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Response function of a two-dimensional electron gas in a unidirectional periodic potential

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The dynamical density-response function of a periodically modulated two-dimensional electron gas under a perpendicular magnetic field is calculated within the random-phase approximation. It is found that the response function is not only broadened by the periodic potential, it also contains a series of subsingularities at the band edges. The maximum number of subsingularities is $2n_{\max}$, where $n_{\max}$ is the number of occupied Landau levels (the last level may be partially filled). It is further proposed that light-scattering or electromagnetic absorption experiments can be performed to study these predicted structures.

A two-dimensional electron gas (2DEG) in a magnetic field can exhibit many physical phenomena of fundamental importance and interest, such as the integer and fractional quantum Hall effects[1,2] and various kinds of magnetic quantum oscillations in the optical and transport coefficients. If the system is further subjected to an additional periodic potential, even richer information can be revealed in the energy spectra and the density of states. This additional periodic potential broadens, in a nonuniform way, the original infinitely sharp Landau levels (LL's) into so-called Landau bands. Both the bandwidths and the maxima of the density of states of the Landau bands are oscillatory functions of the applied magnetic field and the periodicity of the modulation potential.[3] Two van Hove singularities (inverse-square-root divergence) appear at the band edges. This oscillation in the density of states (both in width and in height) leads to the observed additional oscillation in dc magnetotransport,[4–6] in magnetocapacitance,[7] and in magnetoplasmon dispersion.[8,9] Such additional oscillations are often referred to as commensurability oscillations owing to the fact that they are natural consequences of the interplay of two different length scales: the magnetic length ($l=\sqrt{\hbar/eB}$) and the periodicity of the modulation potential (a). Although the commensurability oscillations in the static limit have been extensively studied,[3–13] the dynamical properties of this interesting system have yet to be studied.

In this paper, we shall present a first-principles calculation of the response function for a spatially modulated electronic system within the random-phase approximation (RPA). Our primary task is to evaluate the following quantity ($T=0$):

$$\mathrm{Im}\left[\frac{1}{\epsilon(q,\omega)}\right]=\frac{2\pi^2e^2}{q}\int dt e^{i\omega t}\langle n(\mathbf{q},t)n(-\mathbf{q},0)\rangle, \tag{1}$$

where $\epsilon(q,\omega)$ is the frequency- and wave-number-dependent dielectric-response function and $n(\mathbf{q},t)$ is the density operator. In the absence of a modulation potential and other disorders, the density response contains only contributions from the magnetoplasmon excitation, i.e., $\mathrm{Im}[1/\epsilon(q,\omega)]\sim\delta(\omega-\omega_{\mathrm{mp}})$ where ω_{mp} is the frequency of the magnetoplasmon. The application of the modulation potential broadens the spectrum and reintroduces the particle-hole excitation into the density-response function. The main purpose of this work is to obtain a qualitative and quantitative knowledge of these particle-hole excitations.

While it is known that under a one-dimensional periodic potential the density of states have two van Hove singularities at the band edges, it is not known whether the dynamical properties of these systems, such as the light-scattering cross section and electromagnetic absorption, will exhibit this double singularity feature. In what follows we shall show that the response function has a much more complex structure under a modulation potential. It contains previously unreported subsingularities (fine structure) at the band edges. The number of singularities at each band edge varies in an increasing even sequential order, starting at the resonance frequency, from four (or two for integer filling factors) to a maximum of $n_{\max}$, where $n_{\max}$ is the number of occupied LL's. We further predict that such fine structure can be revealed in light-scattering or electromagnetic absorption measurements.

