Magnetorotons in quasi-one-dimensional electron systems in the absence of Kohn's theorem

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Using a time-dependent Hartree-Fock approximation we have investigated the inter-Landau-level collective excitation spectrum of quasi-one-dimensional electron gases where Kohn's theorem is violated. We find that the spectrum develops a *roton minimum* at finite wave vectors. In addition to the main magnetoroton, *extra* collective modes are found. Also we find that it is important to include both the Hartree and exchange local-field corrections in a calculation of the cyclotron resonance.

A magnetoroton minimum exists in intra-Landau-level collective excitations of the fractional quantum Hall effect (FQHE) state[1] and in inter-Landau-level collective excitations of quasi-two-dimensional (Q2D) (Ref. 2) and quasi-three-dimensional (Q3D) (Ref. 3) electron gases. The magnetoplasmon dispersion displays a roton minimum around a wave vector $q \sim 1/r_0$ when the pair-correlation function is strongly peaked near the mean particle distance r_0. A roton minimum has been observed[3] in the dispersion relation of inter-Landau-level collective excitations of a Q3D electron gas in a wide parabolic quantum well. In the FQHE state and in Q2D electron gases Raman scattering experiments[4] have been interpreted as showing the existence of a roton minimum.

Recent advances in semiconductor fabrication techniques have made possible the growth of quasi-one-dimensional (Q1D) electron systems in the quantum limit[5] where only one subband is occupied. In particular, cleaved edge overgrowth[6] may be used to grow periodically modulated Q1D electron wires with a period of order 100 Å. The experimental investigation of magnetorotons in Q1D gases has thus become a relevant issue.

It has not been established theoretically whether many-body correlations in Q1D electron gases can give rise to magnetorotons. Furthermore, our understanding of the inter-Landau-level collective excitations in quantum wires has been quite limited in situations where Kohn's theorem[7] is violated.[8] We have investigated this problem in large magnetic fields using a time-dependent Hartree-Fock approximation with a parabolic Hartree-Fock self-consistent (HFSC) lateral confinement potential. In the presence of a parabolic HFSC potential Kohn's theorem is violated, in contrast to the case[7] of a parabolic *bare* lateral confinement potential. In our work we have used normal Fermi-liquid theory because finite temperature and impurity scattering[9] effects suppress instabilities toward broken symmetry states and Tomonaga-Luttinger liquid behavior. A Fermi-liquid picture is also supported by recent experimental investigations in Q1D wires.[5] Our main results are as follows. We find, using finite-temperature Fermi-liquid theory, that the inter-Landau-level collective modes develop a *roton minimum* at finite wave vectors. As a consequence of the violation of Kohn's theorem, *extra* collective modes are found in addition to the main magnetoroton mode. In addition, we find in the presence of local exchange (excitonic) and Hartree (depolarization) fields that the collective excitation energies lie below the single pair excitation energies.

Our model Hartree-Fock (HF) Hamiltonian is

$$H_{\rm HF}=-\frac{\hbar^2}{2m}\nabla^2-i\hbar\omega_c x\frac{\partial}{\partial y}+\frac{1}{2}m(\omega_c^2+\omega_0^2)x^2\ , \tag{1}$$

where the HFSC lateral potential is taken to be parabolic $1/2m\omega_0^2x^2$. Here ω_c and m are the cyclotron frequency and electron effective mass. The wire extends along the y axis and the Landau gauge $A=(0,Hx,0)$ is used (magnetic field along z axis). The advantage of this model Hamiltonian is that the eigenstates and eigenenergies of $H_{\rm HF}$ can be found exactly[10]

$$\begin{aligned}&\Psi_{n,k}(\mathbf{r})=\Phi_n(x-R^2k)e^{iky}\delta(z)\ ,\\ &\epsilon_n(k)=(n+\tfrac{1}{2})\hbar\Omega+\frac{\hbar^2}{2m}\left[\frac{\omega_0}{\Omega}\right]^2k^2\ ,\end{aligned} \tag{2}$$

where $\Omega=(\omega_c^2+\omega_0^2)^{1/2}$, $R^2=\hbar\omega_c/(m\Omega^2)$, and Φ_n are the wave functions of a harmonic oscillator with characteristic frequency Ω[the magnetic length is $l=(\hbar/m\Omega)^{1/2}$]. The quantity ω_0 is to be chosen such that the true HF energy separation[11] between the first and second subbands is given by $\hbar\Omega$. The density for either spin can be expressed as

$$\rho(\mathbf{r})=\sum_{m,k,m',k'}\Psi^*_{m',k'}(\mathbf{r})\Psi_{m,k}(\mathbf{r})\rho_{m,k;m',k'}\ . \tag{3}$$

