Magnetoconfined levels in a parabolic quantum dot: An analytical solution of a three-dimensional Fock–Darwin problem in a tilted magnetic field

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The energy spectrum of an electron confined in a quantum dot (QD) with a three-dimensional anisotropic parabolic potential in a tilted magnetic field was found analytically. The theory describes exactly the mixing of in-plane and out-of-plane motions of an electron caused by a tilted magnetic field, which could be seen, for example, in the level anticrossing. For charged QDs in a tilted magnetic field we predict three strong resonant lines in the far-infrared-absorption spectra.

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The Fock–Darwin (FD) problem[1] is a famous example of an exactly solvable quantum-mechanical problem, which is broadly used in solid-state physics for modeling of many charge and spin properties of singly and multiply charged quantum dots (QD) in a magnetic field.[2–5] Fock and Darwin independently found the exact eigenfunctions and eigenstates of an electron confined in a two-dimensional parabolic potential and submitted to a magnetic field normal to the two-dimensional plane. Despite the fact that an electronic-confined potential in real self-organized QDs is obviously three-dimensional, it is found that the FD formula describes excellently the electron-energy levels, if a correction due to a small in-plane anisotropy is taken into account.[6] This model even more impressively allows us to describe the collective properties of multielectrons localized in a QD,[7,8] such as, for example, the collective oscillation of their center-of-mass motion.[4]

The high symmetry of the FD problem, which allows us to separate variables, is broken, however, if an external magnetic field is tilted away from the normal to the plane containing self-organized QDs, which makes the problem much more difficult to solve. To circumvent this difficulty, an approximate solution is commonly used,[9,10] whereby the normal component of the magnetic field gives rise to FD states, whereas the in-plane component adds a weak diamagnetic shift of the electron-energy levels $\sim(d/L)^2$, where d is the quantum-well thickness and L is the magnetic length. This approximation is only valid in weak tilted fields *and* when the out-of-plane confinement is much larger than the in-plane one. However, depending on the preparation method, the frequency of out-of-plane confinement in self-assembled InAs/GaAs QDs can be as small as 30 meV,[11] which is comparable to typical frequencies of in-plane confinement: 20 (Ref. 5) and 30 meV.[4] Moreover, the in-plane component of the magnetic field has an even more fundamental effect upon an electron confined in the QD because it mixes the electron in-plane and out-of-plane motions. Even in a weak magnetic field the level mixing leads to anticrossings between spatially confined level of the quantum well (QW) and of the two-dimensional magnetoconfined levels of the FD problem.

The level mixing underlies such phenomena as electric-dipole spin resonance (EDSR), which can be used for electron-spin manipulation by applying an electric field perpendicular to the QW plane.[12] In parabolic QW's the mixing of in-plane and out-of plane motions in a tilted magnetic field can be described exactly,[13] and the EDSR magnitude can be precisely calculated.[12] Even more important is the electric field manipulation of an electron spin confined in QDs, which is a promising candidate for solid-state-based qubit[14–19] due to its very long decoherence time, T_2, at cryogenic temperatures. In a single GaAs/AlGaAs gated QD (Ref. 20) and in InGaAs self-organized QDs (Ref. 21) T_2 reaches the microseconds range. An analytical description of the QD electronic structure in a tilted magnetic field would therefore be most advantageous for electron-spin manipulation modeling.

This Brief Report reports an analytical description of magnetoconfined levels in three-dimensional anisotropic parabolic QDs exposed to an arbitrarily oriented magnetic field. The exact solution of this problem was found using the general Bogoliubov approach[22] and Colpa's algorithm[23] for quadratic form Hamiltonians.

The Hamiltonian describing an electron confined in a three-dimensional parabolic potential well in an arbitrarily oriented external magnetic field can be written as

$$\mathcal{H}=\frac{[\hat{\boldsymbol{p}}+(e/c)\boldsymbol{A}]^2}{2m}+\frac{1}{2}m\omega_\perp^2(x^2+y^2)+\frac{1}{2}m\omega_z^2z^2, \quad (1)$$

