The effect of confinement on the hyperfine exchange interaction

2003 J. Phys.: Condens. Matter 15 8673

(http://iopscience.iop.org/0953-8984/15/50/001)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) 8673–8677 PII: S0953-8984(03)68681-9

The effect of confinement on the hyperfine exchange interaction

M L Glasser

Department of Physics and Center for Quantum Device Technology, Clarkson University, Potsdam, NY 13699-5820, USA

Received 8 September 2003
Published 3 December 2003
Online at stacks.iop.org/JPhysCM/15/8673

Abstract

We examine the effect of spatial confinement on the hyperfine exchange interaction between two donor nuclei in a semiconductor quantum dot. On the basis of an exactly solvable model we look at the strength of the interaction in the ionized and neutral cases as one of the nuclei approaches the dot surface.

1. Introduction

Among the most promising architectures for the design of scalable units (qubits) for quantum computation are those based on manipulating nuclear spins of donor species embedded in a spatially confined semiconducting medium [1, 2]. Interaction among such spins arises from the hyperfine induced exchange interaction having the form $C\vec{I}_1 \cdot \vec{I}_2$, where $\vec{I}$ denotes a nuclear spin and the coupling constant C depends on the distance between the pair of spins as well as the properties of the medium. Due to spatial confinement, boundary effects may also play a role. A standard way of modelling confinement quantum mechanically is to require the wavefunctions to vanish at the bounding surface. This corresponds to a reduced electron density in this region and suggests that if a nuclear spin approaches such a wall, the hyperfine interaction, which is roughly proportional to the electron density, is also reduced, leading to a reduction in the exchange coupling related to this spin. This could well set a fundamental limit on the size of qubits based on this structural principle.

To estimate the importance of this effect we consider the following very simple model sketched in figure 1. Two point impurities with nuclear spin $\vec{I}$ are fixed at the foci of an ellipsoidal semiconductor dot described by a scalar effective mass m^*, and the wavefunction of a conduction electron is obtained in the effective mass approximation assuming that the donor atoms are singly charged Coulomb centres screened by a scalar dielectric constant κ and that the wavefunction vanishes at the surface. From this wavefunction we can calculate the donor electron's contribution to the exchange coupling constant. By varying the interfocal separation R and the eccentricity of the ellipsoid, one can estimate how C depends on R and the distance s of the nuclear spins from the surface (s is the distance from a focus to the adjacent apex). The case of un-ionized donors is also examined.

0953-8984/03/508673+05$30.00

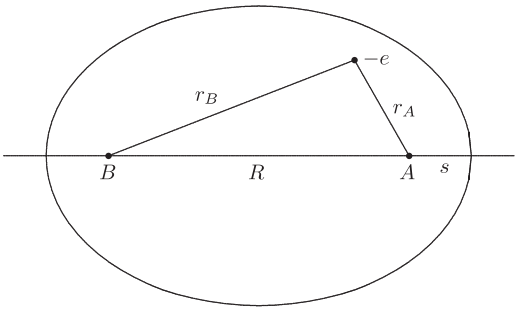

Figure 1. Ellipsoidal geometry.

The following section contains a brief review of the genesis of the dominant term in the hyperfine interaction and presents a formalism for calculating the coupling constant. The next section describes the how the electron wavefunction is calculated for an ellipsoid, and the results are summarized and discussed in the last section.

2. Formalism

Basically, the interaction between an electron and a nuclear magnetic moment, $\vec{\mu}_\mathrm{e}$ and $\vec{\mu}_\mathrm{n}$ respectively, is given by the usual dipole–dipole Hamiltonian

$$H_\mathrm{en} = \frac{\vec{\mu}_\mathrm{e}\cdot\vec{\mu}_\mathrm{n}}{r^3} - 3\frac{(\vec{\mu}_\mathrm{e}\cdot\vec{r})(\vec{\mu}_\mathrm{n}\cdot\vec{r})}{r^5}, \tag{1}$$

where $\vec{r}$ is the location of the electron relative to the nucleus. If the electron wavefunction is the spinor Ψ (with spatial part ψ), the interaction energy is

$$\langle\Psi|H_\mathrm{en}|\Psi\rangle = \vec{\mu}_\mathrm{e}\cdot\vec{\mu}_\mathrm{n}\int|\psi(\vec{r})|^2(1-3\cos^2\theta)\,\frac{\mathrm{d}r}{r}\,\mathrm{d}\Omega. \tag{2}$$

