

Cubic Dresselhaus Spin-Orbit Coupling in 2D Electron Quantum Dots

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We study effects of the oft-neglected cubic Dresselhaus spin-orbit coupling (i.e., $\propto p^3$) in GaAs/AlGaAs quantum dots. Using a semiclassical billiard model, we estimate the magnitude of the spin-orbit induced avoided crossings in a closed quantum dot in a Zeeman field. Using previous analyses based on random matrix theory, we calculate corresponding effects on the conductance through an open quantum dot. Combining our results with an experiment on an $8 \mu\text{m}^2$ quantum dot [D. M. Zumbühl *et al.*, Phys. Rev. B **72**, 081305 (2005)] suggests that (1) the GaAs Dresselhaus coupling constant γ is approximately 9 eV \AA^3 , significantly less than the commonly cited value of 27.5 eV \AA^3 , and (2) the majority of the spin-flip effects can come from the cubic Dresselhaus term.

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Control over electron spin in semiconductors has promise for quantum computing and spintronics. In such applications, it is essential to understand how the transport of an electron through a circuit affects its spin; i.e., we must understand spin-orbit (SO) coupling. In technologically important III-V semiconductor heterostructures, spin-orbit coupling originates in the asymmetry of the confining potential (called the Rashba term), which can be controlled by gates, and in bulk inversion asymmetry of the crystal lattice (called the Dresselhaus term). In quasi-2D systems, the Dresselhaus term has two components, one linear in the electron momentum and the other cubic. The cubic Dresselhaus (CD) term is usually neglected, as it is generally smaller than the linear contribution. Datta and Das proposed a spin-field-effect transistor (SFET) for quasi-1D ballistic wires with Rashba coupling [1]. Schliemann, Egues, and Loss proposed a SFET that can operate in diffusive quasi-2D systems based on tuning the Rashba and linear Dresselhaus (LD) terms to be equal in strength, which produces long spin lifetimes, neglecting CD [2]. The strengths of the SO terms are difficult to measure independently, but a full understanding of their strengths is crucial to making such devices. Additionally, in confined systems such as quantum dots, some effects of the linear SO terms are suppressed [3], and it is important to know the magnitude of the CD contribution, which could limit or even prevent the functioning of spintronic devices.

We characterize the strength of the CD in a confined system by its effect on avoided crossings in an in-plane magnetic field \mathbf{B}_{\parallel} that couples only to the electron spin. With no SO, each eigenstate can be written as a product of orbital state $|\alpha\rangle$ and spin quantized along \mathbf{B}_{\parallel} . Eigenstates $|\alpha \uparrow\rangle$ and $|\beta \downarrow\rangle$ become degenerate when $\epsilon_{\alpha} - \epsilon_{\beta} = E_Z$, where $\epsilon_{\alpha,\beta}$ are the orbital energies and E_Z is the Zeeman energy [4], but SO leads to avoided crossings.

In the first half of this Letter, we estimate the CD contribution to the avoided crossings, which can be larger than the linear terms' contribution since the latter are sup-

pressed for small \mathbf{B}_{\parallel} [3]. In the second half of this Letter, we relate these avoided crossings in closed quantum dots to the mean and variance of the conductance when the quantum dot is connected to ideal leads. We compare these predictions to the results of Zumbühl *et al.* [5,6] and find that agreement is possible only if the CD coupling constant in GaAs γ is considerably less than the frequently cited value of 27.5 eV \AA^3 [7,8] from $\mathbf{k} \cdot \mathbf{p}$ theory. A smaller value of γ has also been suggested by experiments [9,10] and band structure studies [11–13]. Even with this smaller value of γ , we find that CD is the dominant spin-flip mechanism in the sample considered.

We consider conduction electrons in a 2D electron system (2DES) grown on a (001) surface of a III-V semiconductor confined to a small area by a potential $V(\mathbf{r})$. We use an effective Hamiltonian

$$\mathcal{H} = \frac{(\mathbf{p} - \mathbf{A}_{\text{so}})^2}{2m} + \frac{\gamma}{2\hbar^3}(p_2^2 - p_1^2)(\mathbf{p} \times \boldsymbol{\sigma}) \cdot \hat{\mathbf{e}}_3 + V(\mathbf{r}) + \frac{1}{2}g\mu_B \mathbf{B} \cdot \boldsymbol{\sigma}, \quad (1)$$

