Effect of modulation and magnetic field on the properties of two-dimensional Coulomb systems

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A two-dimensional (2D) electron system in a modulation potential and a weak uniform perpendicular magnetic field is studied by a molecular-dynamics simulation method. The simulation results clearly demonstrate some interesting oscillations in the diffusion coefficient, which we interpret in terms of the orbital motion of the electrons on the modulated 2D system. [S0163-1829(98)07607-3]

In recent years, there has been growing interest in the effect of electrostatic and magnetic modulation on the transport properties of charged carriers in two-dimensional (2D) electron systems from both an experimental and theoretical perspective. Specifically, there have been several investigations on the effect of a static field modulation potential on the static, thermodynamic, and dynamical properties of the 2D electron system. The reason for the interest in modulation effects is that recent advances in submicron lithography and nanofabrication techniques have made it possible to create lateral surface superlattices with modulation periods much smaller than the elastic mean free path and comparable with the cyclotron radius at low magnetic fields.[1–4] This gives rise to a new class of effects. For example, when a perpendicular magnetic field B is applied to a homogeneous 2D electron gas (EG), the Shubnikov–de Haas (SdH) oscillations associated with the filling of successive Landau levels (LL's) are exhibited in the resistivity. If a weak periodic one-dimensional (1D) modulation is applied to a homogeneous 2DEG, a new kind of magnetoresistance oscillations (Weiss oscillations) are obtained below the SdH oscillations.[1] These oscillations were attributed to the commensurability between the lattice period and the cyclotron radius of the electrons at the Fermi energy.[2,5–9] Streda and MacDonald[10] used a semiclassical theory to explain the oscillations for a unidirectionally modulated 2D electronic system by interpreting these as a consequence of oscillations in the probability of magnetic breakdown. Results for a weak periodic 2D modulation have also been reported[4,11–13]. The work of Fleischmann, Geisel, and Ketzmerick.[14] is devoted to a calculation of the magnetoresistance of an electron system with a strong periodic 2D modulation to simulate an array of antidots on semiconductor heterojunctions. The present work is for the diffusion coefficient with weak bilateral modulation using a classical approach like Fleischmann, Geisel, and Ketzmerick[14] which neglects quantum coherence effects that would become significant in the high-density regime. For antidots, quantum oscillations superimposed on the classical peaks of the magnetoresistance have been observed by Weiss *et al.*[15] and explained theoretically by Hackenbroich and von Oppen.[16]

Many calculations have used a quantizing magnetic field to calculate the transport coefficients of a 2D electron system with a modulation potential. However, in this paper, we use a classical magnetic-field approach that is described by its effect through a Lorentz force for a system with low electron density in a weak magnetic field. The strength of the modulation potential is chosen so that quantum-mechanical effects do not change our results. The advantage of our method is that it allows us to observe the system evolving in real time which consequently makes it possible to calculate various time correlation functions needed for comparison with experimental results. The lateral modulation potential is simulated by a product of cosine functions raised to some even power so that the potential does not change sign. This is, of course, just one term in the Fourier expansion of a periodic potential and is taken as the principal contribution. One may also represent the modulation potential by a sum of cosine functions.[11] In this paper, we will report the effect due to modulation on the properties of a 2D electron system when the Coulomb interaction and the magnetic field are included directly into the electron dynamics. As far as we know, the calculated static properties as a function of the magnetic field strength and modulation potential that we present are the only simulation results available.

In 2D, the Coulomb interaction between two electrons of charge $-e$ separated by a distance r is given by $V_{e-e}(r)=-e^2\ln(r/L)$, where L is a scaling length chosen as the length of the simulation cell. The 2D models of logarithmically interacting charges have found widespread application in understanding the behavior of many different physical systems via a mapping to the XY model, Josephson-function arrays in

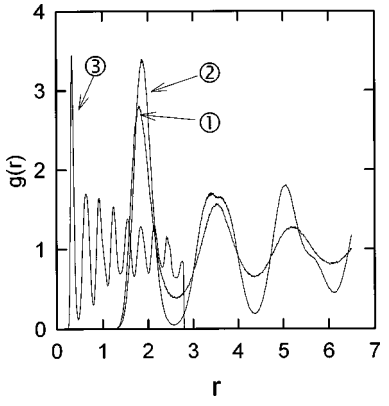

FIG. 1. The pair-correlation function vs particle separation for the following pairs of values of modulation strength V_0 and applied magnetic field B: (1) $V_0=0$ and $B=0$, (2) $V_0=0$ and $B=1.0$ T, (3) $V_0=1.0$ K and $B=1.0$ T. The value of β used in Eq. (3) is chosen as $\beta=1$.

