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Spin excitations in multilayered ferromagnetic electron gases

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Spin excitations in a periodic array of layered ferromagnetic electron gases are discussed within the generalized Hubbard approximation. It is shown that the Stoner gap and the spin waves display appropriate crossover behavior (from two to three dimensions) on going from the weak- to strong-coupling regime. Their anisotropic behavior depends not only on the electron tunneling between adjacent layers, but on the screened Coulomb potential as well. The screening anisotropy even affects the existence of the collective modes.

I. INTRODUCTION

Molecular-beam epitaxy allows the fabrication of electronic systems with anisotropic dispersion intermediate between two and three dimensions (2D and 3D). Such structures are referred to as superlattices, where a weak periodic potential is imposed onto the electronic system in the z direction, parallel to the growth. Phenomenologically, they can be regarded as a simple extension of the quasi-2D case. But the transparency of neighboring barriers and the strong interlayer coupling change qualitatively the character of the system; therefore, such a system provides a way of studying the crossover behavior in the collective mode spectrum as the layer thickness is reduced.

Much attention has been devoted so far to the charge density excitations of a layered electron gas, and various investigations have been reported on plasmons and the associate dielectric screening in the last decade.[1-5] Research on other types of excitations (say, spin waves,[6,7] magnetorotons,[8] etc.) has only started recently.

The purpose of this paper is to investigate the magnetic excitations of such an electron gas in its ferromagnetic phase, which is promising since an important rule is played by the spin-density fluctuation[9] in addition to the charge-density fluctuation. By being able to carry their spin bias to nearby regions, moving electrons bring about spin correlations in the system that can lead to collective spin-wave modes. Using the Feynman diagram technique, we study the spin excitations of a layered ferromagnetic electron system in the generalized Visscher-Falicov (VF) model[10] and analyze the effects of the electron tunneling and the modulation of the superlattice on the spectra. The paper is divided as follows: The spin correlation function is evaluated at first (Sec. II), then in Sec. III the spectra of the excitations are determined; the last section is devoted to the concluding remarks.

II. TRANSVERSE SPIN CORRELATION FUNCTION

Considering a periodic array of ferromagnetic layers of quasi 2D electron gas, in which the electrons move freely in each layer, the single-particle wave function can then be written as

$$\psi_K(\mathbf{r},z)=\frac{1}{\sqrt{A}}e^{i\mathbf{k}\cdot\mathbf{r}}\xi_{k_\perp}(z)\ , \tag{1a}$$

$$\xi_{k_\perp}(z)=\frac{1}{\sqrt{N}}\sum_{l=1}^{N}e^{ik_\perp ld}\phi(z-ld)\ , \tag{1b}$$

where $\mathbf{r}$ stands for the position variable in the electron layer plane, $\mathbf{K}=(\mathbf{k},k_\perp)$ is the wave vector, A and N are the area of the layer and the number of the layers, respectively. $\phi(z-ld)$ confines the electrons in the lth layer which adopts the atomic wave function in the generalized VF model, it is assumed only the lowest band is occupied, so the band index in Eq. (1) has already been omitted.

Assuming further a very small overlap between the wave functions of two neighboring layers, and retaining only the wave functions belonging to the same layers in the interacting Hamiltonian, we can readily obtain the total Hamiltonian of the system:[6]

$$H=H_0+H_{\text{int}}\ , \tag{2a}$$

$$H_0=\sum_{K,s}\left[\frac{\hbar^2k^2}{2m_e}+2T\cos(k_\perp d)\right]C^\dagger_{Ks}C_{Ks}\ , \tag{2b}$$

$$H_{\text{int}}=\frac{1}{V}\sum_{\substack{K,K'\\ \mathbf{Q},\\ s,s'}}\frac{2\pi e^2}{q}\frac{d\sinh(qd)}{\cosh(qd)-\cos(q_\perp d)}\times C^\dagger_{Ks}C^\dagger_{K's'}C_{K'-Qs'}C_{K+Qs}\ . \tag{2c}$$

$C^\dagger_{Ks}$ (C_{Ks}) is the creation (annihilation) operator for an electron in the single-particle state with spin s, T is the hopping integral between the nearest-neighbor layers, $\mathbf{Q}=(\mathbf{q},q_\perp)$ is the momentum transfer. The anisotropy of superlattices is naturally reflected in the dispersion relation ε_K and the Coulomb potential $V(\mathbf{Q})$.

