Solid State Communications, Vol. 88, No. 10, pp. 765-768, 1993.
Printed in Great Britain.

0038-1098/93$6.00+.00
Pergamon Press Ltd

COLD MELTING OF TWO-DIMENSIONAL WIGNER CRYSTALS

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(Received 29 September 1993 by A. Okiji)

The melting criterion of the two-dimensional Wigner crystals is studied at zero temperature by taking into account of phonon anharmonicity. The lowest order anharmonic corrections do not lead to the phonon instability, where the shear modulus of the Wigner crystal vanishes, in contrast to the earlier calculation by Chang and Maki, and the next order corrections are shown to be important to have the phonon instability. On the assumption that the phonon instability causes melting, we find that the melting occurs at $r_s \sim 8.7$. This value is in good agreement with the recent experiment in Si MOSFET's by Pudalov et al.

Melting of two-dimensional electron crystals, i.e., the phase transition from the Wigner crystal to liquid has attracted much attention recently. The melting of classical two-dimensional Wigner crystals as found in the electron system on liquid He is understood to be the dislocation mediated melting proposed by Kosterlitz-Thouless[1-5]. The theoretical understanding of the quantum melting in two-dimensions, on the other hand, is not clear in our opinion because no standard theory comparable to the Kosterlitz-Thouless theory exists. In order to understand the quantum melting, several melting criteria have been proposed [6-10]. In particular, the relation between the quantum melting and the phonon instability of two-dimensional Wigner crystals was discussed by Platzmann and Fukuyama[6] within the self-consistent harmonic approximation and by Chang and Maki[7] with a perturbational method including the lowest order correction of the anharmonic interactions among Wigner phonons. Both of the studies report a relatively small value of r_s for the phase transition, where r_s is defined by

$$r_s = \frac{e^2 m}{\epsilon \hbar^2 \sqrt{\pi n}}, \tag{1}$$

with e being the elecronic charge, m the electron effective mass, ϵ the dielectric constant and n the electron areal density. Numerical analysis of the ground state energy was performed by Tanatar and Ceperley[10] who showed that the transition is of first order and $r_s \sim 30$. If this is the case, there should be a critical point which separates the first order and the Kosterlitz-Thouless transitions on the phase transition line.Whether or not the critical point exists is an open question and is beyond the scope of the present note. The recent experiment in Si MOSFET's by Pudalov et al.[11] reports that the melting occurs at $r_s \sim 10$, and seems to indicate that the transition is of second order in view of their data of the activation energy and the threshold electric field.

In this work, we present the calculation of the shear modulus of the Wigner phonons to include the higher order anharmonic corrections and try to discuss the melting from the view point of the instability of the transverse mode of the Wigner phonon.

We assume that electrons form a 2-dimensional triangular crystal and phonons are created by the oscillations of the lattice points. We consider here the transverse mode, because the vanishing of the shear modulus is essential in the melting of solids. We write the phonon dispersion ω_t^2 of the transverse mode by the sum of the harmonic term Ω_t^2 and the anharmonic correction $\Sigma(\boldsymbol{p})$:

$$\omega_t^2(\boldsymbol{p}) = \Omega_t^2(\boldsymbol{p}) + \Sigma(\boldsymbol{p}), \tag{2}$$

where $\Omega_t^2(\boldsymbol{p})$ is given by

$$\begin{aligned}\Omega_t^2(\boldsymbol{p}) &= -\frac{1}{m}\sum_{R\neq 0}\sum_{\boldsymbol{q}\neq 0}\frac{2\pi e^2}{Aq}e^{i\boldsymbol{q}\cdot\boldsymbol{R}}(\boldsymbol{q}\cdot\boldsymbol{\epsilon}_t(\boldsymbol{p}))\\ &\quad\times(1-\cos\boldsymbol{p}\cdot\boldsymbol{R}),\end{aligned} \tag{3}$$

where $\boldsymbol{\epsilon}_t(\boldsymbol{p})$ is the polarizaion vector of the transverse phonon, $\boldsymbol{R}$ the lattice point vector and A the area of the system. From the dimensional analysis, it is found that the expansion parameter of $\Sigma(\boldsymbol{p})$ is found to be $r_s^{-1/2}$. The lowest order anharmonic correction in $r_s^{-1/2}$ is written as

$$\Sigma^{(1)}(\boldsymbol{p}) = \sum_{\lambda_1}\Sigma_{\lambda_1}^{\text{quartic}}(\boldsymbol{p}) + \sum_{\lambda_1,\lambda_2}\Sigma_{\lambda_1,\lambda_2}^{\text{cubic}}(\boldsymbol{p}), \tag{4}$$