In the presence of an external time-potential $V_{\rm ext}(y,t)=V_{\rm ext}e^{i(Qy-\omega t)}$, the time evolution of the change in $\rho_{n,k+Q;m,k}$ is given by

$$\begin{aligned}\delta\rho_{n,k+Q;m,k}=&\frac{f_n(k+Q)-f_m(k)}{\epsilon_n(k+Q)-\epsilon_m(k)-\hbar\omega-i\gamma}\\ &\times\langle n,k+Q|\delta H_{\rm HF}|m,k\rangle\ ,\end{aligned} \tag{4}$$

where γ is a linewidth and $f_m(k)$ is the Fermi function. Here the common factor $e^{-i\omega t}$ has been canceled. In the absence of spin splitting the change in $H_{\rm HF}$ induced by the external time-dependent potential is given by

$$\langle n,k+Q|\delta H_{\rm HF}|m,k\rangle = V_{\rm ext}\langle n,k+Q|e^{iQy}|m,k\rangle + \sum_{m',n',k'}[2\langle n,k+Q;m',k'|V|m,k;n',k'+Q\rangle - \langle n,k+Q;m',k'|V|n',k'+Q;m,k\rangle]\delta\rho_{n',k'+Q;m',k'}\ , \tag{5}$$

where the first (second) term in the summation is the Hartree (exchange) local-field correction. The Coulomb matrix elements are given by

$$\langle n_1,k_1;n_2,k_2|V|n_3,k_3;n_4,k_4\rangle = \frac{1}{A}2\pi\delta(k_4+k_3-k_2-k_1)\int_{-\infty}^{\infty}\frac{dq_x}{2\pi}\frac{2\pi e^2}{\epsilon[q_x^2+(k_1-k_3)^2]^{1/2}} \times\exp[iq_x(k_1-k_4)R^2]F_{n_1,n_3}(q_x,k_1-k_3)F_{n_2,n_4}(-q_x,-k_1+k_3) \tag{6}$$

and

$$F_{n,m}(q_x,q_y)=F_{n,m}(\mathbf{q})=\left[\frac{m!}{n!}\right]^{1/2}\left[\frac{(-q_y+iq_x)l}{\sqrt{2}}\right]^{n-m}\exp\left[-\frac{q^2l^2}{4}\right]L_m^{n-m}\left[\frac{q^2l^2}{2}\right] \tag{7}$$

for $n>m$ [one can use $F_{m,n}(\mathbf{q})=F^*_{n,m}(-\mathbf{q})$ for $n<m$]. A is the area of the xy plane on which the electrons reside, ϵ is the background dielectric constant, and L_m^n is a Laguerre polynomial. $\delta\rho_{n,k+Q;m,k}$ satisfies the equation

$$\sum_{m',n',k'}K_{m,n,k;m',n',k'}(Q)\delta\rho_{n',k'+Q;m',k'}=[f_n(k+Q)-f_m(k)]\langle n,k+Q|e^{iQy}|m,k\rangle V_{\rm ext}\ , \tag{8}$$

where the kernel is

$$K_{m,n,k;m',n',k'}(Q)=[\epsilon_n(k+Q)-\epsilon_m(k)-\hbar\omega-i\gamma]\delta_{nn'}\delta_{mm'}\delta_{kk'} - [f_n(k+Q)-f_m(k)][2\langle n,k+Q;m',k'|V|m,k;n',k'+Q\rangle - \langle n,k+Q;m',k'|V|n',k'+Q;m,k\rangle\ . \tag{9}$$

The sum in Eq. (8) is over indices such that $f_n(k+Q)-f_m(k)\neq 0$. Due to the exchange contribution the kernel of this integral equation is found to be *singular* when $k=k'$. This singularity can be treated using the modified quadrature method.[12] The response function for either spin can be found from

$$\delta\rho(Q)=\frac{1}{A}\sum_{m',n',k'}\delta\rho_{n',k'+Q;m',k'}\langle n',k'|e^{-iQy}|m',k'+Q\rangle = \chi(Q,\omega)V_{\rm ext}\ , \tag{10}$$

which yields

$$\chi(Q,\omega)=\frac{1}{A}\sum_{m,n,k}\sum_{m',n',k'}[K]^{-1}_{m,n,k;m',n',k'}(Q)[f_{n'}(k'+Q)-f_{m'}(k')]\langle n',k'+Q|e^{iQy}|m',k'\rangle\langle n,k|e^{-iQy}|m,k+Q\rangle\ . \tag{11}$$

