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Spin-wave excitations in quantum dots

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The transverse response function for a quantum dot in a uniform magnetic field B is calculated using current-density-functional theory. The poles corresponding to the $\Delta L_z = \pm 1$ and $\Delta S_z = \pm 1$ spin waves are investigated as a function of B. [S0163-1829(98)52812-3]

Transverse spin excitations in Fermi liquids have been extensively studied in the last few years in liquid ^{3}He (Refs. 1 and 2), ^{3}He-^{4}He solutions,[3,4] paramagnetic metals,[5,6] and finely layered heterostructures[7,8] both theoretically and experimentally. The same excitations in finite Fermi systems have been, however, much less studied. In particular, the transverse spin dipole modes excited by the operator $D_\pm = x\sigma_\pm$, where x is the Cartesian component of the position vector and $\sigma_\pm$ the spherical components of the vector of Pauli matrices, giving rise to spin-flip transitions, are practically unexplored. The reason for that is twofold: to study these modes one needs a spin polarized ground state and a complicated experiment to detect the excited states as, e.g., inelastic scattering of polarized light. In atomic nuclei, for example, these measurements have become accessible only in recent years in small systems as polarized deuteron and ^{3}He.[9]

A much easier detection of spin modes in finite Fermi systems should be possible in quantum dot structures that have been successfully built in the last few years using advanced technologies.[10–13] In fact, these structures are easily spin polarized with a perpendicular magnetic field B and the transverse response can be detected via inelastic scattering of polarized light, which is commonly used in condensed matter physics.[7]

The purpose of this paper is to provide a theoretical study of the propagation of spin waves in quantum dots as a function of the applied static magnetic field. Our investigation is based on the study of the transverse spin response function, or dynamical polarizability $\alpha(\omega)$. This quantity is defined in terms of the polarization

$$\langle D_+ \rangle = \tfrac{1}{2} g^* \mu_B h \alpha_-(\omega) e^{-i\omega t}, \tag{1}$$

induced by a transverse oscillating magnetic field h interacting with the system through the Hamiltonian $H_{\rm int} = \frac{1}{2} g^* \mu_B h D_- e^{-i\omega t}$, where g^* is the effective gyromagnetic factor and μ_B the Bohr magneton. Standard perturbation theory yields the following expression for the transverse polarizability:

$$\alpha_-(\omega) = \sum_n \frac{|\langle n|D_-|0\rangle|^2}{\omega - \omega_{n0} + i\eta} - \frac{|\langle n|D_+|0\rangle|^2}{\omega + \omega_{n0} + i\eta}, \tag{2}$$

where $|n\rangle$ and ω_{n0} are eigenstates and eigenvalues of the Hamiltonian of the system. The positive and negative poles of α_- correspond to elementary excitations induced by the operators D_- and D_+, respectively. Starting from an external field D_+ and in a completely analogous way we define $\alpha_+(\omega)$, the poles of which are placed symmetrically from the $\omega = 0$ axis with respect to those of α_-. In the following we provide an explicit evaluation of α in the framework of the time-dependent current-density-functional theory (TDCDFT), which includes the effect of correlations through a self-consistent treatment of the mean field and has already been used in Ref. 14 to study far-infrared absorption of light in quantum dots.

In CDFT,[15] the single-particle wave functions $\varphi_{i\sigma}$ corresponding to the two-dimensional motion [$\vec{r} = (r, \theta)$, $r = \sqrt{x^2 + y^2}$] of the electrons in the $z = 0$ plane in the presence of a constant magnetic field B in the z direction are given by the solutions of the Kohn-Sham equations

$$\left\{ -\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}\omega_c \ell_z + \tfrac{1}{8}\omega_c^2 r^2 + V_+(r) + V_H(r) + \frac{e}{c}\frac{A_{\rm xc}(r)}{r}\ell_z + V_{\rm xc}(r) + [f_{\rm xc}(r)\vec{m} + \tfrac{1}{2} g^* \mu_B \vec{B}] \cdot \vec{\sigma} \right\} \varphi_{i\sigma} = \varepsilon_{i\sigma} \varphi_{i\sigma}, \tag{3}$$

where V_+ is the dot confining potential, $V_H = \int [\rho(r')/|\vec{r} - \vec{r}'|] d\vec{r}'$ is the Hartree potential, while $V_{\rm xc} = \partial E_{\rm xc}/\partial\rho - (e/c) A_{\rm xc} j_p/\rho$ and $f_{\rm xc}\vec{m} = \partial E_{\rm xc}/\partial\vec{m}$ are the exchange-correlation potentials in the local approximation appropriate for a two-dimensional system in a magnetic field.[16] $A_{\rm xc}$ is the exchange-correlation vector potential of CDFT,[15] and $j_p(r) = -1/r \Sigma_{n\ell\sigma} \ell u^2_{n\ell\sigma}$ is the orbital paramagnetic current density. As shown in Ref. 15, CDFT has proved to be very accurate, even for such few-electron systems as two- and three-electron quantum dots.