a transverse applied magnetic field. Vortices induced by magnetic fields and other physical systems, such as 2D melting, surface roughening, and liquid crystals can also be described in terms of logarithmically interacting topological defects. This is why we use the logarithmic potential. Because of the long-range nature of the Coulomb interaction, we use an Ewald summation to take account of the interaction between an electron and an infinite array of periodic images of the other electrons. The Coulomb energy of the system, consisting of N particles of charge $-e$, is given by

$$V_C=\frac{e^2}{2}\sum_{\mathbf{n}}\sum_{i=1}^{N'}\sum_{j=1}^{N'}\ln|\mathbf{r}_{ij}+\mathbf{n}| + \frac{Ne^2}{A}\sum_{\mathbf{n}}\sum_{j=1}^{N}\int_A d\mathbf{r}\,\ln|\mathbf{r}_j-\mathbf{r}+\mathbf{n}| - \frac{N^2e^2}{A^2}\sum_{\mathbf{n}}\int_A d\mathbf{r}\int_A d\mathbf{r}'\ln|\mathbf{r}-\mathbf{r}'+\mathbf{n}|, \tag{1}$$

where $\mathbf{r}_{ij}$ is the vector between electrons i and j, $\mathbf{n}$ is a vector whose components are (n_xL,n_yL); n_x and n_y are integers. The first term on the right-hand side of Eq. (1) arises from the interactions between pairs of electrons. The sum over $\mathbf{n}$ is carried out over all lattice vectors. The primes on the summation signs indicate that, when $n=0$, the terms with $i=j$ have to be excluded. The second term arises from the interaction between the electrons and a uniform positive jellium background. The integrals over $\mathbf{r}$ and $\mathbf{r}'$ are carried out over the rectangular unit cell of area $A=L_xL_y$. The third term represents the interaction of the background with itself. The sum in Eq. (1) is conditionally convergent and the energy V_C depends on the shape of the macroscopically large periodic system.

We now investigate the effect of a 2D modulation potential, based on the following simple harmonic ansatz for the superlattice potential:

$$V_M(\mathbf{r})=V_0\left[\cos\left(\frac{2\pi x}{a_x}\right)\cos\left(\frac{2\pi y}{a_y}\right)\right]^{2\beta}, \tag{2}$$

where a_x and a_y are the lattice periods and β is an integer. The reason for choosing the form in Eq. (2) is to ensure that the potential is either attractive or repulsive, depending on the sign of V_0. Although Eq. (2) is only one term in the Fourier expansion of a periodic potential, it could be used to study the effect of the size of the scatterers by varying the value of β and the strength of the scatterers by changing V_0. Effects from higher-potential harmonics are neglected in this model.

We have carried out a molecular-dynamics (MD) simulation experiments for the 2D Coulomb system in a uniform perpendicular magnetic field $\mathbf{B}$ and applied modulation potential. Our calculations were done for 256 particles in a rectangular cell with periodic boundary conditions and $a_x=a$, $a_y=\sqrt{3}a/2$. A predictor-corrector method involving up to five time derivatives of the positions was used to integrate Newton's equation of motion. The total force on an electron is the sum of the forces arising from the modulation potential and the Coulomb interaction, i.e., $\mathbf{F}(V_M+V_C)$, and the Lorentz force so that $\mathbf{F}_T=\mathbf{F}(V_M+V_c)-(e/c)(\mathbf{v}\times\mathbf{B})$, where $\mathbf{v}$ is the velocity of the electron.

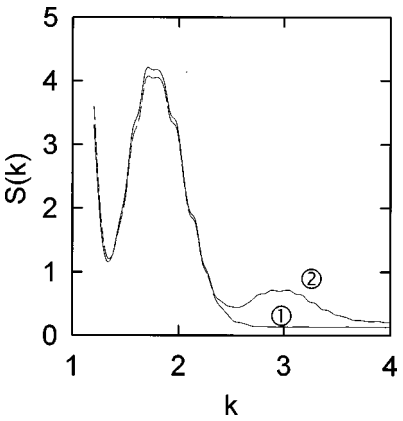

FIG. 2. Plot of the static structure factor vs wave number for the following pairs of values of modulation strength V_0 and applied magnetic field B: (1) $V_0=0$ and $B=1$ T and (2) $V_0=0.1$ K and $B=1$ T. The value of β used in Eq. (3) is chosen as $\beta=1$.