This is generally negligible except for an s state where $\psi(0)\neq 0$ and the integral is undefined. The resolution of this difficulty is well established [3] and leads to

$$\langle\Psi|\mathcal{H}_\mathrm{en}|\Psi\rangle = -\frac{8\pi}{3}\vec{\mu}_\mathrm{e}\cdot\vec{\mu}_\mathrm{n}|\psi(0)|^2. \tag{3}$$

Thus, effectively, the hyperfine interaction is dominated by the Fermi contact Hamiltonian

$$H_\mathrm{en} = -\frac{8\pi}{3}\vec{\mu}_\mathrm{e}\cdot\vec{\mu}_\mathrm{n}\delta(\vec{r}). \tag{4}$$

An electron described by Hamiltonian H_0 in the presence of nuclear moments $\vec{\mu}_1$ at $\vec{r}=\vec{R}_1$ and $\vec{\mu}_2$ at $\vec{r}=\vec{R}_2$ thus has the Hamiltonian

$$H = H_0 + H_\mathrm{n}, \qquad H_\mathrm{n} = \frac{16\pi}{3}\mu_0\sum\vec{\mu}_j\cdot\vec{S}\delta(\vec{r}-\vec{R}_j). \tag{5}$$

Expanding the partition function $Z(\beta)=\mathrm{Tr}\{\mathrm{e}^{-\beta H}\}$ in powers of H_n, the bilinear term is

$$Z_{12}(\beta) = \beta^2\left(\frac{16\pi}{3}\right)^2\mu_0^2\int_0^1\mathrm{d}u\,\mathrm{Tr}\{\vec{\mu}_1\cdot\vec{S}\delta(\vec{r}-\vec{R}_1)\mathrm{e}^{-\beta H_0(1-u)}\vec{\mu}_2\cdot\vec{S}\delta(\vec{r}-\vec{R}_2)\mathrm{e}^{-\beta H_0 u}\}. \tag{6}$$

If H_0 does not depend on $\vec{\mu}_j$,

$$Z_{12} = \left(\frac{16\pi\beta\mu_0}{3}\right)^2\mathrm{Tr}\{(\vec{\mu}_1\cdot\vec{S})(\vec{\mu}_2\cdot\vec{S})\int_0^1\mathrm{e}^{-\beta H_0 u}\delta(\vec{r}-\vec{R}_1)\mathrm{e}^{-\beta H_0(1-u)}\delta(\vec{r}-\vec{R}_2)\,\mathrm{d}u\}. \tag{7}$$

The spin trace is $\hbar^2\vec{\mu}_1\cdot\vec{\mu}_2/2$ and evaluating the spatial trace with respect to the eigenstates $|a\rangle$, E_a of H_0, we find

$$Z_{12} = 2\left(\frac{8\pi\hbar\beta\mu_0}{3}\right)^2 \vec{\mu}_1\cdot\vec{\mu}_2 \int_0^1 \Psi(\vec{R}_1, \vec{R}_2; \beta u)\Psi(\vec{R}_2, \vec{R}_1; \beta(1-u))\,\mathrm{d}u \quad (8)$$

where $\Psi(\vec{r}, \vec{r}'; s) = \sum_a \exp(-E_a s)\psi_a^*(\vec{r})\psi_a^*(\vec{r}')$ is the propagator. The contribution of (8) to the electron free energy is

$$F_{12} = \frac{\mathrm{i}}{\beta}\left(\frac{8\pi\mu_0\hbar}{3}\right)^2 \vec{\mu}_1\cdot\vec{\mu}_2 \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \frac{s\,\mathrm{d}s}{\sin\pi s}\mathrm{e}^{\beta\zeta s}\int_0^1 \mathrm{d}u\,\Psi(\vec{R}_1, \vec{R}_2; \beta s u)\Psi(\vec{R}_2, \vec{R}_1; \beta s u'), \quad (9)$$

where $u' = 1-u$ and ζ is the chemical potential.