In Eq. (3), $\omega_c = eB/mc$ is the cyclotron frequency and $\vec{\sigma}$ the vector of Pauli matrices. As a consequence of circular symmetry, the $\varphi_{i\sigma}$ are eigenstates of the z component of orbital angular momentum ℓ_z, i.e., $\varphi_{i\sigma}(r, \theta) = u_{i\sigma}(r) e^{-i\ell\theta}$, $i \equiv (n\ell)$, with possible values $\ell = 0, \pm 1, \pm 2, \ldots$. The ground-state density is given by $\rho = \Sigma_{n\ell\sigma} |u_{n\ell\sigma}|^2$ and the ground-state magnetization, defined

as $\vec{m}=\Sigma_{n\ell\sigma}(\varphi^*_{n\ell\sigma}\vec{\sigma}\varphi_{n\ell\sigma})$, has $m_x=m_y=0$ and $m_z\equiv m_0=\rho_\uparrow-\rho_\downarrow$. We have used effective atomic units defined by $\hbar=e^2/\epsilon=m=1$, where ϵ is the dielectric constant of the semiconductor and m is the electron effective mass. In units of the bare mass m_e it is $m=m^*m_e$. In this unit system the length unit is the effective Bohr radius $a_0^*=a_0\epsilon/m^*$ and the energy unit is the effective Hartree energy $\mathcal{H}^*=\mathcal{H}m^*/\epsilon^2$. For GaAs one has $\epsilon=12.4$, $m^*=0.067$, and $g^*=-0.44$, which imply $a_0^*=97.9$ Å and $\mathcal{H}^*=11.9$ meV.

The CDFT ground state is an eigenstate of $L_z=\Sigma_i\ell_{z,i}$ and $S_z=\Sigma_i\sigma_{z,i}/2$, which eigenvalues are predicted by the calculation at each value of B. Besides spin, the dipole transverse operator can be further separated in its orbital parts, i.e., in its $L_z=\pm1$ and $S_z=\pm1$ parts as

$$D_{L_z=\pm1,S_z=\pm1}=\sum_{i=1}^{N} r_i e^{\pm i\theta_i}\sigma_{\pm,i}. \tag{4}$$

Acting on the ground state with angular momenta L_0 and S_0 for orbital and spin components, respectively, $D_{\pm,\pm}$ excites states with $L_z=L_0\pm1$ and $S_z=S_0\pm1$.

In TDCDFT when the system interacts with the oscillating external field $D_{\pm,\pm}e^{-i\omega t}$ the potential $2f_{\rm xc}(m_+\sigma_-+m_-\sigma_+)$, entering the scalar product $f_{\rm xc}\vec{m}\cdot\vec{\sigma}$ of Eq. (3) and statically equal to zero, changes due to the variations $\delta m_\pm(\vec{r},\omega)$ dynamically induced in the magnetization. The transverse linear-response function associated, for instance, to the particular case of $D_{+,-}$ is defined by

$$\alpha_{+,-}(\omega)=\langle D^\dagger_{+,-}\rangle=\int d\vec{r}re^{-i\theta}\delta m_+(\vec{r},\omega), \tag{5}$$

with

$$\delta m_+(\vec{r},\omega)=\int d\vec{r}'\chi(\vec{r},\vec{r}',\omega)r'e^{+i\theta'}. \tag{6}$$

The correlation function χ is the solution of the Dyson-type integral equation

$$\chi(\vec{r},\vec{r}',\omega)=\chi^0(\vec{r},\vec{r}',\omega)+\int d\vec{r}_1d\vec{r}_2\chi^0(\vec{r},\vec{r}_1,\omega)\times2f_{\rm xc}({\rm g.s.})\delta(\vec{r}_1-\vec{r}_2)\chi(\vec{r}_2,\vec{r}',\omega), \tag{7}$$

where

$$\chi^0(\vec{r},\vec{r}',\omega)=\sum_{hp}\left[\frac{(h|\sigma_+|p)_{\vec{r}}(p|\sigma_-|h)_{\vec{r}'}}{\omega+i\eta-\varepsilon_p+\varepsilon_h}-\frac{(p|\sigma_+|h)_{\vec{r}}(h|\sigma_-|p)_{\vec{r}'}}{\omega+i\eta+\varepsilon_p-\varepsilon_h}\right] \tag{8}$$

