In addition it follows from the orthonormalization $\langle\Psi_i|\Psi_j\rangle = \delta_{ij}$ and equation (6) that

$$(B_k)_{i,j} = (B_k)_{j,i}^* \qquad \text{for } i \neq j. \tag{34}$$

Using these results we find that the NAVPs, equations (5) and (8), are off-diagonal:

$$A_1 = \begin{pmatrix} 0 & P \\ P & 0 \end{pmatrix}, \qquad A_2 = \begin{pmatrix} 0 & Q \\ Q & 0 \end{pmatrix} \tag{35}$$

with $P$, $Q$ real. The time-dependent Schrödinger equation for the expansion coefficients $C_1$ and $C_2$, given by equation (2), can then be written as

$$\frac{{\rm d}C_1}{{\rm d}t} = {\rm i}f(t)C_2, \qquad \frac{{\rm d}C_2}{{\rm d}t} = {\rm i}f(t)C_1, \tag{36}$$

where the function

$$f(t) = P\frac{{\rm d}\lambda_1}{{\rm d}t} + Q\frac{{\rm d}\lambda_2}{{\rm d}t}. \tag{37}$$

For each point $(\lambda_1(t), \lambda_2(t))$ on the adiabatic path the off-diagonal elements of the NAVPs are evaluated numerically, as described in steps (a), (b), (c) and (d) above. As the strength of the Coulomb interaction $\kappa = \frac{e^2}{\epsilon\ell_y}/E_0$ increases $f(t)$ varies more significantly, see figure 1. The calculated matrix Berry phase for $\kappa \leqslant 1$ is given as follows[5]:

$$\begin{pmatrix} C_1(T) \\ C_2(T) \end{pmatrix} = \begin{pmatrix} \cos\chi & {\rm i}\sin\chi \\ {\rm i}\sin\chi & \cos\chi \end{pmatrix} \begin{pmatrix} C_1(0) \\ C_2(0) \end{pmatrix}, \tag{38}$$

where $T$ is the period of the adiabatic cycle. The parameter $\chi = \int_0^T f(t){\rm d}t$ of equation (38) is shown in figure 2. For $\kappa > 1$ Slater determinant states with higher total confinement energies than those four we have used need to be included in the many-body basis set. This also implies that single-electron states with higher energies than those six we have used must be included.

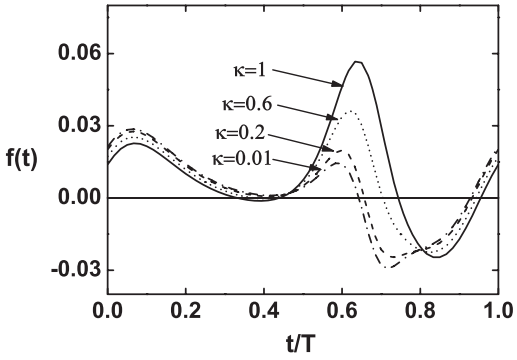


**Figure 1.** $f(t)$ as a function of $t/T$ for $\kappa = 0.01, 0.2, 0.6, 1$.

[5] Our matrix Berry phase is parameterized by a single parameter $\chi$ for the special choice of basis vectors given in equations (17)–(19).

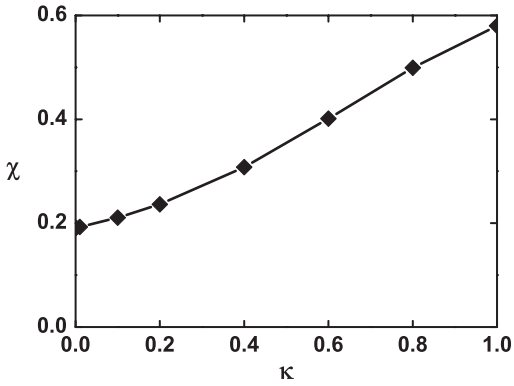


**Figure 2.** The dependence of $\chi$ on $\kappa$, where $\chi$ characterizes the $2 \times 2$ matrix Berry phase and $\kappa$ is the ratio between the Coulomb energy scale and single-electron level spacing. $\kappa$ measures the strength of quantum fluctuations.