The Hamiltonian of the system, when the Landau gauge is chosen, can be written as

$$H=\frac{1}{2m_b}\left[-\hbar^2\frac{d^2}{dx^2}+\left(\frac{\hbar}{i}\frac{d}{dy}+\frac{e}{c}Bx\right)^2\right]+V_0\cos(Kx), \tag{2}$$

where V_0 is the amplitude of the modulation potential, m_b is the static electron effective band mass, and $K=2\pi/a$. The single-electron eigenfunctions are of the form $\psi_{nk}(x,y)\propto\exp(ik_yy)\phi_{nx_0}(x)$ where $x_0=k_yl^2$ is the center coordinate and $\phi_{nx_0}(x)$ is the eigenfunction of the one-dimensional Hamiltonian

$$H_{x_0}=-\frac{\hbar^2}{2m_b}\frac{d^2}{dx^2}+\frac{1}{2}m\omega_c^2(x-x_0)^2+V_0\cos(Kx) \tag{3}$$

with eigenvalue $E_n(x_0)$. In the following, we shall treat the modulation potential within first-order perturbation theory to calculate the energy spectrum $E_n(x_0)$:

$$E_n(x_0)=E_n^{(0)}+E_n^{(1)}=\varepsilon_n+U_n\cos(Kx_0), \tag{4}$$

where $\varepsilon_n=(n+1/2)\hbar\omega_c$, $U_n=V_0\exp(-\mathscr{X}/2)L_n(\mathscr{X})$, $\mathscr{X}=(Kl)^2/2$, and $L_n(\mathscr{X})$ is a Laguerre polynomial. This is a reasonable approximation to use provided the cyclotron energy is not too small.[6]

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Within the random-phase approximation, the dielectric-response function is given as

$$\epsilon(q,\omega)=1+2\pi r_s\frac{k_F}{q}\hbar\omega_c \times\sum_{n\geq n'}\sum_{x_0} C_{nn'}\left[\frac{f_{n,x_0}-f_{n',x_0+x_0'}}{E_{n,x_0}-E_{n',x_0+x_0'}+\hbar\omega}+\frac{f_{n,x_0}-f_{n',x_0+x_0'}}{E_{n,x_0}-E_{n',x_0+x_0'}-\hbar\omega}\right], \quad (5)$$

where k_F is the Fermi wave vector, $r_s=m_b e^2/(\hbar^2 k_F)$ is the plasma parameter, $\omega_c=eB/m_b$ is the cyclotron frequency, $x_0'=q_y l^2$, and f_{n,x_0} is the Fermi-Dirac distribution function. It should also be understood that ω means $\omega+i0$. The matrix element $C_{nn'}$ is given by $(n>n')$

$$C_{nn'}=(n'!/n!)X^{n-n'}e^{-X}[L_{n'}^{n-n'}(X)]^2$$

with $X=(ql)^2/2$ and $L_n^{(\alpha)}(X)$ is an associated Laguerre polynomial.

After separating the above equation into the real part and the imaginary part, the x_0 integration can be carried out. For the imaginary part, only those x_0 satisfying energy conservation (enforced by the δ function) contribute. For the real part, the principal-value integration is solved via a contour integral method. By choosing a new set of variables ($m=n-n',m'=n'$) we obtain

$$\begin{aligned}\mathrm{Re}\,[\epsilon(q,\omega)]=&1-4\pi^2 r_s(k_F/q)\,\omega_c\sum_{m=1}^{\infty}\sum_{m'=0}^{n_F+1}C_{m+m',m'}(f_{m+m',x_i}-f_{m',x_i+x_0'})\,\theta(1-1/|\zeta_1|)/(m\omega_c+\omega)\sqrt{1-1/\zeta_1^2}\\&-4\pi^2 r_s(k_F/q)\,\omega_c\sum_{m=1}^{\infty}\sum_{m'=0}^{n_F+1}C_{m+m',m'}(f_{m+m',x_j+x_0'}-f_{m',x_j})\,\theta(1-1/|\zeta_3|)/(m\omega_c-\omega)\sqrt{1-1/\zeta_3^2}\\&-4\pi^2 r_s(k_F/q)\,\omega_c\sum_{m'=0}^{n_F+1}e^{-X}[L_{m'}(X)]^2(f_{m',x_k}-f_{m',x_k+x_0'})\,\theta(1-1/|\zeta_5|)/\omega\sqrt{1-1/\zeta_5^2}\end{aligned} \quad (6)$$

