Theory of discommensurations and the commensurate-incommensurate charge-density-wave phase transition*

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The lowest-energy state of the incommensurate charge density wave (CDW) near the lock-in transition is found to be a distorted plane wave. An exact solution is found in the weak-coupling limit and the lock-in phase transition is continuous. A new defect is found in the commensurate CDW, a discommensuration, in which the phase of the CDW slips by $2\pi/3$ relative to the perfectly locked in CDW. The lock-in phase transition is interpreted as a defect melting transition with a finite density of discommensurations in the incommensurate state.

I. INTRODUCTION

Recently, the anomalous properties of the layered transition-metal dichalcogenides such as $2H$-$TaSe_2$ have been attributed to charge-density-wave (CDW) formation.[1] In $2H$-$TaSe_2$ an incommensurate CDW state is formed at 122 °K which locks in to the lattice to form a commensurate CDW state at 90 °K.[2] Wilson, DiSalvo, and Mahajan have studied the susceptibility, resistivity, and electron diffraction pattern of this material. Barmatz, Testardi, and DiSalvo[3] have observed an anomaly in the Young's modulus at the lock-in transition. Moncton, Axe, and DiSalvo[2] have made a careful study of $2H$-$TaSe_2$ using neutron diffraction to study the periodic lattice-distortion associated with the CDW. These authors observed an interesting distortion of the incommensurate CDW near the lock-in transition and explained this distortion as arising from the lock-in energy term in a Landau free-energy expansion. Independently the present author developed a more complete Landau theory to describe CDWs.[4]

The purpose of the present paper is to present a careful study of the commensurate-incommensurate (lock-in) phase transition using the author's Landau theory. We show that the phase transition is continuous (second order) in contrast to the earlier approximate treatments[3,4] which yielded a first-order phase transition. In addition we define and study a new defect in the commensurate CDW state state, the discommensuration (DC). The commensurate-incommensurate transition is naturally described as a DC melting transition with no DCs in the commensurate state and a finite density of DCs in the incommensurate state. This second-order phase transition is interesting in that it cannot be described in the conventional Landau sense[5] using an order parameter. We show that three DCs can terminate in a CDW dislocation. The model provides a qualitative explanation of the neutron diffraction data and the Young's modulus data.

II. INCOMMENSURATE PHASE

The free-energy expression was discussed thoroughly in an earlier paper[4] and we include it here for completeness. The free energy of the lth layer is

$$F_l = \int d^2r \Big(a\alpha_l^2 - b\alpha_l^3 + c\alpha_l^4 + d(|\psi_{l1}\psi_{l2}|^2 + |\psi_{l2}\psi_{l3}|^2 + |\psi_{l3}\psi_{l1}|^2) + e\sum_i |(\vec{q}_i\cdot\vec{\nabla} - iq_i^2)\psi_{li}|^2 + f\sum_i |(\vec{q}_i\times\vec{\nabla}\psi_{li})|^2 \Big), \tag{1}$$

where

$$\alpha_l(\vec{r}) = \mathrm{Re}[\psi_{l1}(\vec{r}) + \psi_{l2}(\vec{r}) + \psi_{l3}(\vec{r})], \tag{2}$$

and the three complex order parameters $\psi_{li}(\vec{r})$ represent the three coexisting CDWs in the lth layer. The conduction band electron density is

$$\rho_l(\vec{r}) = \rho_0(\vec{r})[1 + \alpha_l(\vec{r})], \tag{3}$$

where $\rho_0(\vec{r})$ is the normal-state conduction-electron density. The three $\vec{q}_i$ vectors are the wave numbers of the three incommensurate CDWs and they lie in the ΓM directions 120° apart. The coefficients a, b, etc., are periodic in $\vec{r}$ with the periodicity of the crystal lattice. We write

$$b(\vec{r}) = b_0 + b_1\sum_i e^{i\vec{K}_i\cdot\vec{r}} + 1\cdots, \tag{4}$$

where the $\vec{K}_i$ are the six shortest reciprocal-lattice vectors characteristic of the planar hexagonal transition-metal lattice. For $2H$-$TaSe_2$ $|q_1|$ is 2%

less than $\frac{1}{3}K_1$ so that the CDW can lock in to the lattice by decreasing its wavelength by 2%. The cubic "umklapp" term (proportional to b_1) provides the lock-in energy. This change in wavelength is opposed by the gradient term (proportional to e_0) which is minimized when the CDW wave number is $\vec{q}_1$. These two terms in the free energy are of central importance for the present discussion.