As a check on the correctness of our numerical procedures we have verified numerically that the value of $\cos(\chi)$ is independent of the choice of the set of degenerate ground states. (Although the elements of the matrix Berry phase depend on the choice of the basis states the trace of it is independent of the basis states.) By taking the limit of the vanishing strength of Coulomb interaction $\kappa \to 0$ in equations (25) and (27) we see that the degenerate ground states are $(c_1, c_2, c_3, c_4) = (\alpha, \beta, 0, 0)$ and $(d_1, d_2, d_3, d_4) = (-\beta^*, \alpha^*, 0, 0)$. (This limit is somewhat delicate since $N_1$ and $K$ diverge.) We can also use another possible set for degenerate ground states: $(c_1, c_2, c_3, c_4) = (1, 0, 0, 0)$ and $(d_1, d_2, d_3, d_4) = (0, 1, 0, 0)$. The elements of the NAVPs with respect to these new degenerate ground states are $(\tilde{A}_k)_{11} = (\tilde{B}_k)_{11} = 0$, $(\tilde{A}_k)_{12} = (\tilde{B}_k)_{12} = (a_k)_{34}$. However, we find that the value of $\cos(\chi)$ is the same in these different sets of ground states.

Using the computed matrix Berry phase, equation (38), we now evaluate the single-electron occupation numbers, which can be measured in tunneling experiments. Combining equations (1) and (4) we find that the many-body ground state at each time instant is given by

$$|\Psi\rangle = C_1 \sum_i c_i |\Psi_i\rangle + C_2 \sum_i d_i |\Psi_i\rangle. \tag{39}$$

The probabilities that a single-electron eigenstate $p$ is occupied at $t = 0$ and $T$ are, respectively

$$\begin{aligned} f_p(0) &= \sum_i |(C_1(0)c_i(0) + C_2(0)d_i(0))|^2 \theta_{ip} \\ f_p(T) &= \sum_i |(C_1(T)c_i(0) + C_2(T)d_i(0))|^2 \theta_{ip}, \end{aligned} \tag{40}$$

where $f_p = \langle\Psi|a_p^+ a_p|\Psi\rangle$, $c_i(T) = c_i(0)$ and $d_i(T) = d_i(0)$ ($c_i$ and $d_i$ are given in equations (25) and (27)). If the single-electron eigenstate $p$ is occupied (unoccupied) in the Slater determinant state $|\Psi_i\rangle$ we define $\theta_{ip} = 1(0)$. At $\kappa = 1$ we find for the occupation number of the third single-electron level $f_3(0) = 0.0266$ and $f_3(T) = 0.4494$. For the fourth single-electron level we find $f_4(0) = 0.9492$ and $f_4(T) = 0.5264$. The difference between $f_p(0)$ and $f_p(T)$ reflects the presence of a matrix Berry phase. It would be interesting to measure these differences in the single-electron occupation numbers before and after an adiabatic cycle.

## 4. Discussions

The Hamiltonian of II–VI and III–V n-type semiconductor quantum dots with spin–orbit terms are not invariant under two-dimensional inversion operators. Despite this, whether the lateral confinement potential is or is not invariant has important consequences on the matrix Berry phase. Our investigation shows that many-body correlation effects do not generate a matrix Berry phase when the confinement potential is invariant under two-dimensional parity operation. This is an exact result. It holds despite that the *inter-shell* single-electron NAVPs couple different single-electron energy levels. However, when the confinement potential is not invariant under parity operation our approximate calculation indicates that correlations can affect the matrix Berry phase significantly.

Our results can be tested experimentally in self-assembled dots with wetting layers [31, 32] or in gated n-type semiconductor dots [33]. These quantum dots have several attractive features: the lateral shape of the dot can be distorted electrically to induce breaking of two-dimensional inversion symmetry. Moreover, the electron number can be varied from one to several electrons. These electric means for control provide excellent opportunities to test systematically the effect of many-body correlations. We have investigated quantitatively how quantum fluctuations affect the matrix Berry phase when the strength of Coulomb interaction is smaller or comparable to the single-electron level spacing. In self-assembled dots the characteristic scale of the single-electron level spacing is 10–40 meV, which is larger than or comparable to the Coulomb energy scale of 10 meV. However, in gated semiconductor quantum dots [33] the characteristic scale of the single-electron level spacing is a few meV, which is smaller than the Coulomb energy scale. In order to obtain accurate results for these dots one needs to include a large number of Slater determinant basis states and single-electron states. Nonetheless, even for these systems the matrix Berry phase should be absent when two-dimensional inversion symmetry is present, which should be experimentally testable. It should be noted that the matrix Berry phase depends on the geometric properties of an adiabatic path [34].

