# Effect of interplane coupling in quasi-two-dimensional systems

S. T. Chui
*Bartol Research Foundation of The Franklin Institute, University of Delaware, Newark, Delaware 19711*
(Received 14 January 1983)

There are many divergent susceptibilities in two-dimensional systems that are not associated with phase transitions. We propose that when stacks of planes of these two-dimensional systems are coupled together, these divergences indicate genuine phase transitions. Applications to melting, commensurate-incommensurate transitions, and superconductivity are pointed out.

Divergent susceptibilities quite often indicate the onset of an instability. However, this is not necessarily so. In fact, there are many two-dimensional systems whose correlation function shows divergence at certain temperatures and yet no phase transitions. For example, the structure factor $S_q = \langle \rho_q \rho_{-q} \rangle$ for a two-dimensional "solid" is known to exhibit a power-law divergence $(q-G)^{\eta_G - 2}$,[1,2] where $G$ is a reciprocal-lattice vector,

$$\eta_G = T|G|^2(3\mu+\lambda)/4\pi\mu(2\mu+\lambda) \quad , \tag{1}$$

and $\mu$ , $\lambda$ are Lamé constants. Yet no phase transition occurs at a temperature $T_0$ determined by $\eta_G = 2$ because the divergence is not intensive, i.e., $S/N \rightarrow 0$ as $N \rightarrow \infty$, where $N$ is the size of the system. In fact, the Kosterlitz-Thouless (KT) transition occurs when $\eta_G < 2$. We call this a pseudoinstability. There are many quasi-two-dimensional systems that consist of planes of coupled two-dimensional systems. These occur, for example, in the graphite intercalation compounds, in heterojunctions, etc. We propose here that the two-dimensional (2D) pseudoinstabilities become genuine three-dimensional instabilities when the two-dimensional systems are stacked up to form a quasi-two-dimensional system.

This has some rather amusing consequences. For example, for coupled planes of atoms, the 3D "melting" transition will occur at $\eta_G = 2$, whereas the Kosterlitz-Thouless transition occurs at $\eta_G \cong \frac{1}{3}$ for a hexagonal lattice. The melting transition that one sees in quasi-two-dimensional systems probably is then not related to the dislocation unbinding or grain boundary picture at all.[3]

There are other interesting applications of this idea to other situations such as the commensurate-incommensurate transition, superconductivity, and so on. For example, whereas it is quite difficult to observe 2D melting in a quasi-2D system, it is possible to observe 2D commensurate-incommensurate transitions. We propose that there is a new phase transition in which one goes from a 3D incommensurate phase to a 2D incommensurate phase for a high enough temperature in that case. A recent experiment by Kortan[4] *et al.* sees only 2D incommensurate behavior in bromine intercalated graphite, whereas Fleming *et al.*[5] found 3D incommensurate behavior in $2H$-$TaSe_2$, suggesting that both possibilities exist, consistent with our picture. However, the transition from 3D to 2D behavior in a single material has not been observed.

We also obtained the reduction of the superconducting transition temperature ($T_c$) from the mean-field ($T_0$) temperature of planes, viz.,

$$T_c = T_0[1 + T_0(m_x m_y)^{1/2}/2\pi n h^2]^{-1} + O(\eta) \quad . \tag{2}$$

Here $\eta$ is the interplane coupling, $n$ the electron density, and $m_x$ and $m_y$ the effective masses in the plane. This may be of relevance to recent experiments of superconductivity in di-tetramethyltetraselenafulvalium salts $(TMTSF)_2X$ ($X = PF_6$, $ClO_4$, etc.). For example, it may be possible to relate the pressure dependence of $m_x$ and $m_y$ to that of $T_c$. We shall first focus on the melting transition.

Our result is obtained by treating the interplane interaction in a mean-field manner. Calculations using this have been carried out for coupled chains previously.[6] Let us briefly recapitulate the basic idea here. Suppose there is an interplane interaction of the form $V_q \rho_q \rho_{-q}$, where $\rho_q$ is the $q$th Fourier transform of the density. The effective field $h_{\text{eff}}$ acting on a plane is then the sum of the external and the internal field, viz.,

$$h_{\text{eff}}(G) = h_{\text{ext}}(G) + 2V\langle \rho_{-G} \rangle \quad . \tag{3}$$

Note that the component of the wave vector perpendicular to the planes is zero. The response $\langle \rho_{-G} \rangle$ of an array of atoms is, in turn, related to the effective field through the two-dimensional response function $\chi_{\parallel}(q)$:

$$\langle \rho_{-G} \rangle = \chi_{\parallel}(-G) h_{\text{eff}}(-G) \quad . \tag{4}$$