is the free transverse correlation function built with the solutions of Eq. (3) and in Eq. (8) the label $p(h)$ refers to unoccupied (occupied) single-particle states. Only spin variables are summed in the single-particle matrix elements of Eq. (8), while space variables are indicated as a subindex. The kernel $2f_{\rm xc}({\rm g.s.})\delta(\vec{r}_1-\vec{r}_2)$ can be interpreted as the residual two-body interaction in the spin transverse channel. The study of the response [Eqs. (5)–(8)] allows us to investigate the excitations induced by the operators $D_{+,-}$ and $D_{-,+}$ with excited states of angular momentum (L_0+1, S_0-1) and (L_0-1, S_0+1), respectively. In an analogous way, starting from the operator $D_{+,+}$, instead of $D_{+,-}$, one can study the excitation modes with (L_0+1, S_0+1) and (L_0-1, S_0-1).

It is also interesting to investigate the properties of the response function in terms of sum rules. For this it is useful to consider the $\omega\to\infty$ expansion of α. From Eq. (2) one finds[17]

$$\lim_{\omega\to\infty}\alpha_{+,-}(\omega)=\frac{1}{\omega}S_0+\frac{1}{\omega^2}S_1+\cdots, \tag{9}$$

with

$$\begin{aligned}S_0&\equiv S_0^{+,-}-S_0^{-,+}=\sum_n(|\langle n|D_{+,-}|0\rangle|^2-|\langle n|D_{-,+}|0\rangle|^2)\\&=\langle0|[D_{-,+},D_{+,-}]|0\rangle,\\S_1&\equiv S_1^{+,-}+S_1^{-,+}=\sum_n\omega_{n0}(|\langle n|D_{+,-}|0\rangle|^2+|\langle n|D_{-,+}|0\rangle|^2)\\&=\langle0|[D_{-,+},[H,D_{+,-}]]|0\rangle,\end{aligned} \tag{10}$$

where we have used the completeness relation. Analogous expressions for the sum rules corresponding to the $D_{+,+}$ and $D_{-,-}$ operators are obtained. The occurrence of the term in $1/\omega$ in Eq. (9) is peculiar to polarized systems and is associated with the fact that for such systems the transverse response is not an even function of ω.

The sum rules in Eq. (10) can be evaluated in the framework of CDFT and one can demonstrate rigorously that the expectation value of the commutators in Eq. (10) on the CDFT ground state is equivalent to the sum on the left-hand side evaluated with TDCDFT excitation energies and matrix elements. We find the following results:

$$\begin{aligned}S_0^{+,-}-S_0^{-,+}&=S_0^{-,-}-S_0^{+,+}=\int d\vec{r}r^2m_0(r),\\S_1^{+,-}+S_1^{-,+}&=N-g^*\mu_BB\int d\vec{r}r^2m_0(r)+\int d\vec{r}r[j_\uparrow(r)-j_\downarrow(r)]+\frac{\omega_c}{2}\int d\vec{r}r^2m_0(r),\\S_1^{-,-}+S_1^{+,+}&=N-g^*\mu_BB\int d\vec{r}r^2m_0(r)-\int d\vec{r}r[j_\uparrow(r)-j_\downarrow(r)]-\frac{\omega_c}{2}\int d\vec{r}r^2m_0(r),\end{aligned} \tag{11}$$

where $j_\sigma(r)=-1/r\Sigma_{n\ell}u^2_{n\ell\sigma}$.

In the following numerical application we consider a dot of $N=11$ electrons confined in a parabolic potential given by $V_+=\frac{1}{2}\omega_0^2r^2$ with $\omega_0=3.51$ meV. This potential reproduces near the origin a jellium disk with radius $R=r_s\sqrt{N}\approx500$ Å, with $r_s=1.51a_0^*$. We have solved self-consistently the ground state and then the transverse response equations (5)–(8) for this dot in an external magnetic field of magnitudes $B=0$, 1.5, 3, and 5.4 T. Figure 1 displays the strength func-