In large magnetic fields, where the Landau-level separation $\hbar\Omega$ is large compared to the characteristic Coulomb energy, inter-Landau-level excitations may be investigated by restricting Landau-level indices to $(m,n)=(0,1)$. This implies that the excitations in the lowest Landau level may be ignored (note that in the 2D case with partially filled Landau levels this approximation fails due to the singular density of states). In the strong-field limit the numerically calculated $\mathrm{Im}\chi$ obeys the f-sum rule. Figure 1(a) shows $\log_{10}[-\mathrm{Im}\chi]$ as a function of energy $\hbar\omega$ for different values of Q with $\hbar\omega_0=1$ meV and at a temperature $k_BT\ll E_F$. We see that as Q varies the main peak for each Q traces out a magnetoroton dispersion relation $\omega(Q)$. The presence of several weaker collective modes beside the main peak can be attributed to the violation of Kohn's theorem; excitations other than the center-of-mass modes become visible. Figure 2(a) shows, for each value of Q, the two largest peak values from Fig. 1(a). The magnetoroton dispersion relation is clearly visible with a minimum at $Ql\sim 2.3$. As an indication of temperature effects we show in Fig. 2(b) a dispersion curve for $k_BT=E_F$ with all other parameters unchanged (strictly speaking, in the Hartree-Fock-approximation ω_0 should depend on temperature). We observe that the roton dip has decreased somewhat at the higher temperature but qualitatively the dispersion rela-

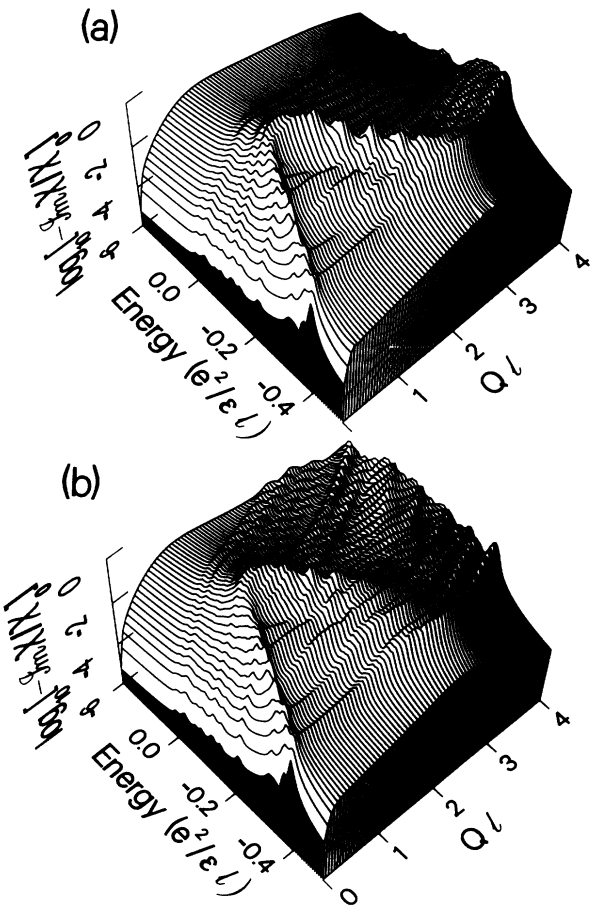

FIG. 1. Plot of $\log_{10}[-\mathrm{Im}\chi/\chi_0]$ as a function of Ql and energy $\hbar\omega$ for (a) $\hbar\omega_0=1$ meV, and (b) $\hbar\omega_0=2$ meV ($\chi_0=1$ $\mathrm{eV}^{-1}\mathrm{\AA}^{-1}$). The other parameters are $\gamma=0.1$ meV, $B=10$ T, $k_BT\ll E_F$, and $N=1.3\times10^6$ cm^{-1} (the Fermi energy E_F is in the lowest Landau level). We have subtracted $\hbar\Omega$ from the energies for the sake of clarity. In this plot the smallest value shown for Ql is greater than zero.