## Acknowledgments

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## Appendix A. Single-electron states and lateral inversion symmetry

When the lateral confinement potential $U(\vec{r})$ has inversion symmetry the single-electron eigenstates simplify. For a given

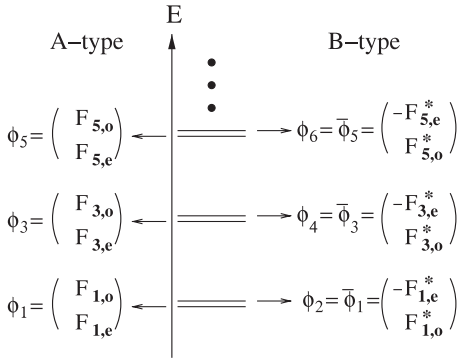


**Figure A.1.** Each degenerate pair of eigenstates consists of A and B types. These two types of eigenstates are time-reversed states of each other. As the subscript $i$ in $\phi_i$ increases the transformation properties of $\phi_i$ alternate between A and B types.

twofold degenerate energy shell we choose [30] one of the eigenstates as

$$|\phi\rangle = \begin{pmatrix} F_o(\vec{r}) \\ F_e(\vec{r}) \end{pmatrix}, \qquad \text{or} \qquad |\phi\rangle = \begin{pmatrix} F_e(\vec{r}) \\ F_o(\vec{r}) \end{pmatrix}, \tag{A.1}$$

where $F_e(\vec{r})$ and $F_o(\vec{r})$ are even and odd functions of $\vec{r}$. Although $|\phi\rangle$ has even and odd spinor components it is not an eigenstate of the parity operator since the Hamiltonian is not invariant under two-dimensional inversion operation due to the Rashba term. (Note that any linear combination of the two states of equation (A.1) can also be chosen as a single-electron basis state in the degenerate Hilbert subspace.)

We define a single- or many-electron wavefunction to have a A-type property under parity operation if the spin-up part changes sign under parity operation:

$$\begin{pmatrix} F_o(\vec{r}) \\ F_e(\vec{r}) \end{pmatrix} \to \begin{pmatrix} -F^*_o(\vec{r}) \\ F^*_e(\vec{r}) \end{pmatrix} \Rightarrow \text{A-type}. \tag{A.2}$$

A wavefunction has a B-type property under parity operation if the spin-down part changes sign under parity operation:

$$\begin{pmatrix} F_e(\vec{r}) \\ F_o(\vec{r}) \end{pmatrix} \to \begin{pmatrix} F^*_e(\vec{r}) \\ -F^*_o(\vec{r}) \end{pmatrix} \Rightarrow \text{B-type}. \tag{A.3}$$

Each eigenstate $|\phi_p\rangle$ can be labeled by a subscript $p$. When $p$ is odd the spin-up and-down components of the wavefunction are, respectively, odd and even functions of $\vec{r}$. When $p$ is even the odd and even properties are reversed.

In order to include many-electron physics we need to fix single-electron eigenstates of not only the first shell, but also of the second, third, etc, energy shells. Here we choose them in the following specific order:

$$|\phi_1\rangle = \begin{pmatrix} F_{1,o}(\vec{r}) \\ F_{1,e}(\vec{r}) \end{pmatrix}, \qquad |\phi_2\rangle = \begin{pmatrix} -F^*_{1,e}(\vec{r}) \\ F^*_{1,o}(\vec{r}) \end{pmatrix}, \tag{A.4}$$

$$|\phi_3\rangle = \begin{pmatrix} F_{3,o}(\vec{r}) \\ F_{3,e}(\vec{r}) \end{pmatrix}, \qquad |\phi_4\rangle = \begin{pmatrix} -F^*_{3,e}(\vec{r}) \\ F^*_{3,o}(\vec{r}) \end{pmatrix}, \tag{A.5}$$

$$|\phi_5\rangle = \begin{pmatrix} F_{5,o}(\vec{r}) \\ F_{5,e}(\vec{r}) \end{pmatrix}, \qquad |\phi_6\rangle = \begin{pmatrix} -F^*_{5,e}(\vec{r}) \\ F^*_{5,o}(\vec{r}) \end{pmatrix}, \tag{A.6}$$

etc.

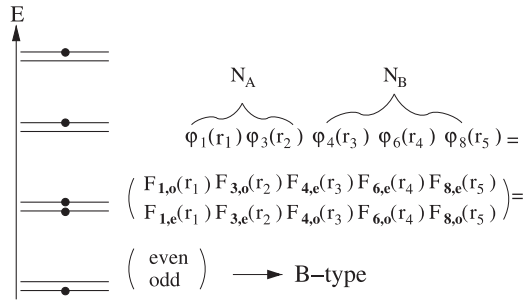


**Figure A.2.** A B-type Slater determinant is a sum of $N!$ terms. One of these terms is shown.

Note that the wavefunctions of a degenerate pair are chosen to be time-reversed states of each other. We have chosen the single-electron wavefunctions $\phi_1, \phi_3, \ldots$ to have A-type property, and $\phi_2, \phi_4, \ldots$ to have B-type property under parity operation, as shown in figure A.1. This particular choice simplifies the calculation of matrix Berry phases in the presence of many-body correlation effects. This corresponds to fixing a convenient 'gauge', i.e. a single-electron basis set.