where x and y are the coordinates in the plane of QD self-organization, and z is coordinate perpendicular to this plane; $\hat{\boldsymbol{p}}=-i\hbar\boldsymbol{\nabla}$ is the momentum operator; $\omega_\perp$ and ω_z are the characteristic frequencies for lateral and vertical parabolic confinement, respectively; m is the effective mass and e is the charge of the electron; c is the speed of light, and $\boldsymbol{A}$ is the vector potential. A magnetic field $\boldsymbol{B}$ is tilted at an angle θ from the vertical direction z: $\boldsymbol{B}=B(\hat{\boldsymbol{z}}\cos\theta+\hat{\boldsymbol{y}}\sin\theta)$ and the vector potential gauge can be written as $\boldsymbol{A}=B(-\frac{y\cos\theta}{2},\frac{x\cos\theta}{2},-x\sin\theta)$. To find the spectrum of Hamiltonian (1), we first express the Hamiltonian via six Bose operators, $\hat{a}_\xi,\hat{a}_\xi^\dagger$, connected with coordinates, $\xi=x,y,z$, and momentum operators by the standard relationships

$$\xi = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_\xi + \hat{a}_\xi^\dagger), \quad \hat{p}_\xi = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}_\xi^\dagger - \hat{a}_\xi), \tag{2}$$

where $\omega^2 = \omega_\perp^2 + (0.5\omega_c \cos\theta)^2$ and $\omega_c = (eB)/(mc)$ is the cyclotron frequency. The Hamiltonian takes the form

$$\hat{\mathcal{H}} = \frac{\hbar\omega}{4}(\hat{a}_x^\dagger \hat{a}_y^\dagger \hat{a}_z^\dagger \hat{a}_x \hat{a}_y \hat{a}_z)\boldsymbol{D}\begin{pmatrix}\hat{a}_x\\ \hat{a}_y\\ \hat{a}_z\\ \hat{a}_x^\dagger\\ \hat{a}_y^\dagger\\ \hat{a}_z^\dagger\end{pmatrix} \equiv \frac{\hbar\omega}{4}\hat{\boldsymbol{a}}^\dagger \boldsymbol{D}\hat{\boldsymbol{a}}, \tag{3}$$

where

$$\boldsymbol{D} = \begin{pmatrix}\boldsymbol{D}_1 & \boldsymbol{D}_2\\ \boldsymbol{D}_2^* & \boldsymbol{D}_1^*\end{pmatrix}, \tag{4}$$

$$\boldsymbol{D}_1 = \begin{pmatrix}2+\beta^2\sin^2\theta & -i\beta\cos\theta & i\beta\sin\theta\\ i\beta\cos\theta & 2 & 0\\ -i\beta\sin\theta & 0 & 1+\gamma\end{pmatrix}, \tag{5}$$

$$\boldsymbol{D}_2 = \begin{pmatrix}\beta^2\sin^2\theta & 0 & -i\beta\sin\theta\\ 0 & 0 & 0\\ -i\beta\sin\theta & 0 & \gamma-1\end{pmatrix}, \tag{6}$$

$\boldsymbol{D}_i^*$ is the complex-conjugated matrix $\boldsymbol{D}_i$, $\beta = \omega_c/\omega$ and $\gamma = \omega_z^2/\omega^2$. Next, we apply a linear Bogoliubov transformation of six Bose operators $\hat{a}_\xi$ and $\hat{a}_\xi^\dagger$ into another six Bose operators $\hat{b}_j$ and $\hat{b}_j^\dagger$ $(j=1,2,3)$ (Ref. 22)

$$\hat{\boldsymbol{b}} = \boldsymbol{T}\hat{\boldsymbol{a}} = \begin{pmatrix}\boldsymbol{T}_1 & \boldsymbol{T}_2\\ \boldsymbol{T}_2^* & \boldsymbol{T}_1^*\end{pmatrix}\hat{\boldsymbol{a}}, \tag{7}$$

where $\boldsymbol{T}_i (i=1,2)$ are 3×3 matrices and $\boldsymbol{T}_i^*$ are the complex-conjugated ones. Matrix $\boldsymbol{T}$ allows us to express the Hamiltonian via occupation number operators $\hat{N}_j = \hat{b}_j^\dagger \hat{b}_j$. Substituting Eq. (7) in Eq. (3) we get