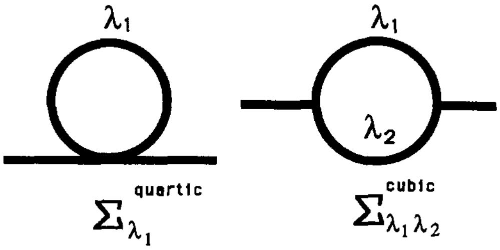

Figure 1 Diagrams of the lowest order anharmonic corrections

where λ_i denote the phonon polarizations, either longitudinal (l) or transverse (t). $\Sigma^{\rm quartic}_{\lambda_1}$ and $\Sigma^{\rm cubic}_{\lambda_1\lambda_2}$ are shown in the diagrams in Fig.1. They are explicitly written as

$$\Sigma^{\rm quartic}_{\lambda_1}(\boldsymbol{p}) = \frac{4}{m^2\beta N}\sum_{p_1}\sum_{\nu_1} g_{\lambda_1,\nu_1}(\boldsymbol{p}_1) \times V^{\lambda_1,\lambda_1,t,t}_{\boldsymbol{p}_1,\boldsymbol{p}_1,\boldsymbol{p},\boldsymbol{p}}, \tag{5}$$

$$\Sigma^{\rm cubic}_{\lambda_1,\lambda_2}(\boldsymbol{p}) = \frac{8}{m^3\beta N}\sum_{p_1}\sum_{\nu_1} g_{\lambda_1,\nu_1}(\boldsymbol{p}_1) \times g_{\lambda_2,\nu_1}(\boldsymbol{p}+\boldsymbol{p}_1)\left(V^{t,\lambda_1,\lambda_2}_{\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}+\boldsymbol{p}_1}\right)^2. \tag{6}$$

Table I The numerical results of each diagram in Fig. 1

λ	$\sqrt{r_s}\,\Sigma^{\rm quartic}_{\lambda}/\Omega_t^2$
t	3.907
l	−1.452

$\lambda_1\ \lambda_2$	$\sqrt{r_s}\,\Sigma^{\rm cubic}_{\lambda_1\lambda_2}/\Omega_t^2$
$t\ t$	-5.147×10^{-4}
$t\ l$	−2.119
$l\ l$	-5.987×10^{-2}

$\lambda_1\ \lambda_2\ \lambda_3$	$r_s\,\Sigma^{(a)}_{\lambda_1\lambda_2\lambda_3}/\Omega_t^2$
$t\ t\ t$	−1.075
$t\ t\ l$	−1.339
$t\ l\ l$	-4.868×10^{-1}
$l\ l\ l$	-3.418×10^{-2}

$\lambda_1\ \lambda_2\ \lambda_3$	$r_s\,\Sigma^{(b)}_{\lambda_1\lambda_2\lambda_3}/\Omega_t^2$
$t\ t\ t$	-9.582×10^{-2}
$t\ t\ l$	6.630×10^{-1}
$t\ l\ l$	-1.367×10^{-2}
$l\ t\ t$	-1.120×10^{-1}
$l\ t\ l$	5.536×10^{-1}
$l\ l\ l$	-1.751×10^{-1}

$\lambda_1\ \lambda_2\ \lambda_3$	$r_s\,\Sigma^{(c)}_{\lambda_1\lambda_2\lambda_3}/\Omega_t^2$
$t\ t\ t$	6.004×10^{-1}
$t\ t\ l$	1.120
$t\ l\ l$	-5.732×10^{-1}
$l\ l\ l$	-1.538×10^{-1}

$\lambda_1\ \lambda_2$	$r_s\,\Sigma^{(d)}_{\lambda_1\lambda_2}/\Omega_t^2$
$t\ t$	-1.119×10^{1}
$t\ l$	2.743
$l\ l$	2.600×10^{-1}

