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LETTER TO THE EDITOR

A quantitative study of pinning of a 2D electron crystal in heterojunctions

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Abstract. We study numerically the relaxation and the pinning gap of a 2D electron crystal in the presence of randomly distributed distant dopants. Our results agree with experiments and with analytic calculations based on a perturbation in the deviations of the particle positions $\delta r/a$ from the lattice positions. For parameters corresponding to the recent experimental studies ($d/a \simeq 3$), the relaxation is dominated by the *longitudinal* mode.

Recently there has been much interest in the low-density limit of 2D electrons in GaAs heterojunctions in an external magnetic field [1–11] and Si-MOSFETs in high [12–14] and zero [15, 16] fields where a freezing transition to a solid seems to occur as the density is lowered.

To investigate the pinning of the electron crystal by distant dopants of concentration n_i randomly distributed at positions R_j at a setback distance d, we study numerically the relaxation of the lattice of spacing a and density $1/a_c$ [17]. Pinning has been studied qualitatively in the context of charge density waves [18, 19] and more recently for the 2D electron crystals [20–22]. These works focus on the transverse relaxation. We found by our essentially exact calculation that the longitudinal relaxation is larger than the transverse relaxation by two orders of magnitude for parameters corresponding to the experimentally studied systems ($d/a = 3, n_i a_c = 2, r_s = 2.2$) [2]. The average deviation of the particle positions $\delta r/a$ from the lattice positions is 0.05. This suggests that analytic perturbation calculations in the variable are a good approximation. Indeed, the difference between our perturbation result and our numerical result for the relaxation is less than 1%. The numerical pinning gap agrees to within 5% with the perturbation result given by

$$m\Delta^2 = 0.09 n_i a^2 e^2/\epsilon d^3.$$

To compare with experimental results it is necessary to take into account the effect of the quantum fluctuation, which reduces the phonon frequencies by approximately 30%; the fluctuation in the setback distances d, so that $1/d^3$ is replaced by $\langle 1/d^3 \rangle$; and other possible charges which are further away but may be more numerous. For parameters corresponding to the system studied by Paalanen *et al*, we obtain $\Delta = 532\ s^{-1}$ and $\Delta^2/2\pi\omega_c = 0.9$ GHz [19] (filling factor = 0.167) whereas the experimental result is 1 GHz. The agreement is reasonable in view of the fact that there is some uncertainty in our input experimental parameters.

Previous theoretical studies of the gap focused on contributions from transverse relaxation *at long wavelengths* which were identified as the domain size. Our analytic

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results suggest the following picture in the present case: the impurities are coupled to the transverse phonon mode only through large momentum transfer Umklapp processes. Since the Fourier transform of the impurity potential decreases exponentially as the momentum is increased [21, 23] and due to large thermal and quantum fluctuation near melting, the pinning gap is dominated by non-divergent contributions from longitudinal relaxations of *all* length scales larger than d. We now describe our results in detail.

First the numerical calculation. The external impurity potential is given by [21, 23]

