Stabilization of ground-state minimal spin in disordered quantum dots

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Abstract

We investigate the ground-state spin and energy of disordered quantum dots using spin-density-functional theory. With increasing interaction strength, the probability of non-minimal spin increases, but never exceeds 50%. Within a two-orbital model, we show that the off-diagonal Coulomb matrix elements help stabilize a ground state of minimal spin by creating a low-energy hybridization of the various minimal-spin basis states.

Key words: quantum dot; ground-state spin; spin-density-functional theory

1. Introduction

Recently spin in semiconductor nanostructures has attracted much attention. The control of spin is essential for a number of applications such as nanoscale spintronics[1] and quantum bits using electron spin in solid-state devices[2]. In disordered or chaotic quantum dots[3], high-spin states are suppressed by the rarity of degenerate or nearly degenerate levels. This is in contrast to clean quantum dots for which high-spin states appear for partly filled shells of degenerate single-particle levels. We find that in disordered quantum dots ground states of minimal spin are further stabilized by off-diagonal Coulomb matrix elements.

2. Calculation Method

The ground-state energy and spin of disordered two-dimensional quantum dots are obtained within spin-density-functional theory(SDFT)[4]. We solve the Kohn-Sham equations self-consistently[5];

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2+\frac{e^2}{\kappa}\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'+\frac{\delta E_{\rm xc}[\rho,\zeta]}{\delta\rho^\sigma(\mathbf{r})}+\frac{1}{2}m^*\omega_0^2r^2+\sum_i\frac{\gamma_i}{2\pi\lambda^2}\mathrm{e}^{-\frac{|\mathbf{r}-\mathbf{r}_i|^2}{2\lambda^2}}\right]\Psi_i^\sigma(\mathbf{r})=\epsilon_i^\sigma\Psi_i^\sigma(\mathbf{r}), \tag{1}$$

where the density is $\rho(\mathbf{r})=\sum_{i,\sigma}|\Psi_i^\sigma(\mathbf{r})|^2$, σ is the spin index, $\zeta(\mathbf{r})$ is the local spin polarization, and $E_{\rm xc}[\rho,\zeta]$ is the exchange-correlation energy functional[6]. The ground-state energy $E(N)$ is obtained from

$$E(N)=\sum_{i,\sigma}\epsilon_i^\sigma-\frac{e^2}{2\kappa}\int\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}'-\sum_\sigma\int\rho^\sigma(\mathbf{r})\frac{\delta E_{\rm xc}[\rho,\zeta]}{\delta\rho^\sigma(\mathbf{r})}d\mathbf{r}\;+\;E_{\rm xc}. \tag{2}$$

Each impurity potential has a Gaussian profile, with strength γ_i distributed on $[-W/2,W/2]$ with $W=10\hbar^2/m^*$, and width $\lambda=\ell_0/(2\sqrt{2})$ where $\ell_0=\sqrt{\hbar/m^*\omega_0}\simeq 19.5$nm. The density is $n_{\rm imp}=1.03\times10^{-3}\,\mathrm{nm}^{-2}$. The resulting mean free path, $l\simeq 120$nm, is comparable to the dot diameter $L=120-160$nm and thus the dots are marginally in the ballistic regime and have a dimensionless conductance $g\sim 2$[7]. We use $m^*=0.067m$ and $\hbar\omega_0=3.0$meV.

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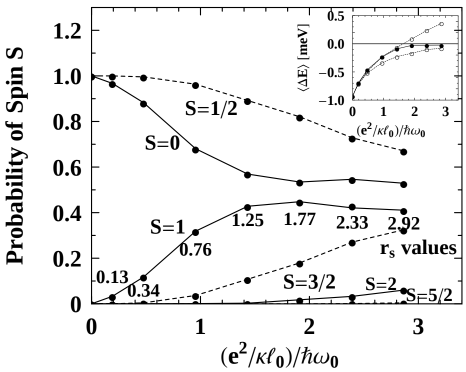

Fig. 1. Probability of a spin S ground state as a function of interaction strength $(e^2/\kappa\ell_0)/\hbar\omega_0$. Solid curves are for $N = 10$ (integer spin) and dashed curves are for $N = 11$ (half-integer spin). (inset) Average total energy difference ΔE between states with $S = 0$ and $S = 1$ as a function of $(e^2/\kappa\ell_0)/\hbar\omega_0$. The solid curve show the SDFT results. Also shown are results of the two-orbital model: exact (low dashed curve) and doubly-occupied lowest orbital (high dashed curve), with parameters evaluated for the $5th$ and $6th$ non-interacting orbitals.

The dimensionless interaction strength is measured by $(e^2/\kappa\ell_0)/\hbar\omega_0$ or $r_s(= 1/\sqrt{\pi\rho_0}a_B^*)$ and is controlled by changing the dielectric κ, where $\kappa = 12.9$ for GaAs[8].