$$\hat{\mathcal{H}} = \frac{\hbar\omega}{4}\hat{\boldsymbol{b}}^\dagger(\boldsymbol{T}^{-1})^\dagger \boldsymbol{D}\boldsymbol{T}^{-1}\hat{\boldsymbol{b}} = \frac{\hbar\omega}{4}\hat{\boldsymbol{b}}^\dagger \boldsymbol{\varepsilon}\hat{\boldsymbol{b}}, \tag{8}$$

where $\boldsymbol{\varepsilon} = (\boldsymbol{T}^{-1})^\dagger \boldsymbol{D}\boldsymbol{T}^{-1}$. For the $\boldsymbol{T}$ matrix of Eq. (7) that transforms $\boldsymbol{D}$ into a diagonal matrix, it can be demonstrated that $\boldsymbol{\varepsilon} = \mathbf{diag}(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_1, \varepsilon_2, \varepsilon_3)$, where all coefficients ε_j $(j=1,2,3)$ are real and positive. Substituting the diagonal form of $\boldsymbol{D}_\mathrm{d}$ into Eq. (8) one obtains the energy spectrum

$$E_{N_1N_2N_3} = \sum_{j=1}^{3}\left(N_j + \frac{1}{2}\right)\hbar\omega_j, \tag{9}$$

where $\hbar\omega_j = \varepsilon_j \hbar\omega/2$ and we set $\omega_1 \le \omega_2 \le \omega_3$ for an unambiguous definition of the energy quanta.

To obtain $\hbar\omega_j$ $(j=1,2,3)$ explicitly, we apply an algorithm suggested by Colpa.[23] First, we Cholesky decompose[24] matrix $\boldsymbol{D} = \boldsymbol{K}^\dagger \boldsymbol{K}$, where $\boldsymbol{K}$ is an upper triangular matrix, which can be done because $\boldsymbol{D}$ is a positive-definite matrix (all its eigenvalues are real and positive). Second, we construct a matrix $\boldsymbol{M} = \boldsymbol{K}\boldsymbol{I}_\mathrm{p}\boldsymbol{K}^\dagger$, where $\boldsymbol{I}_\mathrm{p} = \mathbf{diag}(1,1,1,-1,-1,-1)$ is the *para-unit* matrix. Finally, from the eigenvalues of $\boldsymbol{M}$, $\zeta_k (k=1,\ldots,6)$, we find all ε_j through $\boldsymbol{\varepsilon} = \boldsymbol{I}_\mathrm{p}\boldsymbol{\zeta}$,[23] where $\boldsymbol{\zeta} = \mathbf{diag}(\zeta_1, \zeta_2, \zeta_3, \zeta_4, \zeta_5, \zeta_6)$. The cumbersome but straightforward algebra leads to a cubic equation for the squared eigenvalues: $\sum_{k=0,1,2,3} C_k \varepsilon^{2k} = 0$, where $C_0 = -4\gamma[4-\beta^2(1-S)]^2$, $C_1 = 16+\beta^4(1-6S+5S^2) - 8\beta^2[1-\gamma+(\gamma-3)S] + 32\gamma$, $C_2 = -2[\beta^2(1+S)+2(2+\gamma)]$, $C_3 = 1$, and $S = \sin^2\theta$.[25] Its solution provides analytical eigenvalues, ε_j, whose magnitude increases with j

$$\varepsilon_{j=1,2} = \sqrt{\frac{2F}{3} - \frac{2}{3}\sqrt{G}\cos\frac{\pi+(-1)^j\phi}{3}},$$

$$\varepsilon_3 = \sqrt{\frac{2F}{3} + \frac{2}{3}\sqrt{G}\cos\frac{\phi}{3}}, \tag{10}$$

where

$$F = 2(2+\gamma) + \beta^2(1+S),$$

$$G = 16(\gamma-1)^2 + 8\beta^2[7-\gamma+5(\gamma-1)S] + \beta^4(1+26S-11S^2),$$

$$H = 64(\gamma-1)^3 + 48\beta^2(\gamma-1)[(13+5\gamma)S-\gamma-11)] + 12\beta^4[11+\gamma+(22+8\gamma)S+(7\gamma-25)S^2] - \beta^6(1-69S-33S^2+37S^3),$$

and ϕ is given by the four-quadrant arctan function: $\phi = \arg(H, \sqrt{G^3-H^2})$. When variable separation is possible, Eq. (10) provides well-known analytical results: (i) for $\theta=0$, the FD spectrum, $2\pm\beta$, plus the confinement energy of a parabolic QW $2\sqrt{\gamma}$ and (ii) for $\theta=90°$, the FD solutions in an anisotropic two-dimensional QD (Ref. 26): $\sqrt{2[\beta^2+\gamma+1\pm\sqrt{(\beta^2+\gamma+1)^2-4\gamma}]}$, plus the confinement energy for movement along the magnetic field, equal to 2 in dimensionless units.