Let us assume that $\langle \rho_G \rangle = \langle \rho_{-G} \rangle$ for the sake of simplicity. We then get

$$\langle \rho_G \rangle = h_{\text{ext}}(G)[1 - 2V(G)\chi_{\parallel}(G)]^{-1} = h_{\text{ext}}(G)\chi(G) \quad , \tag{5}$$

where $\chi(G)$ is the three-dimensional response function. It is obvious that $\chi(G)$ becomes infinite when

$$1 = 2V(G)\chi_{\parallel}(G) \quad . \tag{6}$$

So far, everything looks the same as in any ordinary mean-field calculation. However, $\chi_{\parallel}(G)$ becomes very big at the pseudoinstability temperature $T_0$. Hence we expect Eq. (6) to be satisfied at a temperature above $T_0$. Furthermore, in the limit that $V(G) \rightarrow 0$, the three-dimensional ordering temperature approaches $T_0$. Previous investigation shows that

$$\chi(G) = (\gamma k_D/2)^{-\eta_G} 2\pi/(\eta_G - 2)T \quad , \tag{7}$$

where $k_D$ is the Debye wave vector. $\gamma = 1.78$ is the exponential of Euler's constant. The usual argument about the absence of a phase transition for the 2D system at $T_0$ comes from the fact that $\chi_{\parallel}(g, T_0) \sim N^{\alpha}$, where $\alpha < 1$ and $N$ is the total number of atoms in a plane. Even though $\alpha$ is less than 1, $\chi_{\parallel}(G, T_0)$ is still very large so that, unless $V(G)$ is of the order of $N^{-\alpha}$, Eq. (4) will be satisfied for a

 

TABLE I. Transition temperatures of coupled chains and planes of $n$-component spins. $z$ is the number of nearest neighbors; $J_\perp$ ($J_\parallel$) is the intralayer (interlayer) coupling.

| | Chains | Planes |
|---|---|---|
| Ising $n=1$ | $T_c=2J_\parallel/\ln(J_\parallel/J_\perp)$ | $T_c\neq 0$ for $J_\perp=0$ |
| $XY$ $n=2$ | $T_c\cong\left(\frac{z_\perp J_\perp}{nJ_\parallel}\right)^{1/2}$ | $T_c\geq T_{\rm KT}$ |
| $n\geq 3$ | | $T_c=J_\parallel\{[(n-2)/4\pi]\ln(J_\parallel/J_\perp)+\text{const}\}^{-1}$ |

temperature larger than $T_0$.

We next explore the consequences of Eq. (6). The Kosterlitz-Thouless temperature $T_{\rm KT}$ is given by[2] $T_{\rm KT}=a_0^2\mu(\mu+\lambda)/4\pi(2\mu+\lambda)$. For the electron system, $\lambda$ is much larger than $\mu$ so that

$$T_{\rm KT}=a_0^2\,\mu/4\pi\ . \tag{8}$$

From Eqs. (7), (6), and (1), we get

$$T_0=8\pi G^{-2}\mu(2\mu+\lambda)/(3\mu+\lambda)\ . \tag{9}$$

In general, $\mu$ is a function of temperature so that the $\mu$ in Eq. (9) need not be identical to that in Eq. (8).

We note that the core energy of dislocations are larger for coupled planes. Hence they are more difficult to form. The renormalization contribution due to dislocations to the shear modulus is much reduced. For an estimate of the relative magnitude of $T_0$ and $T_{\rm KT}$ we shall assume that the elastic constants are the same. Then, for a hexagonal lattice,

$$T_0/T_{\rm KT}=24/(1+\sigma)(3-\sigma)\ , \tag{10}$$

where $\sigma$ is the Poisson ratio $\lambda/(\lambda+2\mu)$. For Coulomb systms $\sigma=1$, so that $T_0/T_{\rm KT}=6$. A general estimate of $\sigma$ is 0.6. Then $T_0/T_{\rm KT}=6.25$. It is possible to get an estimate of the transition temperature of coupled planes of electrons by use of the estimate $\mu=4\pi e^2(\pi n)^{1/2}/137\epsilon a_0^2$. Then $T_c=T_0+\gamma^{-2}e^2 3/2\epsilon\pi l$, where $l$ is the separation between the layers. This dependence on $n$ and $l$ may be detectable experimentally.

It is possible to test the mean-field method by applying it to systems where the transition temperature has been calculated by other means. In Table I we collected some results obtained with this approximation on the functional dependence of the transition temperatures of coupled layers and chains of $n$-component spins with interplane (intraplane) coupling $J_\perp$ ($J_\parallel$). Some of these results are old, some are new. For a planar collection of Ising chains, our result agrees with the exact solution of the 2D Ising model in the limit $J_\parallel >> J_\perp$. Also, for the case of coupled planes of spins with $\eta>3$, our result agrees with the renormalization group calculation of Kosterlitz and Santos[7] and Ito.[8] Note also that it is always impossible to observe the KT transition for two component spins if the planes are coupled.

Let us now turn our attention to commensurate-incommensurate phase transitions. $\chi$ has been discussed by Chui and Weeks[9] and by Saito.[10] Treating the interplane coupling in mean field we have constructed the phase diagram in Fig. 1.