$\lambda_1\ \lambda_2\ \lambda_3\ \lambda_4$	$r_s\,\Sigma^{(e)}_{\lambda_1\lambda_2\lambda_3\lambda_4}/\Omega_t^2$
$t\ t\ t\ t$	3.171×10^{-4}
$t\ t\ t\ l$	-7.289×10^{-3}
$t\ t\ l\ l$	4.809×10^{-5}
$t\ l\ t\ l$	-4.927×10^{-2}
$t\ l\ l\ l$	-9.922×10^{-4}
$l\ l\ l\ l$	-9.113×10^{-5}

$\lambda_1\ \lambda_2\ \lambda_3\ \lambda_4$	$r_s\,\Sigma^{(f)}_{\lambda_1\lambda_2\lambda_3\lambda_4}/\Omega_t^2$
$t\ t\ t\ t$	1.587×10^{-3}
$t\ t\ t\ l$	-2.011×10^{-1}
$t\ l\ t\ t$	2.301×10^{-1}
$l\ t\ t\ t$	-2.039×10^{-3}
$t\ l\ t\ l$	2.097×10^{-3}
$l\ t\ l\ t$	-4.067×10^{-4}
$l\ t\ t\ l$	8.952×10^{-2}
$l\ l\ t\ t$	-1.138×10^{-2}
$l\ t\ l\ l$	2.370×10^{-2}
$l\ l\ t\ l$	6.973×10^{-3}
$l\ l\ l\ t$	-4.927×10^{-2}
$l\ l\ l\ l$	2.688×10^{-4}

Here the free phonon Green function $g_{\lambda\nu}(\boldsymbol{p})$ is given by

$$g_{\lambda\nu}(\boldsymbol{p}) = \{\nu^2 + \Omega_\lambda^2(\boldsymbol{p})\}^{-1}, \qquad (7)$$

where ν the Matsubara frequency given by $\nu = 2\pi n/\beta$ (n = integer) with β the inverse of temperature. The vertex function V is defined by

$$\begin{aligned} V_{\boldsymbol{p}_1,\ldots,\boldsymbol{p}_n}^{\lambda_1,\ldots,\lambda_n} &= \sum_{\boldsymbol{R}} \sum_{\boldsymbol{q}\neq 0} \frac{2\pi e^2}{Aq} e^{i\boldsymbol{q}\cdot\boldsymbol{R}} \\ &\times \prod_{i=1}^{n} \left\{ (\epsilon_{\lambda_i}(\boldsymbol{p}_i)\cdot\boldsymbol{q}) \sin\frac{\boldsymbol{p}_i\cdot\boldsymbol{R}}{2} \right\}, \qquad (8) \end{aligned}$$

where $\epsilon_\lambda(\boldsymbol{p})$ is the polarizaion vector of the phonon of mode λ. We calculate $\Sigma^{(1)}$ in the limit of small p, since we are interested in the shear modulus. For this, the precise evaluation of the vertex function is most important. We calculate V by several methods: (i) an approximate analytical evaluation to replace the discrete sum over $\boldsymbol{R}$ by the continuum integral, (ii) V is expanded in powers of p's and then their coefficients are estimated by the Ewald summation, and (iii) the direct numerical evaluation. They are checked each other to confirm the final method (iii). The numerical results of each diagram in Fig. 1 are tabulated in Table I.

We obtain by the numerical calculation $\Sigma^{\mathrm{quartic}}/\Omega_t^2 = \sum_{\lambda_1} \Sigma_{\lambda_1}^{\mathrm{quartic}}/\Omega_t^2 = 2.455\, r_s^{-1/2}$, $\Sigma^{\mathrm{cubic}}/\Omega_t^2 = \sum_{\lambda_1,\lambda_2} \Sigma_{\lambda_1,\lambda_2}^{\mathrm{cubic}}/\Omega_t^2 = -2.180\, r_s^{-1/2}$ and hence

$$\Sigma^{(1)}/\Omega_t^2 = 0.275\, r_s^{-1/2}. \qquad (9)$$

Note that $\Sigma^{(1)}$ is positive. This was calculated before by Chang and Maki[7] who obtained $\Sigma^{(1)}/\Omega_t^2 = -2.36\, r_s^{-1/2}$. Discrepancy of the sign and the absolute value from our result arises from their inaccurate estimation of the tt-process in Σ^{cubic}, where the vertex function V^{ttt} was grossly overestimated. In fact the dominant process in Σ^{cubic} comes from the tl-scattering, and $|\Sigma^{\mathrm{cubic}}|$ is smaller than their value, though still negative.