Derivation of coordinate dependencies of the eigenfunctions corresponding to the energy spectrum of Eq. (9) requires matrix $\boldsymbol{T}$ defined by Eq. (7). To obtain $\boldsymbol{T}$ we construct an auxiliary matrix

$$\boldsymbol{U} = \boldsymbol{K}\boldsymbol{T}^{-1}\boldsymbol{\varepsilon}^{-1/2}, \tag{11}$$

where $\boldsymbol{\varepsilon}^r = \mathbf{diag}(\varepsilon_1^r, \varepsilon_2^r, \varepsilon_3^r, \varepsilon_1^r, \varepsilon_2^r, \varepsilon_3^r)$. It can be easily shown that $\boldsymbol{U}$ is right-eigenvector matrix of $\boldsymbol{M}$: $\boldsymbol{M}\boldsymbol{U} = \boldsymbol{\zeta}\boldsymbol{U} = \boldsymbol{I}_\mathrm{p}\boldsymbol{\varepsilon}\boldsymbol{U}$. By reversing Eq. (11) $\boldsymbol{T}$ is obtained

$$\boldsymbol{T} = \boldsymbol{\varepsilon}^{-1/2}\boldsymbol{U}^\dagger \boldsymbol{K}, \tag{12}$$

where the unitarity $\boldsymbol{U}^{-1} = \boldsymbol{U}^\dagger$ was used. Using $\boldsymbol{T}$ we can express $\hat{b}_j$ in coordinate representation. Substituting $\hat{a}_\xi$ and $\hat{a}_\xi^\dagger$ from Eq. (7) into Eq. (2) we get

$$\begin{pmatrix}\hat{b}_1\\ \hat{b}_2\\ \hat{b}_3\end{pmatrix} = \frac{1}{\sqrt{2}}(\boldsymbol{T}_1+\boldsymbol{T}_2)\cdot\boldsymbol{r}' + \frac{1}{\sqrt{2}}(\boldsymbol{T}_1-\boldsymbol{T}_2)\cdot\boldsymbol{\nabla}', \tag{13}$$

where $\boldsymbol{r}' = (x', y', z')$ and $\boldsymbol{\nabla}' = (\partial/\partial x', \partial/\partial y', \partial/\partial z')$ are three-dimensional vectors composed of the dimensionless coordinates, $x'_\xi = x_\xi / L_\omega$, and of the derivatives, $\partial/\partial x'_\xi = L_\omega \partial/\partial x_\xi$, respectively, with $L_\omega = \sqrt{\hbar/m\omega}$.

The ground-state wave function, $\Psi_{000}(x',y',z')$, is found from the condition: $\hat{b}_j \Psi_{000}(x',y',z') \equiv 0$ $(j=1,2,3)$, which after substitution of $\hat{b}_j$ from Eq. (13) leads to three simultaneous differential equations

$$\nabla \Psi_{000}(x',y',z') = \boldsymbol{P} \cdot \boldsymbol{r}' \Psi_{000}(x',y',z'), \tag{14}$$

where $\boldsymbol{P} = -(\boldsymbol{T}_1 - \boldsymbol{T}_2)^{-1}(\boldsymbol{T}_1 + \boldsymbol{T}_2)$ is a symmetric matrix. By resolving Eq. (14) we obtain the normalized wave function for the ground state

$$\Psi_{000}(x',y',z') = C(\boldsymbol{P}) \exp[(\boldsymbol{r}')^{\mathrm{T}} \cdot \boldsymbol{P} \cdot \boldsymbol{r}'], \tag{15}$$

with the normalization coefficient

$$C(\boldsymbol{P}) = \left(\frac{1}{\pi}\right)^{3/4} (\bar{p}_{11}\bar{p}_{23}^2 + \bar{p}_{22}\bar{p}_{13}^2 + \bar{p}_{33}\bar{p}_{12}^2 - \bar{p}_{11}\bar{p}_{22}\bar{p}_{33} - 2\bar{p}_{12}\bar{p}_{13}\bar{p}_{23}), \tag{16}$$

where $\bar{p}_{ij} = Re(p_{ij})$. The exponential factor in Eq. (15) has full quadratic form of variables x', y', and z'.