where $\mathbf{p} = \mathbf{P} - e\mathbf{A}/c$, \mathbf{P} is the canonical momentum, \mathbf{A} is the vector potential from the perpendicular magnetic field, $\boldsymbol{\sigma}$ is the vector of Pauli matrices, m is the effective mass, $\mathbf{A}_{\text{so}} = \hat{\mathbf{e}}_1 \hbar \sigma_2 / 2\lambda_1 - \hat{\mathbf{e}}_2 \hbar \sigma_1 / 2\lambda_2$ is the effective SO vector potential, which contains both the LD and Rashba SO terms, and $\lambda_{1,2}$ are the (linear) SO lengths [14,15]. We choose a coordinate system with axes $\hat{\mathbf{e}}_1 = [110]$, $\hat{\mathbf{e}}_2 = [1\bar{1}0]$, and $\hat{\mathbf{e}}_3 = [00\bar{1}]$. The second term is the CD [16].

In a system of linear size L , the linear SO terms can be gauged away to first order in L/λ by the unitary transformation $\mathcal{H} \rightarrow U\mathcal{H}U^\dagger \equiv \mathcal{H}'$ where $U = \exp(i\mathbf{r} \cdot \mathbf{A}_{\text{so}})$ [14]. Expanding to leading order in L/λ ,

$$\mathcal{H}' = \frac{1}{2m}(\mathbf{p} - \mathbf{a}_{\perp} - \mathbf{a}_{\parallel})^2 + b^Z + b_{\perp}^Z + \frac{\gamma}{2\hbar^3}(p_2^2 - p_1^2)(\mathbf{p} \times \boldsymbol{\sigma}) \cdot \hat{\mathbf{e}}_3 + V(\mathbf{r}), \quad (2)$$

where $\mathbf{a}_\perp = (\hbar\sigma_3/4\lambda_1\lambda_2)[\hat{\mathbf{e}}_3 \times \mathbf{r}]$, $\mathbf{a}_\parallel = (\hbar/6\lambda_1\lambda_2) \times (x_1\sigma_1/\lambda_1 + x_2\sigma_2/\lambda_2)[\hat{\mathbf{e}}_3 \times \mathbf{r}]$, $b^Z = g\mu_B \mathbf{B} \cdot \boldsymbol{\sigma}/2$, and $b_\perp^Z = -g\mu_B(B_1x_1/\lambda_1 + B_2x_2/\lambda_2)\sigma_3/4$.

When we apply a Zeeman field, we can treat each induced degeneracy as a two-level system, assuming the SO matrix elements ϵ_{so} are much less than the single spin mean level spacing, $\Delta = 2\pi\hbar^2/mA$, with m the conduction band effective mass and A the dot area. The magnitude of the avoided crossings at the Fermi energy is given by $\epsilon_{\text{so}} = |\langle \alpha \uparrow | \mathcal{H}^{\text{so}} | \beta \downarrow \rangle|$, where $\epsilon_\alpha - \epsilon_\beta = E_Z$ and $\epsilon_\alpha = E_F$. We want to find the rms value of ϵ_{so} . Following Ref. [3], for a closed chaotic dot we may write $\Lambda^2 \equiv \overline{(\epsilon_{\text{so}}/\Delta)^2}$ as

$$\Lambda^2 = \overline{\sum_{\alpha\beta} |(\mathcal{H}^{\text{so}})_{\alpha\uparrow, \beta\downarrow}|^2 \delta(\epsilon_\alpha - \epsilon_\beta - E_Z) \delta(\epsilon_\alpha - E_F)}, \quad (3)$$

where the overbar indicates ensemble averaging and $O_{a,b} \equiv \langle a|O|b \rangle$.

We rewrite Eq. (3) as in Ref. [3] using the t -dependent representation of the delta function and interaction picture operators, and, after summing over β , find

$$\Lambda^2 = \int_{-\infty}^{\infty} \frac{dt}{\Delta 2\pi\hbar} e^{-i\omega_Z t} \overline{\langle \alpha | \mathcal{H}_{\text{SF}}^{\text{so}}(t) \mathcal{H}_{\text{SF}}^{\text{so}\dagger}(0) | \alpha \rangle}, \quad (4)$$

where $\omega_Z = E_Z/\hbar$ is the Zeeman frequency, $|\alpha\rangle$ is a typical orbital eigenstate with $\epsilon_\alpha \approx E_F$, and $\mathcal{H}_{\text{SF}}^{\text{so}} \equiv \langle \uparrow | \mathcal{H}^{\text{so}} | \downarrow \rangle$ is the spin-flip part of \mathcal{H}^{so} . We consider the CD alone, $\mathcal{H}^c = (\gamma/2\hbar^3)(p_2^2 - p_1^2)(p_1\sigma_2 - p_2\sigma_1)$, and estimate its contribution to Λ , which we call Λ_c .