We have used the following dimensionless units $r^*=r/a$, wave vector $k^*=ka$ and $t^*=t/\tau$, where $\tau^2=ma^3/e^2$ and m is the free-electron mass. The reduced electron density is $N_s^*=N_sa^2$, which corresponds to a value of 1.477×10^8 electrons/cm^2 and a reduced temperature of 2.0 K. The runs for the collection of the data presented here for 256 electrons extended over 15×10^4 time steps, after an initial 10^5 time steps for the system to reach equilibrium. The results reported here are all in reduced units.

In Fig. 1, we have presented our results for the pair-correlation function $g(r)$, through the relation $\langle n(r)\rangle=2\pi r\,\delta r N_s g(r)$. Here, $\langle n(r)\rangle$ is the average number of particles in an annulus of radius r and thickness δr, centered at a given particle. We chose $V_0=0$ and 1.0 K and the magnetic field $B=0$ and 1 T. Our calculations show that, as expected, the magnetic field has no noticeable effect on the pair-correlation function. However, the modulation potential has an appreciable effect on the modulated $g(r)$, which has more oscillations. In the presence of a modulation potential, the first peak of the pair-correlation function shifts to a smaller distance as the modulation strength increases, due to the increased confinement in a unit cell by the walls of the potential barrier. The second peak is reduced, which indicates less confinement at larger distances.

We further analyze the effect of the modulation potential given by Eq. (2), in a uniform perpendicular magnetic field, by calculating the static structure factor defined as the Fourier transform of the pair-correlation function. In 2D, it is given by

$$S(k)=1+2\pi N_s\int_0^\infty dr\; rJ_0(kr)(g(r)-1)=\frac{1}{N}\langle\rho_k\rho_{-k}\rangle, \tag{3}$$

where $J_0(x)$ is the Bessel function of order zero. The pair-correlation function $g(r)$ that is obtained through MD calculations is for half the length of the box. Here, $S(k)$ in Eq. (3) is the zero-time value of the intermediate scattering function. In Fig. 2, we have plotted $S(k)$ as a function of the wave

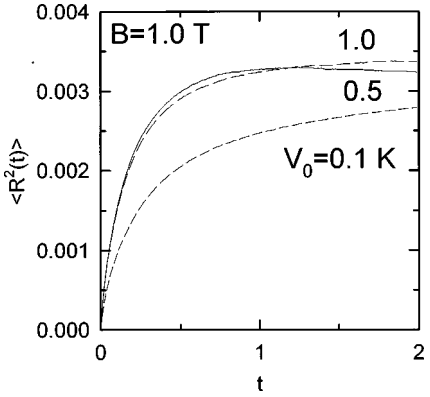

FIG. 3. The mean-square displacement vs time for a magnetic field $B=1.0$ T and with the modulation strengths set equal to $V_0=0.1$, 0.5 and 1.0 K. The value of β used in Eq. (3) is chosen as $\beta=1$.

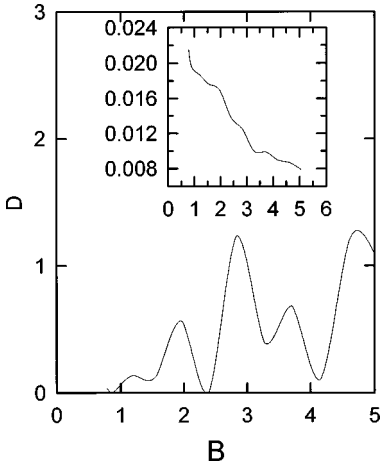

FIG. 4. The diffusion coefficient is plotted as a function of the magnetic field for $V_0=0.5$. The inset is for a homogeneous 2D system. The value of β in Eq. (3) was set equal to unity.

number k in the presence and absence of modulation and for an applied magnetic field $B=1$ T. The value of $S(k)$ in the long- and short-wavelength limits are not appreciably changed by the modulation potential for a fixed magnetic field. However, at intermediate values of k, $S(k)$ is modified by the external potential, as we see by comparing our results when V_0 is zero and when it is finite. This means that the electrons get distributed by the lattice potential over distances determined by the magnetic length and the lattice period. The modification of $S(k)$ at intermediate values of k means that the density correlations are definitely affected by the modulation potential.