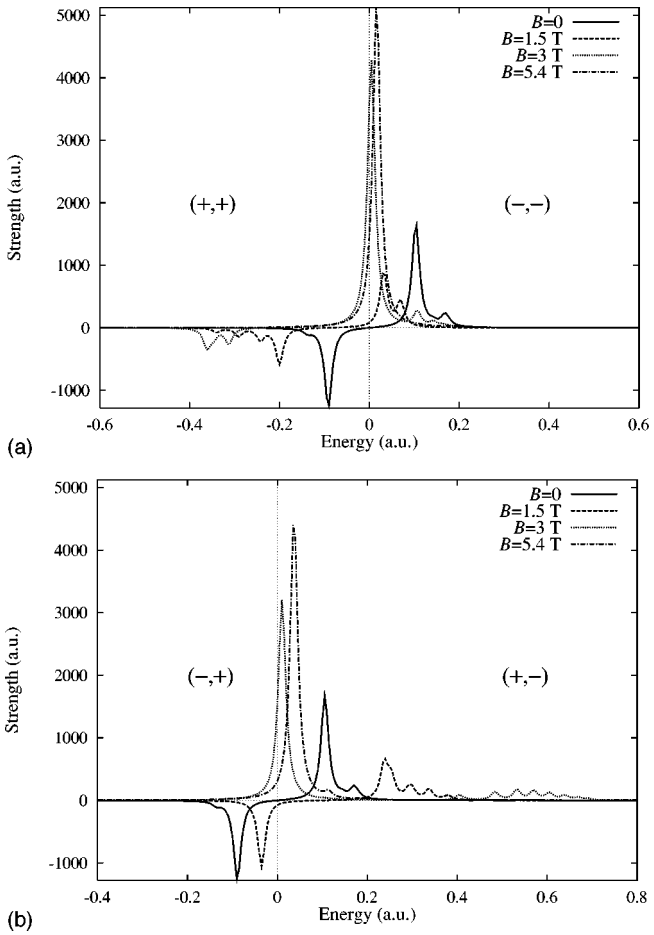

FIG. 1. Strength function $S(\omega)$ for the $(-,+)$ and $(+,-)$ channels (lower) and for the $(+,+)$ and $(-,-)$ ones (upper) for different static magnetic fields and the $N=11$ electron dot discussed in the text. In each case, for the channel on the left part, which is the Hermitian conjugate of the one on the right, the figure shows the negative of the strength as a function of the negative of the energy, i.e., $-S(-\omega)$. With the Lorentzian averaging, in this representation each channel and its Hermitian conjugate are given by a single continuous curve [see Eq. (2)].

tion, related to the polarizability as $S(\omega)\equiv -1/\pi\ \mathrm{Im}[\alpha] = \Sigma_n |\langle n|D|0\rangle|^2 \delta(\omega-\omega_{n0})$. In the actual calculation we have added a small imaginary part (η=0.01 a.u.) to the energy ω that transforms the Δ peaks in Lorentzians. We have checked that the sum rules in Eq. (11) are satisfied by our calculated $S(\omega)$.

From the figure one observes the following behaviors. In all the channels the response is dominated by a single peak at low energy and, in some cases, fragmented high-energy states are also present. At $B=0$ the energy of the peak is the same for both $(-,-)$, i.e., $\Delta L=-1$ and $\Delta S=-1$, and $(+,-)$ channels, as well as for $(-,+)$ and $(+,+)$ ones. There is, however, a small energy difference between the $\Delta S=\pm 1$ cases. Increasing B the peak energies disperse positively for $\Delta L=+1$ transitions and negatively for $\Delta L=-1$, up to $B\approx 3$ T. Then, there is a change of tendency for the $\Delta S=-1$ channel, where at $B\approx 3$ T it appears as a very strong peak at low energy for both $\Delta L=\pm 1$. Furthermore, one notes a vanishing of the strength for the $\Delta S=+1$ channel for both $\Delta L=\pm 1$, but it is faster in the $\Delta L=-1$ case, with a transfer of the strength to the $\Delta S=-1$ channel.