We now introduce the spin correlation function:[11]

$$D^{+-}(\mathbf{x}\tau,\mathbf{x}'\tau')=-\langle T_\tau[S^+(\mathbf{x}\tau)S^-(\mathbf{x}'\tau')]\rangle \ , \tag{3}$$

where the spin-flip operators are defined as

$$S^{\pm}(x)=\tfrac{1}{2}\psi^\dagger(x)\sigma^{\pm}\psi(x) \ . \tag{4}$$

$S^\dagger$ describes a spin-flip process in which a down spin is flipped into an up spin, S^- the reverse process, and σ is the Pauli matrix with

$$\sigma^{\pm}=\sigma_x\pm i\sigma_y \ . \tag{5}$$

Using Wick's theorem and Feynman diagram technique, it is readily verified that all diagrams with more than one bubble have no contributions to the correlation function, that means, the correlation function is related to the proper polarization only by

$$D^{+-}(\mathbf{x}\tau,\mathbf{x}'\tau')=\hbar\Pi^*_{\uparrow\downarrow\downarrow\uparrow}(\mathbf{x}\tau,\mathbf{x}'\tau')\,|_{\text{single bubble}} \ . \tag{6}$$

The latter is obtained by summing up a set of Feynman diagrams shown in Fig. 1, in which we have labeled the right and left particle lines of each diagram with up and down spin indices, respectively, realizing the fact that the spin of each particle is unchanged in scattering.

Evidently, the accuracy of the final result of the correlation function depends entirely on the approximation made in the calculation of the polarization. As a primary approximation, we let $\Pi^*_{\uparrow\downarrow\downarrow\uparrow}\,|_{\text{single bubble}}\approx\Pi^0_{\uparrow\downarrow\downarrow\uparrow}$ (see Fig. 2 for diagramatic representation) and evaluate the basic bubble diagram using the self-consistent Hartree-Fock approximation (SCHFA) Green's function

$$\mathcal{G}_{\alpha\beta}(\mathbf{x},\mathbf{x}';\omega_n)=\delta_{\alpha\beta}\sum_K\frac{\psi_K(\mathbf{x})\psi_K^*(\mathbf{x}')}{i\omega_n-\hbar^{-1}(\varepsilon_{K\alpha}-\mu)} \tag{7}$$

in which

$$\varepsilon_{K\alpha}=\varepsilon_K-\sum_{K'}V(\mathbf{K}-\mathbf{K}')n_{K'\alpha}/V \ . \tag{8}$$

Some straightforward calculations lead to the following form of the polarization in the space-momentum mixed representation:

$$\Pi^0_{\uparrow\downarrow\downarrow\uparrow}(\mathbf{q},\omega_n;z,z')=\frac{1}{A}\sum_{\substack{k_{\perp1},k_{\perp2}\\ p}}\frac{n_{p,k_{\perp1}\uparrow}-n_{p+q,k_{\perp2}\downarrow}}{i\hbar\omega_n-(\varepsilon_{p+q,k_{\perp2}\downarrow}-\varepsilon_{p,k_{\perp1}\uparrow})}\xi_{k_{\perp1}}(z')\xi^*_{k_{\perp1}}(z)\xi_{k_{\perp2}}(z)\xi^*_{k_{\perp2}}(z') \ . \tag{9}$$

Since $\phi(z-ld)$ is highly localized near the lth layer, the system has the superlattice periodicity of supercell d in the z direction, Eq. (9) can further be transferred to the whole momentum space. After introducing the form factor

$$F(q_\perp)=\int dz\, e^{-iq_\perp z}\,|\phi(z)|^2 \ ,$$

we obtain

$$\Pi^0_{\uparrow\downarrow\downarrow\uparrow}(\mathbf{Q},\omega_n)=\frac{|F(q_\perp)|^2}{V}\sum_P\frac{n_{P\uparrow}-n_{P+Q\downarrow}}{ik\omega_n-(\varepsilon_{P+Q\downarrow}-\varepsilon_{P\uparrow})} \ . \tag{10}$$