and

$$\begin{aligned}\mathrm{Im}[\epsilon(q,\omega)]=&2\pi^2 r_s(k_F/q)\,\hbar\omega_c\sum_{m=1}^{\infty}\sum_{m'=0}^{n_F+1}C_{m+m',m'}(f_{m+m',x_i}-f_{m',x_i+x_0'})Q_{12}^{mm'}\\&-2\pi^2 r_s(k_F/q)\,\hbar\omega_c\sum_{m=1}^{\infty}\sum_{m'=0}^{n_F+1}C_{m+m',m'}(f_{m+m',x_j+x_0'}-f_{m',x_j})Q_{34}^{mm'}\\&+2\pi^2 r_s(k_F/q)\,\hbar\omega_c\sum_{m'=0}^{n_F+1}e^{-X}[L_{m'}(X)]^2(f_{m',x_k}-f_{m',x_k+x_0'})Q_{56}^{0m'}\,.\end{aligned} \quad (7)$$

Here

$$Q_{ij}^{mm'}=\frac{\theta(1-|\zeta_i|)}{|U_{m+m'}W_{ij}-U_{m'}\cos(Kx_0')W_{ij}-U_{m'}\sin(Kx_0')Z_{ij}|}$$

with $W_{ij}=\sqrt{(1-\zeta_i^2)/(1+\zeta_j^2)}-(\zeta_i\zeta_j)/\sqrt{1+\zeta_j^2}$, and $Z_{ij}=\zeta_i/\sqrt{1+\zeta_j^2}+\zeta_j\sqrt{(1-\zeta_i^2)/(1+\zeta_j^2)}$. The ζ_i's are given as

$$\zeta_1=\frac{m\hbar\omega_c+\hbar\omega}{\sqrt{U_{m+m'}^2-2U_{m+m'}U_{m'}\cos(Kx_0')+U_{m'}^2}}=-\zeta_3(-\omega),$$

$$\zeta_5=\hbar\omega/[2U_{m'}\sin(Kx_0'/2)],$$

$$\zeta_2=U_{m'}\sin(Kx_0')/[U_{m'}\cos(Kx_0')-U_{m+m'}]=\zeta_4|_{m'\leftrightarrow m'+m},$$

$$\zeta_6=\sin(Kx_0')/[\cos(Kx_0')-1].$$

In Eqs. (6) and (7), x_α (with $\alpha=i,j,k$) denotes the simple roots given by the equations $m\hbar\omega_c+U_{m+m'}\cos(Kx_\alpha)-U_{m'}\cos(Kx_\alpha+Kx_0')\pm\hbar\omega=0$, where the *plus* case corresponds to i and k (with $m=0$ for k only) and the *minus* case corresponds to j, while $\theta(x)$ is the Heaviside step function.

In all of the numerical calculations that are to follow, as an example we have employed the following parameters for a typical modulated GaAs/Al$_x$Ga$_{1-x}$As heterostructure, $\epsilon=13$, $r_s=0.73$, $E_F=10$ meV, and $m_b=0.067m_e$. The amplitude and period of the modulation potential are $V_0=1$ meV, $a=300$ nm. All calculations are done at zero temperature and with $q=0.2k_F$, $q_y=1\times10^6$ m^{-1}.