$$U_i(r) = \sum_{q,j} V_q \exp(iq \cdot [R_j - r_{i0} - \delta r_i])/A$$

where $V_q = 2\pi \exp(-dq)/a_c q$ is the Fourier transform of the Coulomb potential. We looked at systems of 56, 120 and 224 particles under periodic boundary conditions. The Ewald sum technique is used to deal with the long-range nature of the potential U_i as well as the inter-particle Coulomb potential. For each size we investigate 40 samples corresponding to different random distributions of the dopant positions R_j. It is possible to deal with a distribution of setback distance d but for simplicity we assume that it is fixed. We start with a triangular lattice of particles at positions r_{i0}. The relaxation is accomplished with the quasi-Newton method [17] so that the total energy is minimized. We calculate the pinning gap for each sample by computing the sum of the second derivative of the impurity potential over all the electrons. The impurity potential contour and the relaxed particle positions for a typical sample, for parameters corresponding to an experimentally studied system ($d/a = 3$, $n_i a_c = 2$, $r_s = 2.2$) [2] is illustrated in figure 1(a). The average gap as a function of sample size is shown in figure 1(b). We have performed the relaxation calculations with the full inter-particle Coulomb potential $\sum_{i>j} 1/r_{ij}$ as well as with the harmonic approximation for the inter-particle potential $\sum_{i>j,k,l}(r_{ijk} - r_{ijk0})(r_{ijl} - r_{ijl0})\nabla_l \nabla_k (1/r_{ij0})$. The final results differ by less than 1%. For each sample and size we compute the deviation of the lattice position and its longitudinal (l) and transverse (t) Fourier transforms $\delta r_{qj} = \sum_i (r_i - r_{i0}) \cdot e_{qj} e^{iq \cdot r_{i0}}/N^{1/2}$. Here e_{qj} is the polarization vector for mode j =l, t. We found that the longitudinal component is larger than the transverse component by two orders of magnitude. The difference between these and the perturbation results discussed below is then computed numerically.

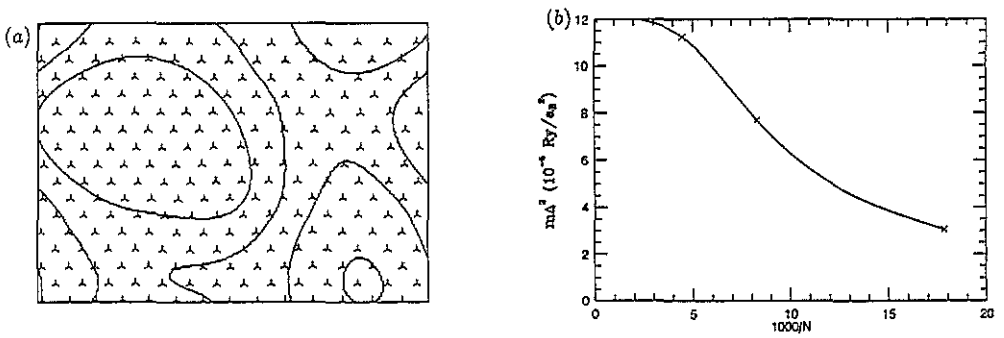

Figure 1. (a) The impurity potential contour at U_i = 3.8, 3.5, 3.2 and 2.9 and the relaxed particle positions for a typical sample at $d/a = 3$, $n_i a_c = 2$, $r_s = 2.2$. (b) The gap in units of $10^{-5}\,\mathrm{Ry}/a_B^2 = 1.46 \times 10^{21}\ \mathrm{s}^{-2} m^*$ as a function of the inverse sample size. The point at $1/N = 0$ is the result from the analytic perturbation calculation. The line is a spline fit throught the points to guide the eye.

We next describe the perturbation calculation. The total energy is

$$m\omega_{qi}^2|\delta_{qi}|^2/2 + \sum V_q \exp(\mathrm{i}\boldsymbol{q}\cdot[\boldsymbol{R}_j - \boldsymbol{r}_{10} - \delta\boldsymbol{r}_1])/A.$$

Here A is the area of the system. Minimizing the energy with respect to δr, we obtain to lowest order in δr the equation

$$\delta r_{qi} = \mathrm{i}\sum_{G,j} V(q+G)[(q+G)\cdot e_{qi}]\exp(-\mathrm{i}\boldsymbol{R}_j\cdot[q+G] - \langle((q+G)\delta r)^2\rangle/2)/[\sqrt{N}a_c m\omega_{qi}^2. \tag{1}$$