As a result, the retarded correlation function has the following simple form:

$$D_R^{+-}(\mathbf{Q},\omega)=\frac{\hbar|F(q_\perp)|^2}{V}\sum_K\frac{n_{K\uparrow}-n_{K+Q\downarrow}}{\hbar\omega-(\varepsilon_{K+Q\downarrow}-\varepsilon_{K\uparrow})} \ . \tag{11}$$

This is precisely the result of the well-known Stoner theory. It gives the Stoner excitations of electron-hole pairs with opposite spins,

$$\hbar\omega=\varepsilon_{K+Q}-\varepsilon_K+\sum_{K'}V(\mathbf{K}-\mathbf{K}')(n_{K'\uparrow}-n_{K'+Q\downarrow})/V \ . \tag{12}$$

The details on these single-particle–like excitations will be examined in the next section.

Equation (11) may be further simplified if the only noninteracting electron gas is concerned. It then becomes,

$$D_R^{+-}(\mathbf{Q},\omega)=\frac{\hbar}{V}\sum_K\frac{n_K-n_{K+Q}}{\hbar\omega-(\varepsilon_{K+Q}-\varepsilon_K)} \ . \tag{13}$$

On this occasion, it is easy to find that the superlattice affects the Stoner excitations only through the anisotropic electronic dispersion [Eq. (2b)].

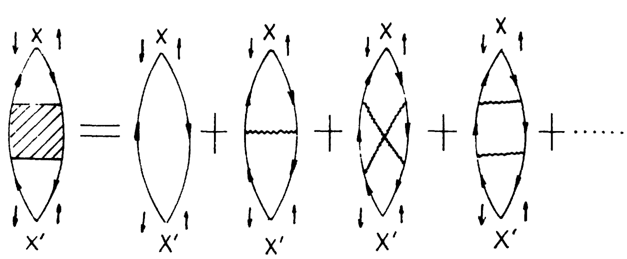

FIG. 1. Diagrams illustrating the single-bubble polarization.

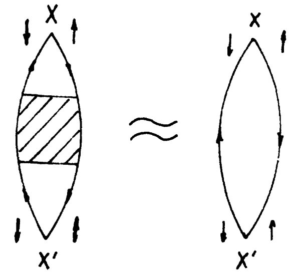

FIG. 2. The lowest approximation of the polarization.

Since the Stoner theory of the itinerant electron magnetism has ignored the correlation among the electrons, we have to go beyond the HFA by taking into account the scattering of electron-hole pairs due to the exchange interaction, so as to search for the information on the collective excitations. A realistic procedure in this direction is to choose a reasonable series of proper polarization insertions, such as those shown in Fig. 3, which, according to Hedin,[12] is a good approximation for the metallic densities.

Again, we incorporate the exchange self-energy contribution by using a SCHF $\mathcal{G}$ instead of $\mathcal{G}^0$ for the propagator, then following the preceding procedures that deduced Π^0, we finally obtain

$$D_R^{+-}(\mathbf{Q},\omega)=\frac{\hbar\,|F(q_\perp)|^2}{V}\sum_{P_1}\mathcal{A}(\mathbf{P}_1)X(\mathbf{P}_1)\;, \tag{14a}$$

where $X(\mathbf{P})$ satisfies an iterative equation

$$X(\mathbf{P})=1-\sum_{P'}V(\mathbf{P}-\mathbf{P}')\mathcal{A}(\mathbf{P}')X(\mathbf{P}')/V\;, \tag{14b}$$

$$\mathcal{A}(\mathbf{P})=\frac{n_{P\uparrow}-n_{P+Q\downarrow}}{\hbar\omega-(\varepsilon_{P+Q\downarrow}-\varepsilon_{P\uparrow})}\;. \tag{14c}$$

It is clear that the correlation function can be evaluated in a number of ways (as in Refs. 6 and 11, for instance). In this paper, we use so-called generalized Hubbard approximation to solve the problem analytically.