For any eigenstate $\Psi_{N_1N_2N_3}(x',y',z')$ can be obtained from ground-state wave function (15) using

$$\Psi_{N_1N_2N_3} = \frac{(b_1^\dagger)^{N_1}(b_2^\dagger)^{N_2}(b_3^\dagger)^{N_3}}{\sqrt{N_1!\,N_2!\,N_3!}} \Psi_{000}, \tag{17}$$

where the coordinate form of the operators $\hat{b}_j^\dagger$ are obtained by conjugating transposing of Eq. (13)

$$\hat{b}_j^\dagger = [\boldsymbol{Q} \cdot \boldsymbol{r}' + \boldsymbol{R} \cdot \nabla']_j, \tag{18}$$

where $\boldsymbol{Q} = \frac{1}{\sqrt{2}}(\boldsymbol{T}_1^* + \boldsymbol{T}_2^*)$ and $\boldsymbol{R} = \frac{1}{\sqrt{2}}(\boldsymbol{T}_1^* - \boldsymbol{T}_2^*)$. As an example, we show the explicit form of the wave functions for the first three excited states. They can be written in a compact vector form

$$\begin{pmatrix} \Psi_{100}(x',y',z') \\ \Psi_{010}(x',y',z') \\ \Psi_{001}(x',y',z') \end{pmatrix} = (\boldsymbol{Q} + \boldsymbol{R}\boldsymbol{P}) \cdot \boldsymbol{r}' \Psi_{000}(x',y',z'). \tag{19}$$

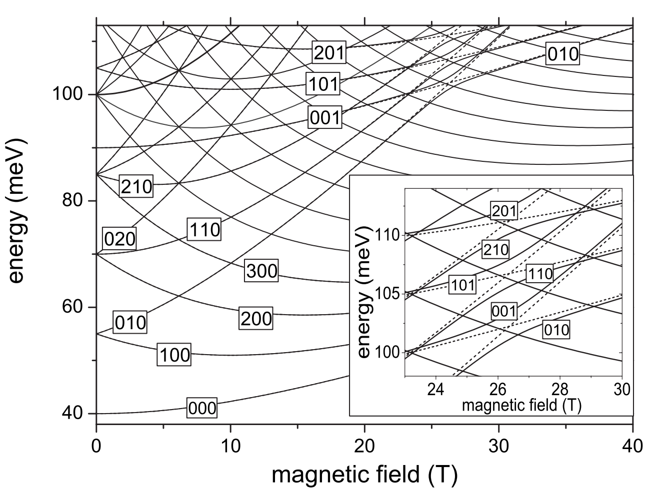

FIG. 1. Energy levels in the QD as a function of magnetic field strength, for a tilt angle of $\theta=3°$. The FD energy levels are shown by the dashed lines.

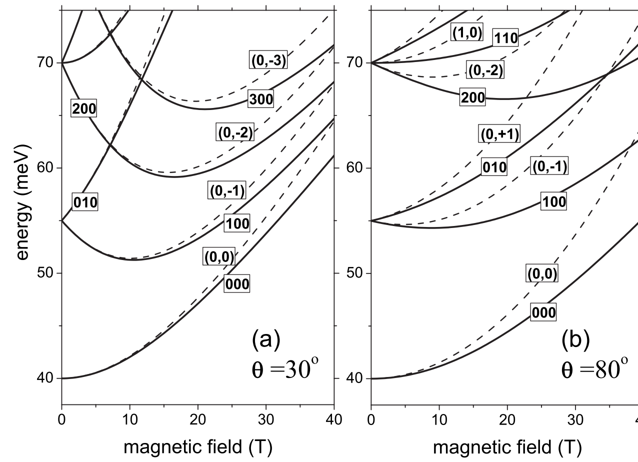

FIG. 2. Dependence of the QD energy levels on magnetic field tilted at (a) $\theta=30°$ and (b) $\theta=80°$. Dashed lines show the (n,ℓ) FD state energies with the diamagnetic shift added.