In this work we deal only with a discrete electron spectrum and the zero-temperature limit where the propagator can be replaced by the ground state term (wavefunction ψ_0). On taking the appropriate limits, the free energy per electron reduces to $2(8\pi\hbar\mu_0/3)^2\vec{\mu}_1\cdot\vec{\mu}_2|\psi_0(\vec{R}_1)|^2|\psi_0(\vec{R}_2)|^2$. The effect of temperature will be examined in a future report. Thus the effective hyperfine interaction between the two nuclear spins is [4]

$$H_{12} = J\vec{\mu}_1\cdot\vec{\mu}_2|\psi(\vec{R}_1)|^2|\psi(\vec{R}_2)|^2 \quad (10)$$

where J is a constant.

3. Electron wavefunction

Now suppose that two singly ionized donor nuclei are located at the foci A and B of an ellipsoid having equal minor axes and filled with a semiconductor described by a scalar effective mass m^*. An electron in the conduction band then obeys the effective mass equation

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\kappa r_\mathrm{A}} - \frac{e^2}{\kappa r_\mathrm{B}}\right)\psi(\vec{r}) = E\psi(\vec{r}), \quad (11)$$

where κ is the dielectric constant. We adopt the modified atomic units $\hbar^2/2m^* = 1$, $e^2/\kappa = 2$. Equation (11) is equivalent to the Schrödinger equation for the hydrogen molecular ion [5] which is separable in ellipsoidal coordinates

$$\xi = \frac{r_\mathrm{A}+r_\mathrm{B}}{R}, \qquad \eta = \frac{r_\mathrm{A}-r_\mathrm{B}}{R}, \qquad \phi. \quad (12)$$

The ground state is independent of ϕ, the rotation angle about the z-axis, so we ignore all ϕ derivatives to obtain a two-dimensional problem. One has

$$\frac{2}{r_\mathrm{A}} + \frac{2}{r_\mathrm{B}} = \frac{8}{R}\frac{\xi}{\xi^2-\eta^2}$$
$$\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \tfrac{1}{8}R^3(\xi^2-\eta^2)\,\mathrm{d}\xi\,\mathrm{d}\eta\,\mathrm{d}\phi \quad (13)$$

and [6]

$$\nabla^2 = \frac{4}{R^2(\xi^2-\eta^2)}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right]. \quad (14)$$

Thus, writing $\psi(\vec{r}) = X(\xi)S(\eta)$ one finds the separated equations

$$[(\xi^2-1)X']' + [2R\xi - p\xi^2 - A]X(\xi) = 0, \quad (15a)$$
$$[(1-\eta^2)S']' + [A + p\eta^2]S(\eta) = 0, \quad (15b)$$

where A is the separation constant and $p = -ER^2/4$. These equations are the same in the neutral case, except that the term $2R\xi$ is absent in (15a).

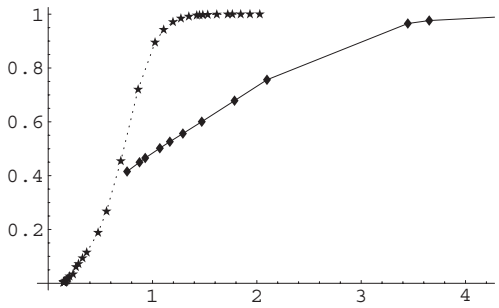

Figure 2. The dependence of the relative HF exchange constant $Q(s)$ versus s, the distance of a nuclear spin from the boundary. Upper curve: $R = 2$; lower curve: $R = 10$.

The surfaces $1 < \xi =$ constant are confocal ellipsoids ($\xi = 1$ is simply the z-axis between the foci). The boundary conditions for equation (15a) are $X(1) < \infty$ ($\xi = 1$ is a regular singular point), and $X(\xi_0) = 0$, where ξ_0 corresponds to the dot boundary. Note that $s = R(\xi_0 - 1)/2$ is the shortest distance from either focus to the boundary. The x–y plane is $\eta = 0$. For the ground state $S(-\eta) = S(\eta)$ and the boundary conditions for equation (15b) are $S(\pm 1) < \infty$ ($\eta = \pm 1$ are regular singular points) and $S'(0) = 0$.