In the Hubbard approximation,[11] the factor $V(\mathbf{P}-\mathbf{P}')$ in the summation is replaced by a screened potential $G(\mathbf{Q})V(\mathbf{Q})$, with $G(\mathbf{Q})$ being the screening factor. By a generalized Hubbard approximation, we assume that the screening effects act only in the 2D charge layer planes. Supposing that $G(\mathbf{q})$ takes the following form:[13,14]

$$G(\mathbf{q})=\frac{q}{q+q_s}\;, \tag{15}$$

where q_s is an appropriate screening wave number, we can then solve the problem [Eq. (14)] exactly. The solution reads

$$D_R^{+-}(\mathbf{Q},\omega)=\frac{\hbar\,|F(q_\perp)|^2}{V}\times\sum_{P}\mathcal{A}(\mathbf{p})\left[1+\frac{G(\mathbf{q})V(\mathbf{Q})}{V}\sum_{P'}\mathcal{A}(\mathbf{p}')\right]^{-1}\;. \tag{16}$$

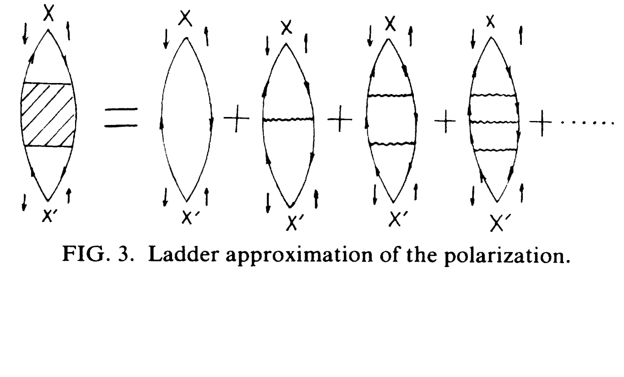

FIG. 3. Ladder approximation of the polarization.

We note that if the screened potential is replaced by a constant effective Coulomb potential, Eq. (16) reduces to the usual RPA results.[15] By introducing the screened potential more explicitly, we attempt to examine how the superlattice structure affects the spin-density fluctuations of the system.

III. SPIN EXCITATIONS OF THE SYSTEM

The excitation spectrum of the system is described by the poles of the correlation function, we then get from Eq. (16),

$$1+\frac{G(q)V(Q)}{V}\sum_{K}\frac{n_{K\uparrow}-n_{K+Q\downarrow}}{\hbar\omega-(\varepsilon_{K+Q\downarrow}-\varepsilon_{K\uparrow})}=0\;. \tag{17}$$

This equation has solutions corresponding to individual modes (or the Stoner excitations) as well as the spin wave modes, as illustrated in Fig. 4.

For the single-particle–like excitations, we have a continuous spectra which lie in the long wavelength limit between

$$E_{\max}=2mG(\mathbf{q})V(\mathbf{Q})+\frac{\hbar^2k_{F\uparrow}Q}{m_e}+\frac{\hbar^2Q^2}{2m_e}\;, \tag{18a}$$

$$E_{\min}=2mG(\mathbf{q})V(\mathbf{Q})-\frac{\hbar^2k_{F\uparrow}Q}{m_e}+\frac{\hbar^2Q^2}{2m_e}\;, \tag{18b}$$

where $m=(n_\uparrow-n_\downarrow)/2$ is the spin density, and an isotropic dispersion other than Eq. (2b) has been assumed for simplicity.[16]

It follows from Eq. (18) that the Stoner gap of the single-particular-like excitations depends on the details of the screened potential. It is thereby a structure-dependent quantity, and the modulation properties of the superlattices should be reflected in the spectra of the Stoner excitations. In the following, we extend our discussions for the two extreme cases.