To understand these behaviors we first notice that the terms in the CDFT single-particle Hamiltonian (3) responsible for the difference between spin-up and -down single-particle wave functions and energies are the Zeeman term $\frac{1}{2}g^*\mu_B B\sigma_z$ and the exchange-correlation potential $W_{xc}\sigma_z \equiv f_{xc}m_0\sigma_z$. This last term is also responsible for the residual interaction in the Dyson-type equation (7). Second, the sum rules of Eq. (11), which are moments of the strength reported in the figure, must be satisfied at each value of B. At $B=0$ the Zeeman term vanishes, but not the exchange-correlation one since in the ground state $S=1/2$ and hence $m_0\neq 0$. This gives rise to a small energy splitting between spin-up and -down single-particle (sp) levels, which is the origin of the small differences of peak energies at $B=0$ between the $\Delta S=\pm 1$ channels. Up to $B\geqslant 1.5$ T the spin of the ground state does not change and the behavior with B can be explained by the splitting between the $\pm\ell$ sp levels originating by the B dependent orbital momentum term in Eq. (3). The situation is similar to the one occurring in the density channel when one studies far-infrared dipole modes excited by a *spin independent* dipole operator $D_\rho=\Sigma_i x_i$, with the difference that now there are four channels instead of two. At $B\approx 3$ T the situation changes, since the spin of the ground state gets larger than 1/2. At $B=5.4$ T the system is completely polarized in spin and angular momentum. The ground state is the maximum density droplet (MDD) with filling factor $\nu=1$, carrying spin $S=11/2$ and angular momentum $L=N(N-1)/2=55$. The $\Delta S=+1$ channels, due to the Pauli blocking of electronic spins, decrease their strength for increasing spin polarization and at $B=5.4$ T, when all the spins are up, no strength is left in these channels. Due to the fact that the sum rules must be fulfilled the strength passes to the $\Delta S=-1$ channels. The $(-,+)$ channel disappears more rapidly than the $(+,+)$ because of the polarization in angular momentum.

The spectacular inversion of tendency of the dispersion with B of the peak energies of $(+,-)$ and $(-,-)$ channels and the simultaneous growth of the strength up to reach at $B\approx 3$ T a very collective state at low energy can be understood as follows. When $B>1.5$ T the spin of the ground state increases and the exchange-correlation potential $W_{xc}\sigma_z$ becomes more and more important and splits the spin-up and -down levels more and more. At a certain point, some of the spin-down levels, previously degenerate with the spin-up ones and below the Fermi level, become unoccupied making possible new low-energy single-particle transitions. These transitions take a lot of strength, also because at the same time in the $\Delta S=+1$ channels the Pauli blocking becomes more and more active. The Zeeman term plays a minor role in determining the single-particle spectrum, since it is much lower than the exchange-correlation one, but it eventually determines the energy of the TDCDFT peak due to the effect of the residual interaction which changes considerably the average energy of the spectrum with respect to that of the free response. This is demonstrated with the sum rules of Eq. (11). In fact, when the system is fully polarized in spin and angular momentum one can estimate the energy of the collective state through the ratio $\overline{\omega}=S_1/S_0$, since then the $\Delta S=+1$ channels are Pauli blocked. One gets for the TDCDFT energies

$$\bar{\omega}_{+,-} = -g^*\mu_B B + \frac{\omega_c}{2} - \frac{1}{2}\frac{N-1}{\langle r^2\rangle} + \frac{1}{\langle r^2\rangle},$$

$$\bar{\omega}_{-,-} = -g^*\mu_B B - \frac{\omega_c}{2} + \frac{1}{2}\frac{N-1}{\langle r^2\rangle} + \frac{1}{\langle r^2\rangle}, \qquad (12)$$

where we have used the definitions $\langle r^2\rangle = 1/N\int d\vec{r}\, r^2\rho$, $\int d\vec{r}\, rj = -L_0$, and the fact that in the polarized system $L_0 = N(N-1)/2$. Equations (12) should be contrasted with those corresponding to the free response, from which they differ for the absence of the term $W_{xc}\sigma_z$, which in TDCDFT is exactly cancelled by the residual interaction. A further simplification of Eq. (12) can be done using for the polarized system the estimate $\langle r^2\rangle = (N+1)/\omega_c$, which is exact for the MDD ground state. One then gets

$$\bar{\omega}_{+,-} = -g^*\mu_B B + \frac{2\omega_c}{N+1},$$

$$\bar{\omega}_{-,-} = -g^*\mu_B B, \qquad (13)$$

from which one can understand the result of our calculation at $B = 5.4$ T displayed in Fig. 1. There the peak energy in the $(-,-)$ channel is at the energy predicted by the sum-rule approach (13), since in the spectrum there are no high-energy states. Conversely, $\bar{\omega}_{+,-}$ takes care, through the presence of the term $2\omega_c/(N+1)$, of the fact that in the $(+,-)$ channel the peak is at higher energy and that there are also other small peaks beyond 0.8 a.u. not seen in the plot.

To summarize, the transverse spin-wave excitations in a quantum dot have been analyzed as a function of the static magnetic field B within the current-density-functional theory. We have shown that at low B there are four dipole channels, two with positive and two with negative dispersion of the energy. At higher B's two of the channels are strongly depressed because of the Pauli blocking and they eventually disappear. This is linked to a dramatic change in the dispersion of the other two channels because of the associated transfer of oscillator strength and of the appearance of low-energy states.

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