3. Results

Fig.1 shows the probabilities of the different ground-state spins S versus electron-electron interaction strength. We see that the probability of $S = 1$ is always higher than that of $S = 3/2$, which shows that it is much more likely to find two orbitals close in energy, producing an $S = 1$ ground state than to find three orbitals close in energy, as required for an $S = 3/2$ ground state. We also see that the probability of an $S = 1$ ground state never exceeds 50%. High-spin ground states are favored by the exchange energy and the enhanced Coulomb repulsion between two electrons in the same spatial orbital and are disfavored by the single-particle energy cost of promoting an electron to a new orbital. This argument[9] is consistent with the present SDFT results up to $r_s \simeq 1$, but does not account for the observed saturation at larger r_s.

To understand this saturation, we consider a two-orbital model where two electrons occupy two non-degenerate orbitals near the Fermi energy. There are three degenerate $S = 1$ states consisting of one electron in each of the two orbitals with the energy $\tilde{E}(S = 1) = \epsilon_n + \epsilon_{n+1} + \tilde{U}^n_{n+1} - \tilde{X}^n_{n+1}$, where $\tilde{U}^n_{n+1}$ is the screened Coulomb interaction and $\tilde{X}^n_{n+1}$ is the screened exchange interaction between two electrons in orbitals n and $n+1$. There are also three, non-degenerate $S = 0$ states. The energy $\tilde{E}(S = 0)$ of the lowest $S = 0$ state is obtained by diagonalizing the following 3×3 matrix;

$$\tilde{H}(S = 0) =$$

$$\begin{bmatrix} 2\epsilon_n + \tilde{U}^n_n & \sqrt{2}\tilde{U}^{n,n}_{n,n+1} & \tilde{X}^n_{n+1} \\ \sqrt{2}\tilde{U}^{n,n}_{n,n+1} & \epsilon_n + \epsilon_{n+1} + \tilde{U}^n_{n+1} + \tilde{X}^n_{n+1} & \sqrt{2}\tilde{U}^{n+1,n+1}_{n+1,n} \\ \tilde{X}^n_{n+1} & \sqrt{2}\tilde{U}^{n+1,n+1}_{n+1,n} & 2\epsilon_{n+1} + \tilde{U}^{n+1}_{n+1} \end{bmatrix}$$

where the off-diagonal Coulomb matrix elements are $\tilde{U}^{n,n}_{n,n'} = e\int \tilde{\varphi}_{n,n}(\mathbf{r})\phi^0_n(\mathbf{r})\phi^0_{n'}(\mathbf{r})d\mathbf{r}$. Here $\tilde{\varphi}_{n,n}(\mathbf{r})$ is the screened potential evaluated by RPA approximation and $\phi^0_n(\mathbf{r})$ is the single-particle eigenstates with ϵ_n. We find that the magnitudes of $\tilde{U}^{n,n}_{n,n'}$ are comparable to the screened exchange energy $\tilde{X}^n_{n+1}$[10]. It is seen in the inset of Fig.1 that the average of $\Delta\tilde{E} = \tilde{E}(S = 0) - \tilde{E}(S = 1)$ for the two-orbital model agrees reasonably well with our SDFT results for all strengths of interaction. In contrast, placing the two electrons in the lowest single-particle orbital $\phi^0_n(\mathbf{r})$ is significantly larger than $\tilde{E}(S = 0)$ at larger r_s. It is evident that for the two-orbital model the off-diagonal Coulomb matrix elements help stabilize the $S = 0$ ground state.

In summary, we have studied ground-state energies and spins in disordered quantum dots. Comparison to a two-orbital model suggests that a ground-state of minimal spin is stabilized by a low-energy hybridization of three low-lying $S = 0$ basis states.

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References

[1] G.A.Prinz, Science **282** (1998) 1660.

[2] D.Loss, D.P.Divincenzo, Phys. Rev. A**57** (1998) 120.

[3] Y.Alhassid, Rev. Mod. Phys. **72** (2000) 895.

[4] K.Hirose, N.S.Wingreen, Phys. Rev. B**59** (1999) 4604.

[5] W.Kohn, L.J.Sham, Phys. Rev **140** (1965) A1133.

[6] We use the local-density approximation: $E_{\rm xc} = \int \rho(\mathbf{r})\,\epsilon_{\rm xc}[\rho(\mathbf{r})]\,d\mathbf{r}$, where $\epsilon_{\rm xc}[\rho(\mathbf{r})]$ is the parameterized form for the two-dimensional electron gas [B. Tanatar and D. M. Ceperley, Phys. Rev. **B39** (1989) 5005].

[7] The dimensionless conductance is given by $g = \hbar/(\tau_L\langle\Delta_0\rangle)$ where τ_L is the time an electron takes to cross the dot and $\langle\Delta_0\rangle$ is the mean level spacing.

[8] K.Hirose, F.Zhou, N.S.Wingreen, Phys. Rev. B**63** (2001) 075301.

[9] R.Berkovits, Phys. Rev. Lett., **81** (1998) 2128.

[10] P.Jacquod, A.D.Stone, Phys. Rev. Lett., **84** (2000) 3380.