Figure 1 shows typical behavior for the imaginary part of the magnetic-field-dependent RPA dielectric function in a unidirectional periodic potential. For a sufficiently small modulation amplitude such that the Landau bands do not overlap, it can be clearly seen that the imaginary part consists of a series of individually isolated double-peak structures about the resonance frequency and each of its harmonics. New subsingularities (fine structure) at either side of the band edges of each main double-peak structure are also resolved. Here the infinities are an artifact of RPA that neglects any intrinsic broadening of the LL. In general, the number of singularities on *each side* of the frequency band is equal to

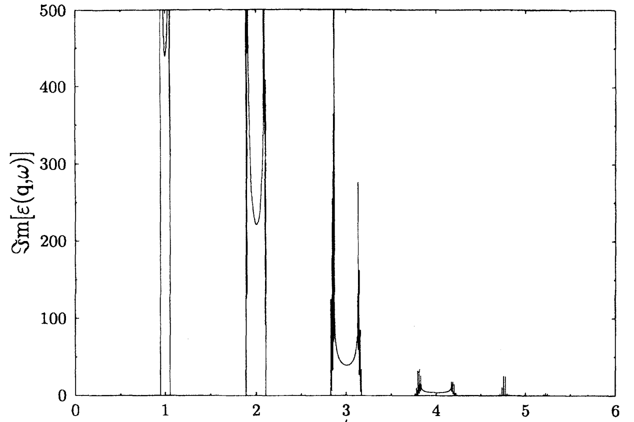

FIG. 1. Imaginary part of the magnetic-field-dependent RPA dielectric function in a unidirectional periodic potential as a function of ω/ω_c for $\nu=5.5$, $V_0=1$ meV, and $T=0$ K.

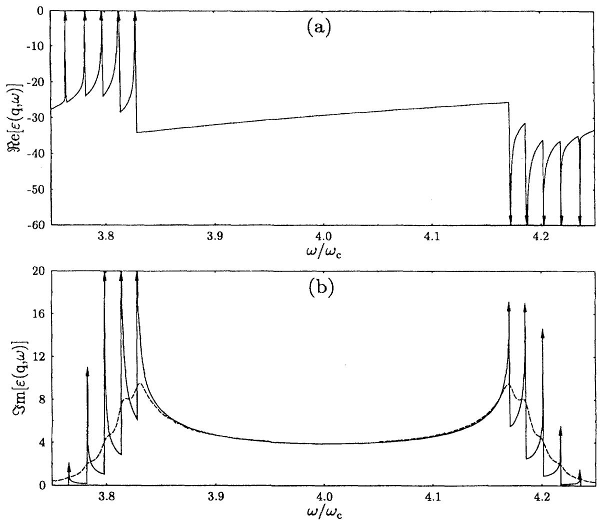

FIG. 3. The real part (a) and imaginary part (b) of the dielectric function around $\omega=4\omega_c$. All parameters are the same as in Fig. 1. The broken line in (b) contains finite impurity broadening, $\Gamma_0=0.01\sqrt{B}$ meV.

$i+1$ (for the special case of integer fillings, this number is i). Here i is an integer and counts the resonance frequency (as $i=1$) and each of its harmonics (as $i=2,3,4,\ldots$). The number of singularities for any i is limited to $n_{\max}$. Figure 2 shows typical behavior for the real part of the magnetic-field-dependent RPA dielectric function in a unidirectional periodic potential. The real part is seen to be qualitatively very similar to the unmodulated case (shown as an inset in Fig. 2) except about the resonance frequency and each of its harmonics, where two new features are seen to be present. The first of these features is the appearance of new subsingularities (fine structure) at the same frequencies. Again, the number of such singularities on *each side* of the band edges is the same as that in the imaginary part. The second feature is the existence of a step region, of finite width, about each of the resonance and harmonic frequencies, that exists between the subsingularities. In Fig. 3, both $\mathrm{Re}[\epsilon(q,\omega)]$ and $\mathrm{Im}[\epsilon(q,\omega)]$ are plotted in expanded form about $\omega=4\omega_c$ to clearly show these new fine structures.