In a similar fashion we calculate numerically the second order anharmonic correction as shown diagramatically in Fig. 2. The result is

$$\begin{aligned} \Sigma^{(2)}/\Omega_t^2 &= (\Sigma^{\mathrm{a}}(p) + \cdots + \Sigma^{\mathrm{f}}(p))/\Omega_t^2 \\ &= (-2.935 + 0.820 + 0.993 \\ &\quad -8.187 - 0.0576 + 0.0885)\, r_s^{-1} \\ &= -9.28\, r_s^{-1}. \qquad (10) \end{aligned}$$

See Table I for detailed results. The main contribution to $\Sigma^{(2)}$ comes from the $ttt-$ and $ttl-$processes in Σ^{a} and the $tt-$process in Σ^{d}.

If we replace $g_{\lambda\nu}$ by the renormalized Green function, i.e., $\Omega_t^2(\boldsymbol{p})$ is replaced by $\omega_t^2(\boldsymbol{p})$ in (6) for the internal lines in the diagrams, we obtain

$$\Sigma^{(2)}/\Omega_t^2 = -9.53\, r_s^{-1}, \qquad (11)$$

instead of (10) and $\Sigma^{(1)}$ remains unchanged. This result

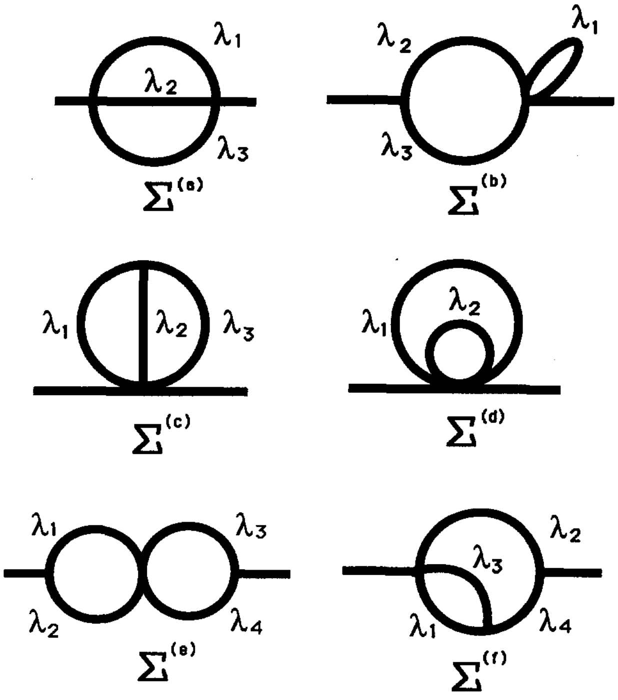

Figure 2 Diagrams of the second order anharmonic corrections. Suffixes of Σ are omitted for brevity.

may be better than (10), since self-consistency within (2) is imposed and part of the higher order corrections which are not considered explicitly in the perturbational calculations will be included.

We estimate the melting point by the condition that the shear modulus of the transverse phonon vanishes:

$$\omega_t^2(p)/\Omega_t^2(p) = 1 + \Sigma(p)/\Omega_t^2(p) = 0. \qquad (12)$$

The solutions with (10) and (11) are obtained as r_s = 8.5 and 8.7, respectively. We prefer r_s = 8.7 for the cold melting criterion as discussed above. Note that $\Sigma^{(1)}$ is positive and this term alone does not lead to the phonon instability, and $\Sigma^{(2)}$ is essential to lead to the phonon instability. This conclusion is different from that of Chang and Maki.

In conclusion we evaluated the critical value of r_s at which the cold melting takes place by assuming that the instability of the transverse phonon causes the melting. Naturally the transition will be of second order. Our value is larger than the values reported by the earlier authors [6,7] who employed the same criterion of the melting, and about 1/3 of the value obtained by the numerical simulation by Tanatar and Ceperley [10]. Our value is in good agreement with the recent observation in Si MOSFET's by Pudalov et al.

We are grateful to Professor H.Kawamura for useful discussions.

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