We have calculated the mean square displacement $\langle R^2(t)\rangle$ as a function of time for several values of the magnetic field and modulation strength to see what is the effect of these variables on the diffusion coefficient. We have

$$\langle R^2(t)\rangle = \frac{1}{N}\left\langle \sum_{j=1}^{N} (\mathbf{r}_j(t)-\mathbf{r}_j(0))^2 \right\rangle, \tag{4}$$

where $\mathbf{r}_j(t)$ is the position vector of the jth electron at time t. The diffusion coefficient D is defined by $D=\langle R^2(t)\rangle/4t$ as $t\to\infty$. Figure 3 is a plot of $\langle R^2(t)\rangle$ versus t for a fixed magnetic field $B=1.0$ T and with the modulation strengths set equal to $V_0=0.1$, 0.5, and 1.0 K. For a uniform homogeneous 2DEG, i.e., $V_0=0.0$ K, our results show that in the absence of modulation, $\langle R^2(t)\rangle$ has a well-established linear behavior for all magnetic fields. We found that the slopes of the linear increments at large times decrease with increasing magnetic field. Our calculations show that in the presence of modulation, the nonlinear behavior in $\langle R^2(t)\rangle$ occurs at all magnetic fields. The diffusion coefficient D is time independent and is plotted as a function of the magnetic field in Fig. 4, for $V_0=0$ and $V_0=0.5$ K. These results show that the diffusion constant is drastically affected by the modulation potential, D has oscillations as a function of B and is not a simple decreasing function of the magnetic field, as it is in the absence of modulation. When V_0 is increased, the electrons tend to remain at the potential minima within a unit cell, resulting in a zero diffusion constant. As V_0 is decreased, some electrons have enough kinetic energy to overcome the saddle point and move to neighboring cells, leading to a finite diffusion constant. The oscillations in D arise when the orbits become commensurate with the lattice. The minima correspond to *pinned* orbits, unlike the scattered open orbits, which can contribute to the transport process. Since the magnetic field introduces another time scale through the cyclotron motion of an electron, our MD simulations were carried out over long-time intervals. For the magnetic fields used in our calculations, the system of particles was simulated for 200 ps.

The static mobility μ_0 can of course be obtained from the Nernst-Einstein relation $D=\mu_0 k_B T$. If we use a relaxation time approximation for μ_0, we can determine the phenomenological scattering time τ from $\mu_0=\tau/m$. For a classical system, the diffusion constant is defined in terms of the velocity autocorrelation function by

$$D=\sum_{\nu}\int_0^{\infty} dt\langle \mathbf{V}_\nu(t)\mathbf{V}_\nu(0)\rangle, \tag{5}$$

where $\mathbf{V}=\Sigma_{j=1}^{N}\dot{\mathbf{r}}_j$ is the total velocity of the system of particles. It is known that the velocity autocorrelation function in 2D has a $1/t$ long-time decay,[17] and thus the diffusion constant as defined in Eq. (5) is not well defined. However, our data on the mean-square displacement shows that after an initial quadratic behavior, $\langle R^2(t)\rangle$ is linear so that we could define a diffusion constant from the slope at long times. The variation of the diffusion coefficient with magnetic field in Fig. 4 is oscillatory. In the absence of modulation, (see the inset of Fig. 4), the diffusion coefficient decreases exponentially with increasing magnetic field.

In summary, we have carried out MD simulations for a 2D Coulomb system in the presence of a modulation potential and a uniform perpendicular external magnetic field. Our calculations show that the diffusion constant is not a simple decreasing function of the magnetic field, but has oscillations like those observed experimentally for the longitudinal magnetoresistance of a modulated 2D electron gas within a semiconductor heterostructure at low magnetic fields. When the Coulomb interaction is neglected the system does not equilibrate and the $\langle R^2(t)\rangle$ curves do not have a constant slope at large time. Our calculations show that the oscillations in D

are classical in nature and are due to the presence of the modulation potential. The oscillations in D arise when the orbits become commensurate with the lattice. The minima correspond to pinned orbits, unlike the scattered open orbits, which can contribute to the transport process. Our simulations were done at low magnetic fields. We do not include quantum interference effects in this Coulomb system. At higher electron densities, exchange and correlation effects should be included through a quantizing magnetic field. Our results were based on the modulation potential in Eq. (2) but our conclusions should not change if we use a different model.[11]

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