To proceed, we specify a value R and integrate equation (15b) numerically starting with $S(-1) = 1$, $S'(-1) = -(A + p)/2$ for a given value p and adjust A until $S'(0) = 0$ (with no intervening nodes). Thus we effectively construct a table of $A(E, R)$. Then a pair of values A, p is inserted into equation (15a) which is integrated numerically with starting values $X(1) = 1$, $X'(1) = -(2R - p - A)/2$ and the pair is adjusted to obtain $X(\xi_0) = 0$ (with no intervening nodes). This gives a table of $E(R, s)$. Then, with A and p determined, the wavefunction $X(\xi)S(\eta)$ is calculated and normalized. As a technical point, since $\xi = 1$ and $\eta = -1$ are singular points, we first obtained X, X' at $\xi = 1 + 10^{-6}$ and S, S' at $\eta = -1 + 10^{-6}$ by series expansion and used these values to start the numerical integration. Finally, the (normalized) wavefunction was evaluated at $\xi = 1, \eta = -1$ ($\psi(0) = \psi(R)$ in (10) by symmetry).

4. Results and discussion

The calculations for the ionized case were carried out for $R = 2$ and 10; the unit of length $\hbar^2\kappa/m^*e^2$ is roughly 10–20 Bohr radii for most common semiconductors. For silicon this corresponds to spacings of about 20 and 100 Å. From the wavefunctions we calculated $Q(s)$, the ratio of the coupling constant to its value at $s = \infty$. The results are shown in figure 2. As expected, the relative values of the coupling constant at these inter-spin separations are reduced substantially when either spin is close to the boundary.

Similar behaviour has also been found for the Knight shift in a metallic particle [7] modelled as an electron gas confined in a spherically symmetric parabolic potential well. There it was found that the shift decreased in a Gaussian fashion as the nucleus moved away from the centre of the sphere. An analogous study of neutral donors in two-dimensional systems has been reported by Pershyn *et al* [8].

Finally, in figure 3 we compare the neutral and ionized donor cases for $R = 2$. The coupling between ionized donors is stronger than in the neutral case, in accordance with a higher electron density attracted to the nuclei, and remains effective for spatially smaller systems, although in the neutral case the coupling constant decays less rapidly as the boundary

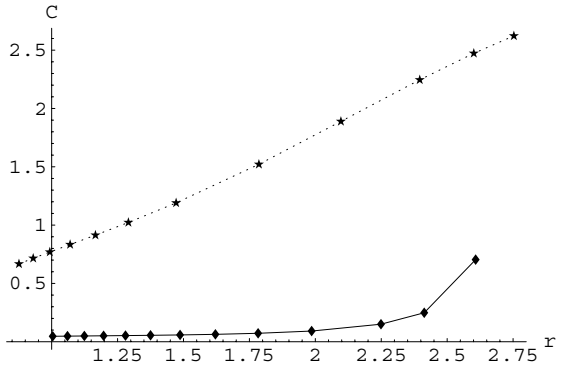

Figure 3. Comparison of the boundary effects for ionized (upper curve) and neutral donors. The vertical axis is in arbitrary units.

is approached. These results suggest that in a Kane model qubit, the imbedded donor nuclei should be located a substantial fraction of their distance from one another from the boundaries to ensure effective hyperfine coupling. In particular, for the model introduced by Mozyrsky *et al* [2], it was suggested that effective coupling between two phosphorus donor nuclear spins could be achieved with separations up to 100 nm in a GaAs quantum well 4 nm thick where the boundary effect examined here is ignored. The present results indicate that this is too optimistic. The spacing between the donors must be reduced by at least a factor of two, or the well thickness must be substantially increased to achieve the same coupling strength. This complicates fabrication of such a device, but does not render it unrealistic.

Acknowledgment

This work was supported by the National Science Foundation under grant DMR-0121146.

References

[1] Kane B H 1998 *Nature* **353** 133
[2] Mozyrsky D, Privman V and Glasser M L 2001 *Phys. Rev. Lett.* **86** 5112
[3] Schiff L I 1955 *Quantum Mechanics* (New York: McGraw-Hill) chapter 12
[4] Ramsey N F and Purcell E M 1952 *Phys. Rev.* **85** 143
Ruderman M A and Kittel C 1954 *Phys. Rev.* **96** 99
Glasser M L 1968 *Phys. Rev.* **174** 424
[5] Pauling L and Wilson E B 1935 *Introduction to Quantum Mechanics* (New York: McGraw-Hill) chapter 12
[6] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* (New York: McGraw-Hill)
[7] Glasser M L 2001 *J. Phys. A: Math. Gen.* **34** 5425
[8] Pershyn Yu V, Vagner I D and Wyder P 2003 *J. Phys.: Condens. Matter* **15** 997