We estimate Λ_c semiclassically using a billiard model for the quantum dot, where the matrix element in Eq. (5) is replaced by the corresponding expectation value for a classical particle moving at the Fermi velocity v_F starting at a random point in phase space. Semiclassical methods using SO have been rigorously justified [18] and used for studying 2D electron SO effects [19]. We consider $B_\perp = 0$ for these simulations. Each of $(2-3) \times 10^5$ such trajectories is followed for an equal amount of time, which is generally about 300 bounces total in the forward and backward directions. Increasing the number of trajectories or bounces does not change the results. We calculate $\int dt e^{-i\omega_Z(t-t')} \mathcal{H}_{\text{SF}}^c(t) \mathcal{H}_{\text{SF}}^{c\dagger}(t')$ for 100 random initial times t' on each trajectory as a function of ω_Z , and their average gives Λ_c^2 when multiplied by the appropriate prefactors. We add a damping function to the integrand that sends it smoothly to zero as t approaches the simulation cutoff.

We consider four billiard shapes and, for specificity, choose parameters corresponding to the largest, highest density dot in Ref. [5], with $A = 8 \mu\text{m}^2$ and $n = 5.8 \times 10^{15} \text{m}^{-2}$. We use $g = 0.44$ and $m = 0.067m_e$, where m_e is the electron mass. Figure 1 shows the resulting $\Lambda_c(E_Z)$ for three orientations of \mathbf{B}_\parallel , with $\gamma = 8.5 \text{eV}\text{\AA}^3$. For other choices, Λ_c scales linearly with γ . For our method to be valid, we must have $\Delta \ll E_Z \ll E_T$, where $E_T = \hbar v_F/\sqrt{A}$

is the Thouless energy. For the case discussed here, $\Delta = 0.9 \mu\text{eV}$ and $E_T \approx 80 \mu\text{eV}$.

We can understand the approximate scale of Λ_c by using a simpler, unphysical billiard. Consider an $L_x \times L_y$ rectangle with specular reflections from the sides and diffuse scattering from the top and bottom. At each collision with a diffuse wall, we choose the tangential momentum from a uniform distribution on $[-p_F, p_F]$ [20]. This choice gives a correct weighting for diffuse scattering and maintains detailed balance. In such a billiard, for $\mathbf{B}_\parallel \parallel \hat{\mathbf{x}}$, in the limit $E_Z \rightarrow 0$,

$$\Lambda_c^2|_{E_Z \rightarrow 0} = \frac{\gamma^2}{\Delta 2\pi\hbar^7} \left\langle \int_{-\infty}^{\infty} dt p_y p_x^2(t) p_y p_x^2(0) \right\rangle, \quad (5)$$

and we can break each trajectory into segments between collisions with the top or bottom walls. Along each segment, p_x^2 and p_y are constant, and the particle takes time $t = mL_y/|p_y|$ to move from one end of the segment to the other, so we can rewrite Eq. (6) as

$$\Lambda_c^2|_{E_Z \rightarrow 0} = \frac{\gamma^2 mL_y}{\Delta 2\pi\hbar^7} \left\langle |p_y(0)| p_x^2(0) \sum_{n=-\infty}^{\infty} (-1)^n p_{x,n}^2 \right\rangle, \quad (6)$$

which we can evaluate explicitly, since the $p_{x,i}^2$ are uncorrelated between segments. The particle begins moving in a random direction with $\mathcal{P}(p_{x,0}) = \pi^{-1}(p_F^2 - p_{x,0}^2)^{-1/2}$, where \mathcal{P} is the probability density on $[-p_F, p_F]$. Since