The first case we are concerned with is the so-called

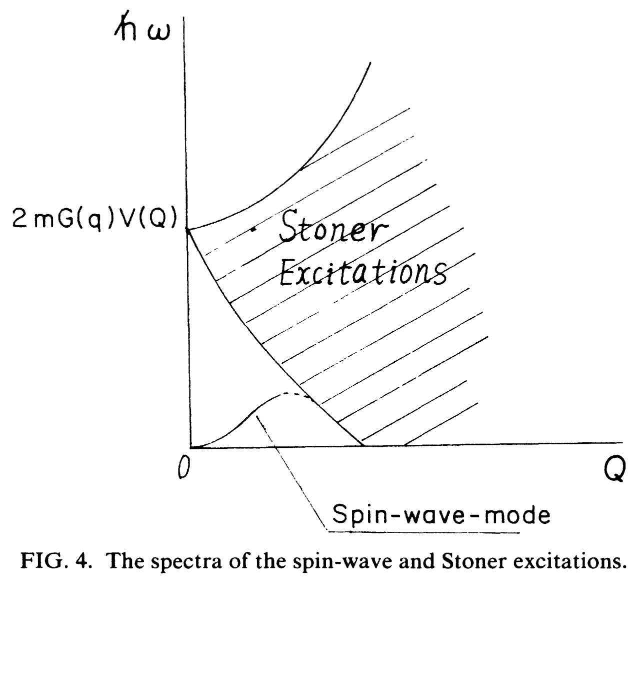

FIG. 4. The spectra of the spin-wave and Stoner excitations.

weak-coupling limit ($qd \gg 1$), taking $qd \to \infty$ limit of $V(\mathbf{Q})$ immediately gives

$$V(\mathbf{Q}) = 2\pi e^2 d/q \ . \tag{19}$$

The single-particle-like excitation energy then approaches gradually that for the 2D electron gas,

$$\hbar\omega = \frac{4\pi m e^2 d}{q} G(\mathbf{q}) + \frac{\hbar^2}{2m_e}(q^2 + 2\mathbf{k}\cdot\mathbf{q}) \ , \tag{20}$$

that is, each layer supports independently its own 2D excitations in this case.

In the opposite limit ($qd \ll 1$), however, the system behaves like a 3D electron gas. For $q_\perp = 0$, we have

$$V(\mathbf{q}) = 4\pi e^2/q^2 \tag{21}$$

and

$$\hbar\omega = \frac{8\pi m e^2}{q^2} G(\mathbf{q}) + \frac{\hbar^2}{2m_e}(q^2 + 2\mathbf{k}\cdot\mathbf{q}) \ . \tag{22}$$

But for $q_\perp \neq 0$, the Coulomb potential becomes

$$V(q_\perp) = \frac{2\pi e^2 d^2}{1 - \cos(q_\perp d)} \ , \tag{23}$$

and the excitation energy becomes

$$\hbar\omega = \frac{4\pi m e^2 d^2}{1 - \cos(q_\perp d)} G(\mathbf{q}) + 2T[\cos(k_\perp + q_\perp)d - \cos(k_\perp d)] \ , \tag{24}$$

which shows precisely the 1D character for the suggested screened potential. All of these results confirm that the Stoner excitations in the superlattice reveal the crossover behavior as the coupling strength varies. Moreover, the Stoner gap is always influenced by the anisotropic screenings as indicated in Eqs. (20), (22) and (24) on which we will make more comments when we deal with the spin-wave excitations.

There are no Stoner excitations for small Q and ω, satisfying the condition"[17,18]

$$2mG(\mathbf{Q})V(\mathbf{Q}) \gg |\varepsilon_{K+Q} - \varepsilon_K|; \hbar\omega \ . \tag{25}$$

With this prerequisite, we finally get the spin-wave spectrum:

$$\hbar\omega = \frac{1}{2mV}\left[\sum_K \frac{n_{K\uparrow} + n_{K\downarrow}}{2}(\mathbf{Q}\cdot\nabla)^2 \varepsilon_K - \frac{1}{2mG(\mathbf{q})V(\mathbf{Q})}\sum_K (n_{K\uparrow} - n_{K\downarrow})(\mathbf{Q}\cdot\nabla\varepsilon_K)^2\right] \ . \tag{26}$$