The many-electron NAVPs contain single-electron NAVPs via equations (6) and (7). So we need to understand first the properties of single-electron NAVPs. We can choose the adiabatic parameters as $\lambda_1 = 2\hbar\omega_x$ and $\lambda_2 = \frac{c_R}{\sqrt{2}\ell_y}$, where the lengths are $\ell_{x,y} = \sqrt{\hbar/m^*\omega_{x,y}}$. (The single-electron Hamiltonian depends on them, see equation (10).) The adiabatic constant $\lambda_1$ may be varied using the gate potential of the dot and $\lambda_2$ may be varied by changing the electric field $E$ along the $z$ axis. The single-electron *intra-shell* NAVP elements [18] are $\mathrm{i}\langle\phi_p|\frac{\partial}{\partial\lambda_k}|\overline{\phi}_p\rangle$, where $\phi_p$ and $\overline{\phi}_p$ are degenerate single-electron eigenstates. The NAVP elements between A and B or B and A states can be shown to be zero [30]. Since $\phi_p$ and $\overline{\phi}_p$ are either of A and B or of B and A the *intra-shell* NAVP elements are zero. On the other hand, from the transformation properties of the eigenstates, given in equations (A.4)–(A.6), we can show that the single-electron *inter-shell* NAVP elements are

$$(a_k)_{p,q} \neq 0 \qquad \text{if } p+q \text{ even}, \tag{A.7}$$

and

$$(a_k)_{p,q} = 0 \qquad \text{if } p+q \text{ odd}, \tag{A.8}$$

where $\phi_p$ and $\phi_q$ belong to different energy shells. Note that different single-electron eigenstates can be coupled through $(a_k)_{p,q}$ if $p+q$ is even. Thus the off-diagonal many-electron NAVPs, equation (8), can be written in terms of *non-zero inter-shell* single-electron NAVPs. Nonetheless it is possible to show that the many-electron matrix Berry phase vanishes.

## Appendix B. Absence of matrix Berry phase and lateral inversion symmetry

Many-electron states can be written as a linear combination of Slater determinant states $|\Psi_i\rangle$. In the following we will choose $|\Psi_1\rangle, |\Psi_3\rangle, \ldots$ as A-type Slater determinant states and $|\Psi_2\rangle = \hat{T}|\Psi_1\rangle, |\Psi_4\rangle = \hat{T}|\Psi_3\rangle, \ldots$ as B-type Slater

determinant states. The time-reversed state of A-type single-electron wavefunctions are of B-type, and vice versa. The Slater determinant states $|\Psi_i\rangle$ are chosen in the order of increasing confinement energy $\langle\Psi_i|H_{\rm K}+V_{\rm C}|\Psi_i\rangle$. The total number of electrons $N = N_{\rm A}+N_{\rm B}$ is odd with the number of A-type single-electron wavefunctions $N_{\rm A}$ and of B-type $N_{\rm B}$. As explained in figure A.2, if $N_{\rm B}$ is odd the Slater determinant transforms like a B-type, i.e. the spin-down part of the wavefunction changes sign. On the other hand, if $N_{\rm A}$ is odd $|\Psi_i\rangle$ transforms like an A-type, i.e. the spin-up part of the wavefunction changes sign. It can be shown that the NAVP between A and B Slater determinant states is zero:

$$(B_k)_{i,j} = \mathrm{i}\langle\Psi_i(\mathrm{A})|\frac{\partial}{\partial\lambda_k}|\Psi_j(\mathrm{B})\rangle = 0. \tag{B.1}$$

This is because NAVPs between A and B single-electron states are zero.

We find that a correlated degenerate ground state, $|\Phi\rangle$ or $|\overline{\Phi}\rangle$, is either A or B type. This is because the many-body Hamiltonian matrix element between A-type and B-type Slater determinant wavefunctions is zero, $\langle\Psi_i(\mathrm{A})|H|\Psi_j(\mathrm{B})\rangle = 0$: if $|\Phi\rangle$ is A type and $|\overline{\Phi}\rangle$ is B type then

$$\begin{aligned}|\Phi\rangle &= c_1|\Psi_1(\mathrm{A})\rangle + c_3|\Psi_3(\mathrm{A})\rangle + \cdots\\ |\overline{\Phi}\rangle &= d_2|\Psi_2(\mathrm{B})\rangle + d_4|\Psi_4(\mathrm{B})\rangle + \cdots.\end{aligned} \tag{B.2}$$

We see from these results that, for a given index $i$, if an expansion coefficient $c_i$ of one degenerate ground state is zero then the expansion coefficient $d_i$ of the other time-reversed ground state is non-zero, and vice versa.

