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2001 J. Phys. A: Math. Gen. 34 5425

(http://iopscience.iop.org/0305-4470/34/26/311)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) 5425–5427 PII: S0305-4470(01)20555-1

Knight shift in a d-dimensional electron gas and quantum dot

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Received 21 December 2000
Published 22 June 2001
Online at stacks.iop.org/JPhysA/34/5425

Abstract

A general expression is derived for the (paramagnetic) shielding factor for a nuclear spin embedded in a d-dimensional noninteracting electron gas and a parabolic quantum dot. We find that for $d = 2$ the Knight shift has no intrinsic magnetic field dependence and that for the quantum dot the shift is negligible unless the nuclear spin is near the centre.

PACS numbers: 0530F, 2110H, 7110C, 7321L

1. Formulation

We shall assume that the interaction of an electron with a nuclear spin, characterized by moment $\mu_N \vec{I}$ aligned along an externally applied magnetic field $\vec{H} = H\hat{k}$ is, in all dimensions $d \geqslant 2$, given by the Fermi contact Hamiltonian

$$\mathcal{H}_N = \frac{16\pi}{3}\mu_0\mu_N \vec{I}\cdot\vec{S}\delta(\vec{r}) \tag{1}$$

where μ_0 is the Bohr magneton, and $\vec{S}$ is the electron spin operator. We identify the Knight shift with the paramagnetic shielding factor given by Das and Sondheimer [1] in terms of the Helmholtz free energy F:

$$\sigma = -\frac{\mathrm{d}F}{H\,\mathrm{d}\mu_N}\bigg|_{\mu_N=0}. \tag{2}$$

At temperature zero, the free energy can be expressed in terms of the chemical potential ζ, particle density n and partition function Z by

$$\begin{aligned} F - n\zeta &= -\frac{1}{2\pi \mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{Z(s)}{s^2}\mathrm{e}^{\zeta s}\,\mathrm{d}s \\ Z(s) &= \mathrm{Tr}\{\mathrm{e}^{-(\mathcal{H}_0+\mathcal{H}_z+\mathcal{H}_N)s}\} \\ \mathcal{H}_0 &= \frac{1}{2m^*}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 \\ \mathcal{H}_z &= 2\mu_0\vec{H}\cdot\vec{S}. \end{aligned} \tag{3}$$

We shall ignore the effect of μ_N on ζ. Then, to linear order in μ_N, the relevant term in the free energy, after performing the spin trace, and inverse Laplace transform, is

$$F_N = \frac{8\pi}{3}\mu_0\mu_N \operatorname{Tr}[\delta(\vec{r})X_{\mu_0 H}(\zeta - \mathcal{H}_0)] \tag{4}$$

where X_a is the characteristic function of the interval $[-a, a]$. By carrying out the trace over the eigenstates $\psi_\lambda(\vec{r}),\quad E_\lambda$ of $\mathcal{H}_0$, we obtain

$$\sigma = \frac{8\pi}{3}\mu_0^2\sum_\lambda |\psi_\lambda(0)|^2\frac{X_{\mu_0 H}(\zeta - E_\lambda)}{\mu_0 H}. \tag{5}$$

In the zero-field limit, this gives

$$\sigma_0 = \frac{16\pi}{3}\mu_0^2\sum_\lambda |\psi_\lambda(0)|^2\delta(\zeta - E_\lambda) \tag{6}$$

from which we easily recover the Towne–Herring–Knight formula [2] $\sigma_0 = (8\pi/3)\chi_p\langle|\psi(0)|^2\rangle_F$.

Continuing in this vein, and noting that

$$\frac{X_a(z)}{a} = 2\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{\sinh(as)}{as}\mathrm{e}^{zs}\frac{\mathrm{d}s}{2\pi\mathrm{i}} \tag{7}$$

we arrive at our basic formula

$$\begin{aligned}\sigma &= \frac{16\pi}{3}\mu_0^2\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{\sinh(\mu_0 Hs)}{\mu_0 Hs}\mathrm{e}^{\zeta s}\Psi(0,0,s)\frac{\mathrm{d}s}{2\pi\mathrm{i}}\\ \Psi(\vec{r},\vec{r}\,',s) &= \sum_\lambda \psi_\lambda^*(\vec{r}\,')\psi_\lambda(\vec{r})\mathrm{e}^{-E_\lambda s}.\end{aligned} \tag{8}$$

2. d-dimensional electron gas

For a d-dimensional ($d \geqslant 2$) electron gas, generalizing Sondheimer and Wilson's calculation [3], we have

$$\Psi(0,0,s) = \left(\frac{m^*}{2\pi\hbar^2}\right)^{d/2}\frac{\mu_0^* Hs}{\sinh(\mu_0 Hs)}s^{-d/2}. \tag{9}$$