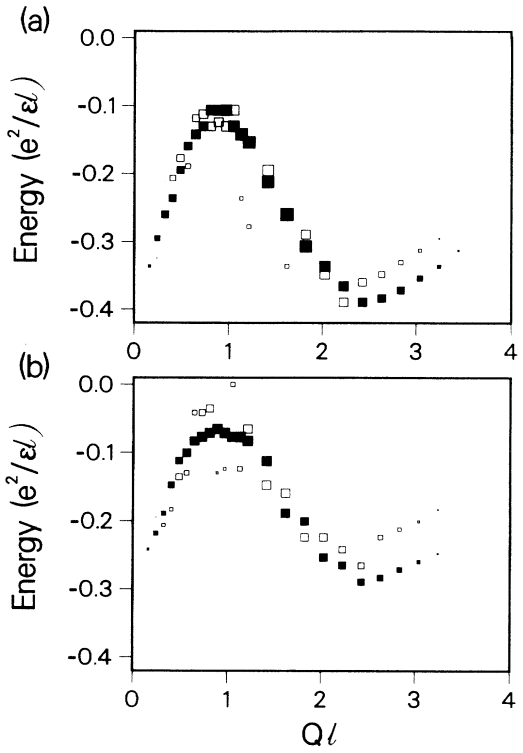

FIG. 2. (a) Plot of the two largest peak values from Fig. 1(a) at each value of Q. The largest and second largest peaks in $-\mathrm{Im}\chi$ are shown respectively as filled and open squares. The size of each square is proportional to $\log_{10}[-\mathrm{Im}\chi/\chi_0]$. All other modes in Fig. 1(a) have much smaller χ compared to those shown. (b) Same as in (a) but with $k_BT=E_F$.

tion remains the same.

The single pair excitations of a 1D wire form a quasicontinuum band in the absence of Coulomb (Hartree and exchange) interactions. For a given Q the bandwidth is given by $W=4E_F(\omega_0/\Omega)^2(Q/k_F)$, where the Fermi wave vector $k_F=N\pi$. In the presence of Coulomb interactions the single pair continuum becomes ill defined. However, for the case shown here, the states that are the most "single-particle-like" occupy a fairly narrow band with very small $-\mathrm{Im}\chi$ near the top of the broad band of states in Fig. 1(a) ($\approx -0.1e^2/\epsilon l$) and are thus not easily distinguished in this representation compared to the modes that are more collective in nature. When this single-particle-like band is broadened, e.g., by increasing ω_0, the single particle and collective modes are even more strongly mixed and it becomes increasingly more difficult to define a clear-cut magnetoroton dispersion. This broadening effect, which is illustrated in Fig. 1(b) for $\hbar\omega_0=2$ meV, can be countered by increasing the magnetic field as can be seen from the expression for W above. It should be noted that we find the collective modes to lie *above* the single pair excitations in the presence of Hartree local fields; it is only when exchange local fields are included that the collective modes lie *below* the single pair excitations. The magnitude of the cyclotron energy can thus be computed correctly only when the exchange local-field corrections are included. Note that in Q2D magnetoplasmas there is no depolarization shift since the Hartree local-field correction at $Q=0$ is zero, in contrast to our Q1D system. In the present work we have ignored finite thickness effects along the z axis, but they may be included by inserting a form factor in the Coulomb matrix elements.

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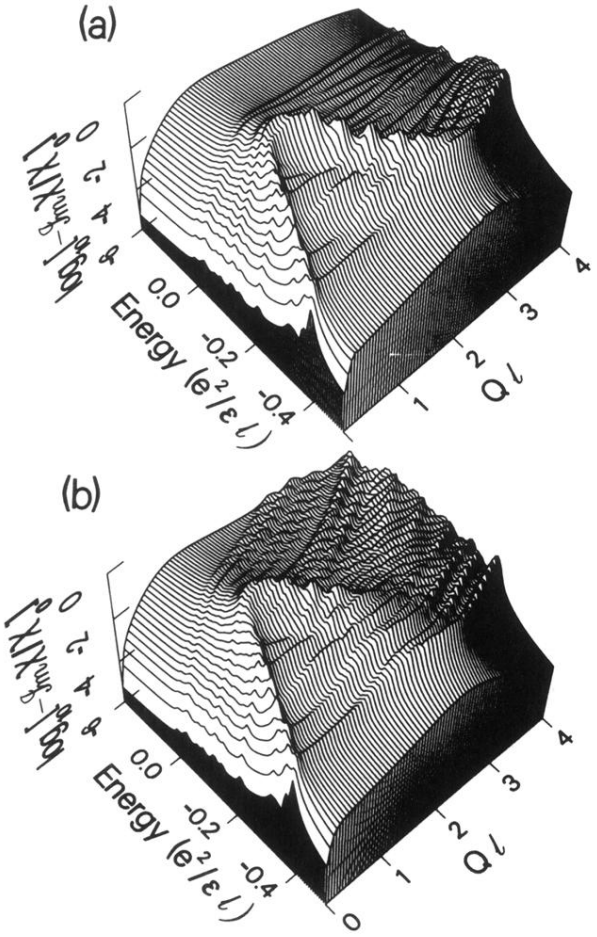

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