Our results indicate that the electron-hole pair excitation is now significantly altered by the spatial periodic modulation. It is well known that for infinitely sharp LL, the electron-hole pair excitation can only occur at frequencies equal to the cyclotron frequency and its harmonics. The imaginary part of the dielectric function $\mathrm{Im}[\epsilon(q,\omega)]$ (which describes the pair excitation), in the absence of a spatial modulation, contains a series of $\delta(\omega-n\omega_c)$ that are highly singular. In the presence of a spatial modulation, the once sharp LL's are broadened into Landau bands with von Hove singularities at the band edges. These broadened Landau bands now allow for pair excitation to occur within a finite frequency bandwidth around the cyclotron frequency and its harmonics. If each Landau band had the same width, one would simply observe a broadened excitation with similar von Hove singularities at the low- and high-frequency sides of the excitation peaks. However, the modulation broadening is dependent on the Landau band index n. This n-dependent level broadening is the origin of these new subsingularities found in the density-response function. For example, if the

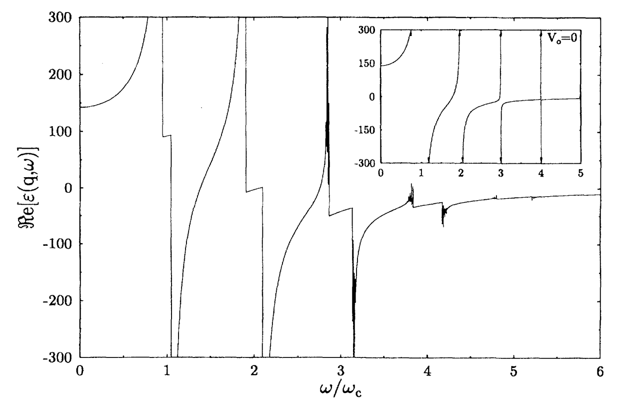

FIG. 2. Real part of the magnetic-field-dependent RPA dielectric function as a function of ω/ω_c. All parameters are the same as in Fig. 1. Inset: The unmodulated (i.e., $V_0=0$) case.

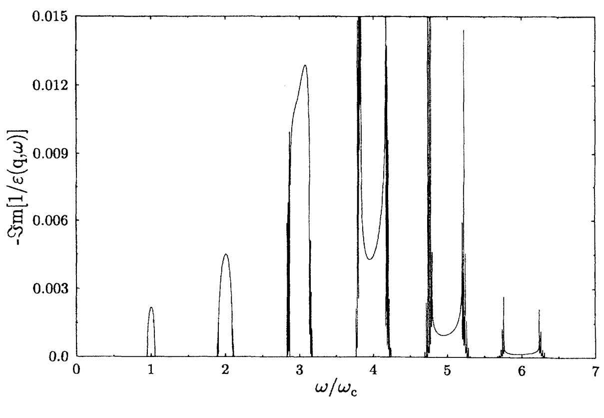

FIG. 4. Plot of $\mathrm{Im}[1/\epsilon(q,\omega)]$ as a function of ω/ω_c. Parameters as in Fig. 1.

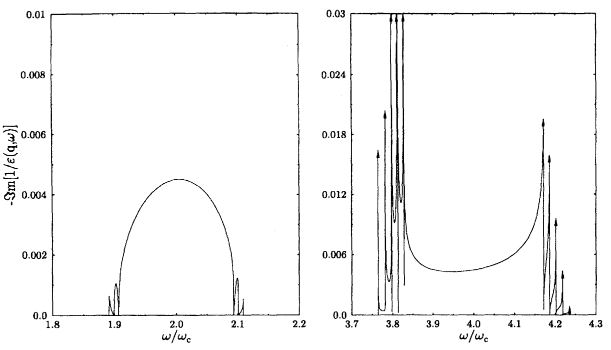

FIG. 5. Two close views of $\mathrm{Im}[1/\varepsilon(q,\omega)]$ about $\omega=2\omega_c$ and $\omega=4\omega_c$ showing the subsingularities that are present on either side of the band edges.