Hence, in terms of the effective mass ratio $\alpha = m^*/m$, we have

$$\sigma^{(d)} = \frac{16\pi}{3}\mu_0^2\alpha\left(\frac{m^*}{2\pi\hbar^2}\right)^{d/2}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{\sinh(\mu_0 Hs)}{\sinh(\mu_0^* Hs)}\frac{\mathrm{e}^{\zeta s}}{s^{d/2}}\frac{\mathrm{d}s}{2\pi\mathrm{i}}. \tag{10}$$

For $d = 2$ it is assumed that the field is normal to the plane of the system. We see that if the mass ratio is unity, σ has no field dependence other than that introduced through the chemical potential. For non-integer mass ratio, the Landau level structure is evident in the step-like behaviour of σ given below. Thus,

$$\sigma^{(d)}(\alpha = 1) = \frac{16\pi}{3}\mu_0^2\left(\frac{m}{2\pi\hbar^2}\right)^{d/2}\frac{\zeta^{d/2-1}}{\Gamma(d/2)}. \tag{11}$$

For non-integer α and $d > 2$,

$$\begin{aligned}\sigma^{(d)} = \frac{16\pi}{3}\frac{\mu_0^2\alpha}{\Gamma(d/2)}\left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2}(\mu_0^* H)^{d/2-1}\sum_{n=1}^{\infty} n[(z+\alpha-2n+1)^{d/2-1}\\ -(z-\alpha-2n+1)^{d/2-1} - (z+\alpha-\min[z+\alpha, 2n+1])^{d/2-1}\\ +(z-\alpha-\min[z-\alpha, 2n+1])^{d/2-1}]\end{aligned} \tag{12}$$

where $z = \zeta/\mu_0^* H$ and the $d/2 - 1$ powers are understood to be 0 if the argument is negative. The corresponding expression for $d = 2$ is

$$\sigma^{(2)} = \frac{16\pi}{3}\mu_0^2\alpha\left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2}\sum_{n=0}^{\infty} n[\Theta(z+\alpha-2n+1)\Theta(2n+1-z-\alpha) \\ -\Theta(z-\alpha-2n+1)\Theta(2n+1-z+\alpha)]. \quad (13)$$

For moderate to high fields, we have the alternative representation

$$\sigma^{(d)} = \frac{32\pi}{3}\mu_0^2\alpha\left(\frac{m^*}{2\pi\hbar^2}\right)^{d/2}\frac{(\mu_0^* H)^{d/2-1}}{\pi^{d/2}}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{d/2}}\sin(k\pi\alpha)\sin\left[\left(kz-\frac{d}{4}\right)\pi\right]. \quad (14)$$

3. Parabolic quantum dot

An electron gas in a spherical well having radius R_0 will be subject to the harmonic potential

$$V(r) = \tfrac{1}{2}m^*\omega_0^2(r^2+z^2) \quad (15)$$

where $\omega_0 = \frac{1}{R_0}\sqrt{\frac{2\zeta}{m^*}}$. In terms of the parameters $\omega_c = 2\mu_0 H$ and $\Omega = \sqrt{\omega_0^2+\omega_c^2}$, we have [4]

$$\Psi(\vec{r}_0,\vec{r}_0,s) = \left(\frac{m^*\omega_0}{2\pi\hbar}\right)^{1/2}\left(\frac{m^*\Omega}{2\pi\hbar}\right)(\operatorname{csch}(\hbar\omega_0 s))^{1/2}\operatorname{csch}(\hbar\Omega s) \\ \times\exp\left[-\left(\frac{m^*}{\hbar}\right)\omega z_0^2\operatorname{sech}(\hbar\omega_0 s/2)\right] \\ \times\exp\left[-\frac{2m^*}{\hbar}\Omega r_0^2\frac{\sinh\frac{1}{2}\hbar(\Omega+\omega_0)s\ \sinh\frac{1}{2}\hbar(\Omega-\omega_0)s}{\sinh\hbar\Omega s}\right]. \quad (16)$$

Here, r_0 and z_0 are the cylindrical coordinates of the nuclear spin site and the magnetic field is along the z-axis. In the zero-field limit (8) becomes

$$\sigma_0(z_0) = \frac{16\pi}{3}\left(\frac{m^*\omega_0}{2\pi\hbar}\right)^{3/2}\mu_0^2\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\frac{\mathrm{e}^{\zeta s}}{(\sinh\hbar\omega_0 s)^{3/2}}\mathrm{e}^{-(m^*\omega_0 z_0^2/\hbar)\operatorname{sech}(\hbar\omega_0 s/2)}\frac{\mathrm{d}s}{2\pi\mathrm{i}}. \quad (17)$$

In the case that the dot radius greatly exceeds the Fermi wavelength, this results in

$$\sigma_0(z_0) = \frac{32\sqrt{\pi}}{3}\mu_0^2\left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2}\zeta^{1/2}\mathrm{e}^{-\frac{m^*\omega_0}{\hbar}z_0^2} \quad (18)$$

showing that the paramagnetic shift decreases dramatically away from the centre of the dot.

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