For later discussion we add the interlayer Coulomb interaction yielding the free energy of the whole crystal

$$F = \sum_l \left(F_l + g\mathrm{Re}\sum_i \int d^2r\, \psi_{li}(\vec{r})\psi_{l+1i}^*(\vec{r}) \right), \quad (5)$$

where $g = 2\rho_0^2 \exp(-q_1 c)/q_1^2\epsilon_\infty$, c is the interlayer spacing, and ϵ_∞ is the dielectric constant of the dichalcogenide matrix in which the conduction electrons move.

In order to simplify the problem enough to actually solve it we will study the lock-in transition of a single CDW in one layer. We will return to the (observed) triple CDW state in three dimensions later. We now substitute

$$\psi_1(\vec{r}) = \psi_0 e^{i\vec{K}_1\cdot\vec{r}/3}\phi(\vec{r}); \quad \psi_2 = \psi_3 = 0 \quad (6)$$

into (1) with $\psi_0^2 = -2a_0/3c_0$ and $\vec{s} = (-q_1 + \frac{1}{3}K_1)\vec{r}$ and find

$$F_l = F^0 \int d^2s[-|\phi|^2 - \beta y\,\mathrm{Re}(\phi^3) + \tfrac{1}{2}|\phi|^4 + \beta|\vec{\nabla}\phi + i\phi|^2 + \gamma|\hat{q}_1\times\vec{\nabla}\phi|^2], \quad (7)$$

where

$$F^0 = a_0^2/[3c_0(q_1 - \tfrac{1}{3}K_1)^2],$$
$$\beta = e_0 q_1^2\psi_0^2(q_1 - \tfrac{1}{3}K_1)^2,$$
$$\gamma = f_0 q_1^2\psi_0^2(q_1 - \tfrac{1}{3}K_1)^2,$$

and

$$Y = b_1\psi_0/[4e_0 q_1^2(q_1 - \tfrac{1}{3}K_1)^2].$$

Writing $\vec{s} = (x,y)$ and taking the $\hat{q}_1$ direction to be the x axis the uniform plane wave solution for the incommensurate phase is $\phi(\vec{s}) = e^{-ix}$ with free energy $F^0(-\frac{1}{2})$. The uniform plane wave solution for the commensurate phase is $\phi(\vec{s}) = 1$ with free energy $F^0(-\frac{1}{2} + \beta(1-Y))$. This simple theory of the lock-in transition predicts a first-order phase transition when $Y = 1$. (The temperature dependence of Y is contained in the temperature dependence of ψ_0.)

Moncton *et al.* were clever enough to notice that the free energy of the incommensurate CDW could be lowered by distorting the plane wave to take advantage of the cubic lock-in term in the free energy. Their trial function was of the form

$$\phi(x) = e^{-ix} + A_1 e^{i2x}, \quad (8)$$

with A_1 determined variationally by minimizing the free energy. The physics of the situation is as follows. The energy of the CDW is lowered when it is "in phase" with the lattice. Here "in phase" means that the peak of the CDW lies between rows of transition metal atoms so that the bond charge is maximized. For the uniform CDW with wavelength 2% longer than the locked in wavelength the CDW will be in phase with the lattice for 25 lattice spacings, out of phase for the next 25 lattice spacings, etc. The umklapp energy is attractive for the in-phase region and repulsive for the out-of-phase region and averages out to zero. However, we can distort the uniform CDW in two ways to gain energy. We can modulate the amplitude of the CDW making it larger in the in-phase region to gain energy. Or we can modulate the phase of the CDW to enlarge the in-phase region and shrink the out-of-phase region to gain energy. It costs much less energy to create a long-wavelength phase distortion (phason) than it does to create a long wavelength amplitude distortion. Therefore, if the modulation wavelength is long compared to the coherence length (i.e., if β is small), the phase variation will be much more important. The ansatz of Moncton *et al.* forces an equal phase and amplitude distortion.