For the dispersion relation given in Eq. (2b), the spectrum becomes

$$\hbar\omega = \frac{1}{2mV}\left[\sum_K n_K \left[\frac{\hbar^2 q^2}{2m_e} - Tq_\perp^2 d^2 \cos(k_\perp d)\right] - \frac{1}{2mG(\mathbf{q})V(\mathbf{Q})}\sum_K (n_{K\uparrow} - n_{K\downarrow})\left[\frac{\hbar^4 k^2 q^2}{2m_e^2} + 4T^2 q_\perp^2 d^2 \sin^2(k_\perp d)\right]\right] \ . \tag{27}$$

The results show clearly the dependence of the spin waves on the supporting periodic structure. It changes from two- to three-dimensional behavior as the coupling between adjacent layers is increased by decreasing the parameter qd.

In the particular $q_\perp = 0$ case, the interlayer Coulomb interaction becomes extremely large compared with the intralayer interaction in the strong-coupling limit ($qd \to 0$). As a consequence, the Stoner gap approaches infinity, and the spin waves dominate the spin excitations of the system. From Eq. (27), we further realize that

$$\hbar\omega = \frac{\sum_K n_K}{m} \frac{\hbar^2 q^2}{2m_e} \ .$$

The spin waves are determined entirely by the additional kinetic energy the electrons develop as they correlate together to form the spin waves; they travel isotropically in the charge layer, being the same as that for 3D strongly interacting electron gases.

A sharp contrast to this situation is the weak-coupling limit ($qd \gg 1$), where the system behaves then as if it were two-dimensional except for the possible tunneling (since $q_\perp$ is arbitrary). In addition, the 2D screened potential makes the Stoner excitations not impossible even in the long-wave limit [see Eq. (20)], which consequently reduces the spin-wave energy by a finite quantity just as Eq. (27) indicates. It is also shown that the spin-wave stiffness in this case is always highly anisotropic no matter what value $q_\perp$ takes.

An important fact we should note is that all the conclusions obtained so far about spin waves are based on the prerequisite Eq. (25). This condition cannot be satisfied for the nonzero $q_\perp$ situation in the strong-coupling limit, since the screened potential and hence the Stoner gap then linearly approach zero at the same speed as $\varepsilon_K(Q) = \varepsilon_{K+Q} - \varepsilon_K$ does. Therefore, Eq. (27) and the relevant conclusions on the spin waves are not suited to this situation. But fortunately, it may be verified that the system cannot support stable spin-wave excitations in this situation, we are thus convinced that Eq. (27) covers all the possible spin-wave modes of the layered ferromagnetic electron gases.

IV. SUMMARY

We have studied in this paper theoretically the spin excitations of a periodic array of layered electron gas in the ferromagnetic phase. The results clearly show the captivating change in dimensionality of the systems from two- to three-dimensional behavior as the coupling between the layers is increased. In the weak-coupling

($qd \gg 1$) limit and the strong-coupling situation ($qd \ll 1$) with $q_\perp = 0$, the band splitting of the Stoner excitations increases as $q \rightarrow 0$, showing a two- and three-dimensional behavior, respectively. The system therefore supports stable collective modes spin wave below the continuous spectra of the single excitations. On the contrary, in the particular $q_\perp \neq 0$ and $qd \rightarrow 0$ case, the screened Coulomb potential lower the Stoner gap to zero due to the screen anisotropy we presupposed. The collective modes are then highly damped and decay into the continuum of the Stoner excitations.

Different from Gasser,[6] we make it clear that the anisotropic stiffness of the existing spin waves is dependent not only on the anisotropic electronic dispersion, but on the screened Coulomb potential as well. Furthermore, we have pointed out that the screen anisotropy even affects the existence of the spin waves in some cases.

Experimentally, the charge-density excitations of layered electron gases have been reported by inelastic light scattering.[4,5] Similar explorations are also expected in order to get a better understanding of the spin excitations of such systems.

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