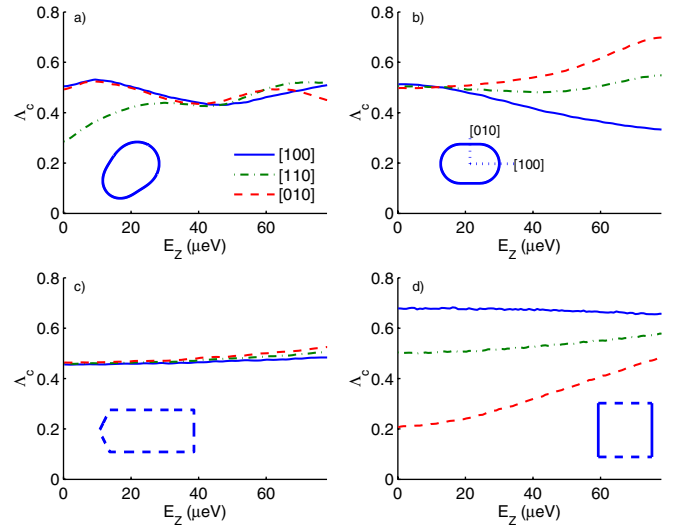


FIG. 1 (color online). Normalized rms avoided crossing Λ_c due to cubic Dresselhaus spin-orbit coupling as a function of Zeeman energy E_Z for four billiards with in-plane magnetic field along the indicated directions, with $\gamma = 8.5 \text{eV}\text{\AA}^3$ [13]. Insets show the billiard shapes with crystal axes. Solid (dashed) lines indicate specular (diffuse) boundary conditions. (a) Has a mixed phase space with small regions of regular trajectories, (b) is a stadium billiard, (c) is similar to the dot in Ref. [5], with diffuse boundaries to ensure chaos, and (d) is a square with diffuse scattering from the top and bottom and specular scattering from the sides (see text).

the diffuse boundaries in this billiard are the top and bottom, $\mathcal{P}(p_{x,i \neq 0}) = 1/2p_F$. We regularize the infinite sum by $\sum_{n=-\infty}^{\infty} (-1)^n = 0$, and, noting that $E_T = \hbar p_F / mL_y$, we find $\Lambda_c^2 = 4\gamma^2 p_F^6 / (45\pi^2 \Delta E_T \hbar^6)$. For the parameters in Fig. 1, this gives $\Lambda_c(E_Z \rightarrow 0) = 0.678$. Finite values of E_Z are not amenable to such simple treatment, but simulations of this billiard appear in Fig. 1(d), where the results for $\mathbf{B}_{\parallel} \parallel \hat{\mathbf{x}}$, shown by the solid trace, approach the analytic prediction for $E_Z \rightarrow 0$.

Avoided crossings have not yet been directly measured in chaotic dots, but our calculations can be related to experiments measuring the conductance g through a quantum dot by Zumbühl *et al.* [5,6]. To make this comparison, we need a connection between avoided crossings in a closed dot and properties of the dot with leads attached. Cremers *et al.*, using random matrix theory (RMT), worked out a similar connection for dots with only LD and Rashba SO [15]. We point out that CD can be added easily into the predictions of Cremers *et al.* without changing their expressions for $\langle g \rangle$ and $\text{var } g$ by reinterpreting one of their RMT energy scales to include both linear and cubic SO terms. We now elaborate.

In Ref. [15], the chaotic quantum dot is connected to two ideal leads with $N \gg 1$ open channels, giving a scattering matrix from the circular orthogonal ensemble. They treat the magnetic field and SO with a stub model [21] in which the stub has the $M \times M$ perturbation Hamiltonian, $\mathcal{H}'_{\text{RMT}}$, given by association to \mathcal{H}' in Eq. (2) (without CD), as

$$\mathcal{H}'_{\text{RMT}} = \frac{\Delta}{2\pi} [i\mathcal{A}_0(x\mathbb{1} + a_{\perp}\sigma_3) + ia_{\parallel}(\mathcal{A}_1\sigma_1 + \mathcal{A}_2\sigma_2) - \mathbf{b} \cdot \boldsymbol{\sigma} + b_{\perp}\mathcal{B}_h\sigma_3], \quad (7)$$

where \mathcal{A}_i , $i = 0, 1, 2$, are real antisymmetric matrices with $\langle \text{tr} \mathcal{A}_i \mathcal{A}_j^T \rangle = \delta_{ij} M^2$, \mathcal{B}_h is a real symmetric matrix with $\langle \text{tr} \mathcal{B}_h^2 \rangle = M^2$, $M \gg 1$ is the number of channels in the stub, and x , a_{\perp} , a_{\parallel} , \mathbf{b} , and b_{\perp} are dimensionless parameters, with x corresponding to B_{\perp} , \mathbf{b} to the Zeeman field, and a_{\perp} , a_{\parallel} , and b_{\perp} to the similarly named terms in Eq. (2) (without CD). Dephasing is included by setting $N_{\text{eff}} = N + 2\pi\hbar/\tau_{\phi}\Delta$, where τ_{ϕ} is the dephasing time. Expressions are then obtained for $\langle g \rangle$ and $\text{var } g$ as functions of x , a_{\perp} , a_{\parallel} , \mathbf{b} , b_{\perp} , and N_{eff} to leading order in $1/N_{\text{eff}}$ [15]. Zumbühl *et al.* use these results to fit their data.