The $x$ axis denotes the force driving the system into the incommensurate phase; the $y$ axis, the temperature. The curve ABC is taken from the previous work. The line $BD$ is the new proposal here. Below $BD$ one has a 3D incommensurate phase, whereas above it one has a 2D incommensurate phase. As one crosses $BC$, the commensurate-incommensurate transition is 3D-like. This has been discussed by several authors[11] for pure systems. In real systems this will probably be masked by other effects such as impurity pinning[12] or effects due to the electronic driving forces. The 2D commensurate-incommensurate behavior marked by the crossed curve AB depends on the commensurability of the system as is previously discussed.[13] It would be interesting to test this phase diagram experimentally.

Finally, let us turn our attention to low-dimensional superconductivity. The order parameter in that case can be written as $\psi=Ae^{i\theta}$. It is the fluctuation of the phase $\theta$ that destroys superconductivity in low-dimensional systems. If we ignore the fluctuation of the amplitude $A$ then the fluctuation of the phase can be described by the $XY$ model. Now $T_{\rm KT}=A^2h^2\pi/2a^2m^*$, where $m^*$ is the effective mass of the electrons.

According to the Landau-Ginsburg therory of superconductivity we get $A^2=n(1-T/T_0)$, where $n$ is the electron planar density. From this, the reduction in $T_c$ can be obtained as

$$T_c=T_0/(1+T_0m^*/2n\pi h^2)\ . \tag{11}$$

Note that $2nh^2/m^*$ is of the order of $E_F$. Hence the reduction in $T_c$ is quite small. This may be why previous studies of quasi-2D superconductivity, which basically ignores the

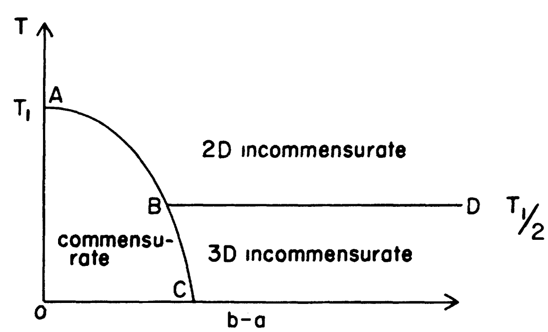


FIG. 1. Phase diagram of commensurate-incommensurate transitions in quasi-two-dimensional systems. The $x$ axis represents driving force towards incommensurability.

2D fluctuations, is successful. It is possible to generalize the above result to planes with anisotropic masses $m_x$ and $m_y$. One gets Eq. (2). This formula may be applicable to $(TMTSF)_2PF_6$ which may actually be two-dimensional.[14] If so, the pressure dependence of $m_x$ and $m_y$ might provide a clue for the pressure dependence of the superconductivity in this compound.

The author was supported in part by the U.S. Department of Energy under Contract No. DE-AC02-82ER12060.

---

[1]B. Jancovici, Phys. Rev. Lett. 19, 20 (1967); Y. Imry and L. Gunther, Phys. Rev. B 3, 3939 (1971).

[2]D. Nelson and B. I. Halperin, Phys. Rev. B 19, 2457 (1979).

[3]For $T < T_0$, the atomic positions are correlated from plane to plane. Dislocations in different layers must line up. The energy to separate dislocation lines of opposite Burger's vectors is of the order $N^{1/3}\ln N^{2/3}$. This is always larger than the entropy gained ($T\ln N^{2/3}$). Hence they always bind. Neither the grain boundary mechanism nor the dislocation mechanism for two-dimensional melting is possible. Hence equation (7) does not contain free dislocation effects.

[4]A. R. Kortan, A. Erbil, R. J. Birgeneau, and M. S. Dresselhaus, Phys. Rev. Lett. 49, 1427 (1982).

[5]R. M. Fleming, D. E. Moucton, D. B. McWhan, and F. J. Disalvo, Phys. Rev. Lett. 45, 576 (1980).

[6]D. J. Scalapino, Y. Imry, and P. Pincus, Phys. Rev. B 11, 2042 (1975).

[7]J. M. Kosterlitz and M. A. Santos, J. Phys. C 11, 2835 (1978).

[8]M. Ito, Prog. Theor. Phys. 65, 1773 (1981).

[9]S. T. Chui and J. D. Weeks, Phys. Rev. B 21, 4413 (1980).

[10]Y. Saito, Prog. Theor. Phys. 63, 831 (1980).

[11]S. T. Chui, in *Melting, Localization and Chaos,* edited by R. K. Kalia and P. Vashishta (North-Holland, Amsterdam, 1982), p. 35; M. E. Fisher, Phys. Rev. B 25, 3192 (1982); F. D. M. Haldane and J. Villain, J. Phys. (Paris) 42, 1673 (1981).

[12]S. T. Chui, Phys. Rev. B 19, 4333 (1979); T. M. Rice, S. Whitehouse, and P. Littlewood, *ibid.* 24, 2751 (1981).

[13]S. N. Coopersmith, D. S. Fisher, B. I. Halprin, P. A. Lee, and W. F. Brinkman, Phys. Rev. Lett. 46, 549 (1981).

[14]K. Bechgaaod, K. Carneiro, M. Olsen, F. B. Rasmussen, and C. S. Jacobsen, Phys. Rev. Lett. 45, 1587 (1980); C. Minot and S. G. Louie, Phys. Rev. B 26, 4793 (1982).