The off-diagonal elements of the many-body NAVPs, equation (8), are zero. This can be shown as follows: according to equation (B.2), for each $i$, we have $c_i = 0$ or $d_i = 0$, which implies that the first term of equation (8) is $\sum_i c_i^*\frac{\partial d_i}{\partial\lambda_k} = 0$. From equation (B.2) we see that, when $i \neq j$ and $c_i^* d_j$ is non-zero, then $\Psi_i$ and $\Psi_j$ are of A and B types, respectively. But this implies $(B_k)_{i,j} = 0$ and the product $c_i^* d_j (B_k)_{i,j} = 0$. The second term of equation (8) is thus $\sum_{i,j} c_i^* d_j (B_k)_{i,j} = 0$. An explicit example of this is given below equation (30). There is thus a delicate interplay between the many-body expansion coefficients $c_i^* d_j$ and the elements of the NAVPs between Slater determinant states $(B_k)_{i,j}$. Since $c_i^*\frac{\partial d_i}{\partial\lambda_k} = 0$ and $c_i^* d_j (B_k)_{i,j} = 0$ the off-diagonal elements of the many-body NAVPs are zero: $(A_k)_{1,2} = 0$. The matrix Berry phase is thus *absent* for doubly degenerate correlated states when inversion symmetry is present. This is true at any level of approximation represented by the number of Slater determinant states, $M$, included in equation (4). Therefore, this is an *exact* result valid for $M \to \infty$.

## Appendix C. Coulomb matrix elements

The diagonal and off-diagonal matrix elements of $H$, equation (21), depend on two-particle Coulomb matrix elements between single-electron eigenstates $p, q, r, s$ that are given in equations (17)–(19):

$$\begin{aligned}\langle pq|v|rs\rangle = &\sum_{\substack{m_p,m_q,m_r,m_s,\\ n_p,n_q,n_r,n_s,\\ \sigma_p,\sigma_q,\sigma_r,\sigma_s}} \delta_{\sigma_p\sigma_r}\delta_{\sigma_q\sigma_s}c^*_{m_pn_p}(p)\\ &\times c^*_{m_qn_q}(q)c_{m_rn_r}(r)c_{m_sn_s}(s)\langle m_pn_p, m_qn_q|v|m_rn_r, m_sn_s\rangle\end{aligned} \tag{C.1}$$

where the Coulomb matrix elements between eigenstates of two-dimensional harmonic oscillators are

$$\begin{aligned}&\langle m_pn_p, m_qn_q|v|m_rn_r, m_sn_s\rangle\\ &= e^2\int \mathrm{d}^2k\,\frac{1}{2\pi k}\,\langle m_p|\mathrm{e}^{\mathrm{i}k_xx_1}|m_r\rangle\langle n_p|\mathrm{e}^{\mathrm{i}k_yy_1}|n_r\rangle\\ &\quad\times\langle m_q|\mathrm{e}^{-\mathrm{i}k_xx_2}|m_s\rangle\langle n_q|\mathrm{e}^{-\mathrm{i}k_yy_2}|n_s\rangle\end{aligned} \tag{C.2}$$

with

$$\begin{aligned}&\langle m|\mathrm{e}^{\mathrm{i}k_xx}|m'\rangle\\ &= \begin{cases}(\frac{m'!}{m!})^{1/2}(\frac{\mathrm{i}k_xl_x}{\sqrt{2}})^{m-m'}\mathrm{e}^{-\frac{k_x^2l_x^2}{4}}L_{m'}^{m-m'}(\frac{k_x^2l_x^2}{2}) & (m' \leqslant m)\\ (\frac{m!}{m'!})^{1/2}(-\frac{\mathrm{i}k_xl_x}{\sqrt{2}})^{m'-m}\mathrm{e}^{-\frac{k_x^2l_x^2}{4}}L_{m}^{m'-m}(\frac{k_x^2l_x^2}{2}) & (m \leqslant m')\end{cases}\end{aligned} \tag{C.3}$$

and Laguerre polynomials $L_m^{m'}(x)$. A similar expression can be found for $\langle n|\mathrm{e}^{\mathrm{i}k_yy}|n'\rangle$ with $\ell_y$ replacing $\ell_x$.

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