Without CD, the correspondence between Eqs. (7) and (2) gives the following mapping from physical parameters to RMT parameters:

$$\begin{aligned} x^2 &= \pi\kappa E_T / \Delta (4\pi\Phi / \Phi_0)^2, \\ b &= \pi E_Z / \Delta, \\ a_{\perp}^2 &= \pi\kappa E_T / \Delta (A / \lambda_{\text{SO}}^2)^2, \\ a_{\parallel}^2 &= a_{\perp}^2 \kappa' [(L_1 / \lambda_1)^2 + (L_2 / \lambda_2)^2], \\ b_{\perp}^2 &= \pi\kappa'' (E_Z)^2 / E_T \Delta (A / \lambda_{\text{SO}}^2), \end{aligned} \quad (8)$$

where Φ is the magnetic flux through the quantum dot, $\Phi_0 = h/e$ is the flux quantum, $\lambda_{\text{SO}} = \sqrt{\lambda_1 \lambda_2}$, $L_{1,2}$ are the linear dimensions of the roughly rectangular dot, oriented along $\hat{\mathbf{e}}_{1,2}$, and κ , κ' , and κ'' are geometric factors of order unity [14,15]. We add CD to this theory by noting that, as a random matrix, the CD in Eq. (2) has the same symmetry as the a_{\parallel} term in Eq. (7); i.e., it contains only σ_1 and σ_2 Pauli matrices. By making the simplest assumption of no correlation between the cubic and linear terms, we include CD in $\mathcal{H}'_{\text{RMT}}$ by setting $a_{\parallel}^2 = a_{\parallel,l}^2 + a_{\parallel,c}^2$, where $a_{\parallel,l}$ is the Rashba and LD contribution, given by Eq. (8), and $a_{\parallel,c}$ is the CD contribution. Since $\mathcal{H}'_{\text{RMT}}$ contains the SO part of the Hamiltonian of the closed quantum dot, we relate $a_{\parallel,c}$ to Λ_c by finding the rms spin-flip matrix element (with spins quantized along \mathbf{B}_{\parallel}) due to $a_{\parallel,c}$, giving $a_{\parallel,c} = 2\pi\Lambda_c$. Including the CD term in $\mathcal{H}'_{\text{RMT}}$ in this way lifts the constraint that $a_{\parallel} \ll a_{\perp}$ [14], similar to spatially varying SO strengths [22].

Zumbühl *et al.* observe weak antilocalization (WAL) in only one of the GaAs/AlGaAs heterostructure quantum dots they study [5,6], and that dot gives the best defined values of the RMT parameters; we use it for the discussion of our results. The other dots do not contradict this discussion. The dot that displays WAL has area $A = 8 \mu\text{m}^2$ and electron density $n = 5.8 \times 10^{15} \text{ m}^{-2}$. The dot has $N = 2$ and $N_{\text{eff}} = 13.9$ [5].

Zumbühl *et al.* measure $\text{var } g$ as a function of \mathbf{B}_{\parallel} with time reversal symmetry broken by a small B_{\perp} . They fit to the expression of Cremers *et al.* [15], with a_{\parallel} (and all parameters except κ'') fixed to the value determined from the $\langle g \rangle$ data. We redo the fits to the $\text{var } g$ data, constraining only $a_{\parallel} \geq a_{\parallel,c}$, with $a_{\parallel,c}$ from our simulations, and τ_{ϕ} fixed to the value determined from $\langle g \rangle$. From Fig. 1, a typical value of Λ_c in all our billiard shapes is 0.4, giving $a_{\parallel,c} = 2.5(8.1)$ for $\gamma = 8.5(27.5) \text{ eV \AA}^3$ (recalling that $\Lambda_c \propto \gamma$). We find that a value of $a_{\parallel,c} \approx 2.5$ is compatible with the experimental data. However, if we require that $a_{\parallel} \geq 8.1$, the fits to the data become markedly worse [17].