Figure 1 shows the energy spectrum of a QD, calculated using Eq. (10), as a function of applied magnetic field tilted by $\theta=3°$. All calculations in this Brief Report where conducted for $m=0.07m_0$ and frequencies of parabolic confinement: $\hbar\omega_z=50$ meV and $\hbar\omega_\perp=15$ meV, which are achievable, for example, in InAs QDs embedded in GaAs.[4,5,11] For comparison, the energy spectra calculated within FD model as a function of the normal component of magnetic field is shown by dashed lines. The FD states are described by the principle quantum number, n, and the azimuthal quantum

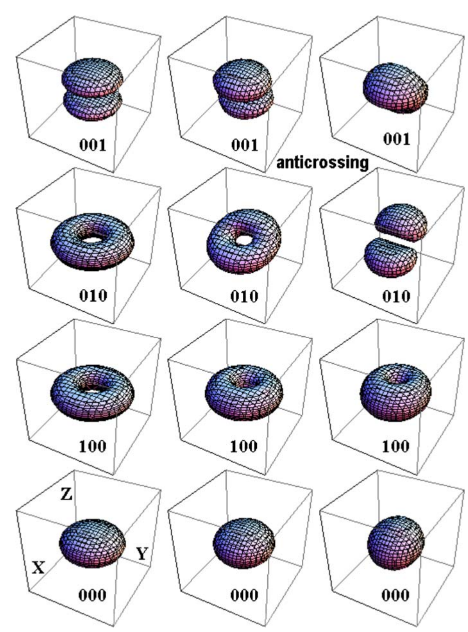

FIG. 3. (Color online) Wave functions as a function of magnetic field strength B, for a tilt angle $\theta=30°$. Left column: $B=0$; middle column: $B=20$ T; and right column: $B=40$ T.

number, ℓ, which are connected with N_1, N_2 through: $\ell = N_2 - N_1$, and n is the smallest element of $\{N_1, N_2\}$. One can see that the exact solution nearly coincides with the FD one for such a small angle, except at certain fields, for which some levels anticross as a result of the lifting of axial symmetry. Our calculations show, however that only levels with the same full occupation number $N_{TOT} = N_1 + N_2 + N_3$ are anticrossed at a tilted magnetic field. This is illustrated in Fig. 1, which depicts the anticrossing of levels 010 and 001, 110 and 101, 210 and 201 for $\theta = 3°$.

Solid lines in Fig. 2 show the energy levels for tilt angles (a) $\theta = 30°$ and (b) $\theta = 80°$, calculated using Eq. (10). Dashed lines show the approximate solutions, which as discussed above consist of a sum of two energy terms: the FD energy, determined by the magnetic field component normal to the interface containing QD's, and the diamagnetic energy $(\hbar\omega_c \sin\theta)^2/(4\hbar\omega_z)$,[27] determined by the in-plane component of the magnetic field. The approximate solution evidently provides a poor description of the levels for large tilted magnetic fields.

Figure 3 shows plots of the boundary surfaces within which the electron-probability densities $|\Psi_{N_1N_2N_3}(x', y', z')|^2 \geq 0.06 L_\omega^{-3}$, for $\theta = 30°$ for the ground and the first three excited states for $B = 0$, 20, and 40 T. One can see that the magnetic field tends to orient 000 and 100 states along it's direction, and compresses them into a smaller volume, as expected. The dramatic modification in the wave functions of the 010 and 001 states is connected with their anticrossing in a magnetic field around 26 T.

Direct confirmation of the developed theory could be obtained in the far-infrared-absorption spectra of charged QDs in tilted magnetic fields. Calculations using wave functions (15) and (17) envisage that these spectra will display three strong resonant lines at the photon energies $\hbar\omega_1$, $\hbar\omega_2$, and $\hbar\omega_3$, instead of only two lines seen in QD ensembles for a magnetic field normal to the QD layer.[28,29] This result is a direct consequence of a mixture of electron in-plane and out-of-plane motions.

In summary, we have found analytical formulas describing electrons in anisotropic parabolic QDs in tilted magnetic fields. Our exact description of the mixing of in-plane and out-of plane motions, induced by the tilted field, opens up the prospect for efficient modeling of electron-spin manipulation using an external electric field. The theory can be verified by studying infrared-absorption spectra of charged QDs in a tilted magnetic field.

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