The factor $\exp[-\langle((q+G)\cdot\delta r_0)^2\rangle/2]$ is obtained from a cumulant expansion. δr_0 includes contributions from both the thermal and the quantum fluctuations. Since the pinning potential is non-linear, it contains a term proportional to $(\delta r)^2$, the coefficient of which provides for the pinning gap. This coefficient is the second derivative of U_i with respect to δr given by

$$m\Delta^2 = -0.5\sum_{qi} V(q)q^2\exp(-\mathrm{i}(\boldsymbol{R}_j - \boldsymbol{r}_{10} - \delta\boldsymbol{r}_1)\cdot q - \langle(q\delta r)^2\rangle/2)/A.$$

The impurity average of this, to the lowest order of δr, is

$$\Delta^2 = 0.5n_i\sum_{p,G,n}[V(p+G)(p+G)\cdot e_{pn}]^2\exp(-\langle((q+G)\delta r)^2\rangle) \times [(p+G)]^2/Am^2\omega_{pn}^2. \tag{2}$$

A similar formula for the gap was derived recently by Ferconi *et al* [22] from density functional considerations. We have computed the difference $\Delta(\delta r)$ between (1) and the results from our numerical relaxation studies and found that the ratio

$$\left[\sum_{q,j}(\Delta(\delta r_{q,j}))^2\right] / \left[\sum_{q,j}(\delta r_{q,j})^2\right] \simeq 0.01.$$

Equation (2) is a sum of contributions from the transverse and the longitudinal phonons: $\Delta^2 = \Delta_t^2 = \Delta_l^2$. The transverse contribution is approximately equal to $\Delta_t^2 = 4\pi V(G)^2\exp(-\langle(G\cdot\delta r)^2\rangle/2)n_i\log(L/a)/3m^2s_t^2a^4$ where L is the lower limit cut-off. It can be the domain or the sample size. The presence of the dot product means that the dominant contribution comes from Umklapp terms with $G \neq 0$. Except for the logarithmic factors, which were emphasized recently by Ferconi *et al*, this expression is essentially that discussed by previous authors [20]. When d/a is small and away from melting, this contribution and the logarithmic factor will be important. This contribution may appear divergent, but for practical purposes is extremely small. Near melting, $G^2\langle(\delta r)^2\rangle/a^2 \simeq 8$; in addition $V(G) = \exp(-2Gd) \propto \exp(-36)$. Thus for this contribution to be significant, $L/a > \exp(\exp(42))$. This is much greater than any normal sample size.

The longitudinal contribution is, in the limit $d \gg a$, approximately given by

$$m\Delta_l^2 = 0.09n_i a^2e^2/(\epsilon d^3)$$

and is not proportional to $V(G)$. Also, the corresponding Debye–Waller factor $\exp(-q^2\langle(\delta r)^2\rangle)$, is close to unity and much larger. Thus the longitudinal contribution is

much larger than the transverse contribution. The same reasoning applies to the displacement $\delta r_{ql,t}$ where we found the longitudinal displacement is larger than the transverse displacement by two orders of magnitude. For the longitudinal component, the sum over the momenta is not divergent even if the gap is equal to zero. Equation (2) contains contributions from *all* wave vectors p less than $1/d$, whereas previous studies emphasized contributions from relaxations of a dominant Fourier component identified as the inverse domain size. The relaxation consists of all Fourier components at length scales larger than the setback distance and is not dominated by a *single* Fourier component. Thus a description in terms of domain may not be appropriate.

In conclusion, we have calculated the relaxation and pinning gap of electron crystals in 2D in the presence of random distant dopants. We found agreement between numerical relaxation studies, analytic self-consistent perturbation calculations, and experimental results. Since the Fourier transform of the potential falls off rapidly with momentum, the longitudinal component of the relaxation dominates over the transverse component. A simple formula that depends on the lattice spacing squared and the setback distance to the inverse third power is derived. The experimentally observed depinning electric field E_{dp} [6, 7] is much smaller than the scale set by the pinning gap $m\Delta^2 a$ [24]; we think the depinning electric field is related to the creation of defects [9–11] but this is beyond the scope of the present paper.

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