last Landau band is partially filled, the allowed transitions about $\omega\sim\omega_c$ are $n_{\max}-1\rightarrow n_{\max}$ and $n_{\max}\rightarrow n_{\max}+1$. The singularities in the pair excitation for the $n_{\max}-1\rightarrow n_{\max}$ transition occur at different frequencies than those for the $n_{\max}\rightarrow n_{\max}+1$ transition. Therefore one observes four singularities, two for each allowed transition, about $\omega\sim\omega_c$. Extending this idea to about $\omega\sim 2\omega_c$, three transition processes are allowed: $n_{\max}-2\rightarrow n_{\max}$, $n_{\max}-1\rightarrow n_{\max}+1$, and $n_{\max}\rightarrow n_{\max}+2$. In this case a total of six singularities can be found in the pair excitation. The number of singularies increases by 2 as ω increases from around $n\omega_c$ to around $(n+1)\omega_c$. If $n>n_{\max}$ the number of singularities cannot further increase due to the limit in initial available occupied states $n_{\max}$. The new subsingularities at the band edges are inverse-square-root divergent. The arrow heads appearing on each singularity in the figures are used to remind one about the existence of infinities here and also to show one the relative weightings of each singularity as it tends to (plus or minus) infinity.

One of the most important quantities in physics is the density-response function $\mathrm{Im}[1/\epsilon(q,\omega)]$. This quantity is plotted in Figs. 4 and 5. It can have either a maximum or a minimum at $\omega=i\omega_c$ depending on the frequency of the dynamical perturbation. These new features contained in the dielectric-response function can be related to several important physically observable quantities.

(i) *Raman scattering intensity and line shape*. The scattering cross section is given as

$$\frac{d\sigma}{d\omega d\Omega}=|\alpha\cdot\alpha'|^2\frac{e^2}{m}\frac{\omega_{\rm out}}{\omega_{\rm in}}\frac{q[\rho(\omega)+1]}{\pi}\,\mathrm{Im}\left[\frac{1}{\epsilon(q,\omega)}\right], \quad (8)$$

where α is the polarization vector of the photons and $\rho(\omega)$ is the photon thermal distribution function. So the results plotted in Figs. 4 and 5 are directly proportional to the light scattering cross section.

(ii) *Electromagnetic absorption*. The absorption of long-wavelength electromagnetic radiation by the electron gas, to the lowest order in plasma parameter, is proportional to $(1/\omega)\Sigma_q F_q \mathrm{Im}[1/\epsilon(q,\omega)]$. Here q is the momentum transfer between the electrons and the heavy impurities (or phonons). The form factor F_q is proportional to the square of the qth Fourier component of electron-impurity (or phonon) interaction. For a magnetically quantized electron system, the singular behavior of $\mathrm{Im}[1/\epsilon(q,\omega)]$ makes the absorption calculation for $\omega\neq\omega_{\rm mp}$ unrealistic. For the present system, due to the modulation broadening, absorption of the electromagnetic radiation by particle-hole excitation becomes possible.

Finally, we would like to discuss the effect of disorder. Theoretically, our result is exact within RPA, and level broadening due to disorder is not included in our formalism. Due to small separations between the subsingularities, these predicted fine structures can only be well resolved in high-mobility samples with minimum disorder. However, it is impossible to avoid disorder altogether in a realistic structure. We demonstrate briefly the effect of disorder on these fine structures by considering short-range impurities within the Born approximation.[8] The result for finite disorder broadening ($\Gamma_0=0.01\sqrt{B}$ meV corresponding to an electron mobility $\mu\sim 6\times 10^6$ cm^2/V s) is plotted as broken lines in Fig. 3(b). We find the modulation-induced fine structures are still present. For the present system under a weak modulation ($V_0=1$ meV), these fine structures will be completely washed out if $\mu<10^6$ cm^2/V s. However, $\mu_{\min}$ decreases as V_0 or q_y increases, e.g., at $V_0=2.5$ meV and $q_y=10^7$/m, the estimated $\mu_{\min}$ is about 2×10^5 cm^2/V s.

In conclusion, we have calculated the dynamical-response function of a spatially modulated 2DEG in a magnetic field. It is revealed that at the cyclotron frequency and its harmonics, the response function contains a series of singularities at the band edges. These singularities should be observable in an optical experiment.

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