Zumbühl *et al.* also measure $\langle g \rangle$ as a function of B_{\perp} , which they use to determine a_{\parallel} , finding $a_{\parallel} = 3.1$ [5,6,23]. Since $a_{\parallel}^2 = a_{\parallel,l}^2 + a_{\parallel,c}^2$, we must have $a_{\parallel} \geq a_{\parallel,c}$, so we conclude that $\gamma = 27.5 \text{ eV \AA}^3$ is inconsistent with these results, while $\gamma = 8.5 \text{ eV \AA}^3$ is consistent with the data. So both $\langle g \rangle$ and $\text{var } g$ data indicate that γ should be closer to 9 eV \AA^3 than 28 eV \AA^3 [24]. Moreover, even with the smaller value of γ , the CD term gives the dominant contribution to a_{\parallel} .

There are only a few other experiments pertaining to the value of γ in GaAs. The best, most direct study is the Raman scattering in a GaAs/AlGaAs quantum well by Richards *et al.* in which they found $\gamma = 11.0 \text{ eV \AA}^3$ [9]; the same group also found $\gamma = 16.5 \text{ eV \AA}^3$ in a different sample [10]. A recent experimental value of $\gamma = 28 \text{ eV \AA}^3$ from transport measurements [25] is less direct, includes

CD only as a density-dependent renormalization of the LD, and assumes the Rashba coupling is independent of gate voltage. Theoretical work has indicated that γ is smaller in AlGaAs/GaAs heterostructures and superlattices than it is in bulk GaAs [11,12,26], so it is possible that experiments are not probing the bulk Dresselhaus coupling, though Ref. [13] predicts $\gamma = 8.5 \text{ eV \AA}^3$ in bulk GaAs. We include as supplementary information a table with experimental and theoretical values of γ in GaAs [17].

Strictly speaking, our calculations are not directly applicable to the $\langle g \rangle$ data of Zumbühl *et al.*, as our calculations assume $E_Z \gg \Delta$, and $\langle g \rangle$ is measured with $\mathbf{B}_{\parallel} = 0$. We do not believe, however, that $a_{\parallel,c}$ changes significantly as $\mathbf{B}_{\parallel} \rightarrow 0$; similarly, Cremers *et al.* consider a_{\parallel} to be constant for all \mathbf{B}_{\parallel} [15]. We believe that $a_{\parallel,c}(\mathbf{B}_{\parallel} = 0)$ can be estimated by simply averaging our results from the different field directions in the limit $\mathbf{B}_{\parallel} \rightarrow 0$.

Our reinterpretation that $a_{\parallel}^2 = a_{\parallel,l}^2 + a_{\parallel,c}^2$ requires, of course, that $a_{\parallel,l}$ be less than 3.1 in the experiment of Zumbühl *et al.* This reduction of $a_{\parallel,l}$ can be absorbed into the geometric parameter κ' (which was set to 1 without fitting in Zumbühl *et al.*) without affecting any of the physical parameters, τ_{ϕ} , λ_{SO} , found by Zumbühl *et al.* Reducing κ' is reasonable, as Ref. [15] predicts $\kappa' = 1/3$ for a circular diffusive system.

Since $\Delta \propto A^{-1}$ and $E_T \propto A^{-1/2}n^{1/2}$, we can see that if the thickness of the 2DES does not change with density, $a_{\parallel,l} \propto A^{7/4}n^{1/4}$, while $a_{\parallel,c} \propto \Lambda_c \propto A^{3/4}n^{5/4}$. We therefore expect that the CD should be relatively more important in small, high density dots, precisely the ones likely to be useful for producing a SFET.

In summary, we have used billiard simulations to estimate the effect of the cubic Dresselhaus term on avoided crossings in a closed chaotic quantum dot. These results are related to the conductance through a dot with ideal leads attached. The CD plays a strong and previously ignored role in observed transport properties. Our calculations suggest that (1) the Dresselhaus SO coupling constant γ in GaAs/AlGaAs heterostructures has a value near 9 eV \AA^3 and not the frequently cited value of 27.5 eV \AA^3 , and (2) even with this smaller value of γ , in the experiments considered the cubic Dresselhaus term provided the bulk of the spin-flip portion of the SO Hamiltonian, which had previously been assigned to the effects of linear SO terms. The value of γ in this technologically important system deserves further study.

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