It turns out that in order to discuss the phase transition we want an exact solution to the problem. This is easy to achieve for the long-wavelength or weak-coupling case where β is small and only phase modulation is important. For that case we substitute $\phi(\vec{s}) = e^{-i\theta(x)}$ and find the free energy relative to the commensurate state

$$\Delta F = F^0\beta \int d^2s\{Y[1 - \cos(3\theta)] + (\nabla\theta - 1)^2\}. \quad (9)$$

Finally we make the ansatz

$$\theta(x) = \delta x + \sum_{n=1}^{N} A_n \sin(3n\delta x), \quad (10)$$

where δ and the A_n are variational parameters. For fixed Y and δ we minimize ΔF with respect to the A_n parameters using the standard nonlinear minimization procedure. Then we minimize ΔF with respect to δ to find the optinum wavelength at a given tempraturee. We retain up to 20 terms in the Fourier series to obtain six place accuracy in the free energy. The integration over x is performed numerically. We find that δ goes continuously to zero at a critical value of Y, $Y_c = 1.2337$, which determines the commensurate-incommensurate transition temperature T_{CI}. Defining the reduced temperature $t = (T - T_{CI})/(T_{IN} - T_{CI})$ we find that δ is a universal function of t and is indepen-

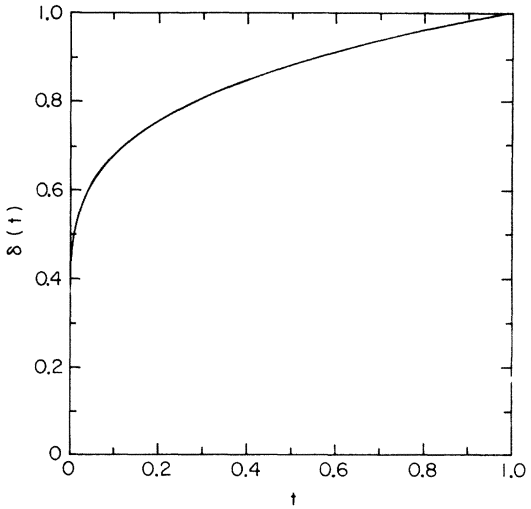

FIG. 1. Wavelength discrepancy δ vs reduced temperature in the incommensurate phase. The density of DCs is proportional to δ which goes continuously to zero at $t = 0$.

dent of the Landau theory parameters. This function is shown in Fig. 1.

Near the transition we can fit the free energy with the following analytic form:

$$\Delta F = F_0 \beta[0.811\delta(Y - Y_c) + 8.0\delta e^{-4.930/\delta}]. \quad (11)$$

The numerical data for $\delta(t)$ can be fit by the following function within ± 1% for $0.005 < t < 0.5$:

$$\delta(t) = 4.62/[4.61 + \ln(1/t)]. \quad (12)$$

The entropy is $s = -\partial \Delta F/\partial t$ and the singular part of the heat capacity is $C_V = \partial s/\partial t$. This function is computed numerically and is shown in Fig. 2. The following function fits the heat capacity within ± 3% for $0.005 < t < 0.5$:

$$C_V = F_0 \beta 1.35/t \ln^2(7.4/t). \quad (13)$$

The phase function $\theta(x)$ for $t \approx 0$, $\delta = 0.2$ is shown in Fig. 3. This function is badly distorted from the linear dependence of an undistorted plane wave. There are wide regions where θ is a multiple of $\frac{2}{3}\pi$ and the CDW is in phase with the lattice and is effectively locked in. There are narrow regions in between where the phase changes by $\frac{2}{3}\pi$ and the CDW is not locked in. These regions appear as defects in a perfectly locked in CDW and we call this new defect a discommensuration. The density of DCs is proportional to δ and is small enough near the phase transition for the defects to be well separated and well defined. In the commensurate phase $\delta = 0$ and there are no DCs in the lowest-energy state. The entropy of these extended defects is insufficient to produce a finite density of DCs in the commensurate state.

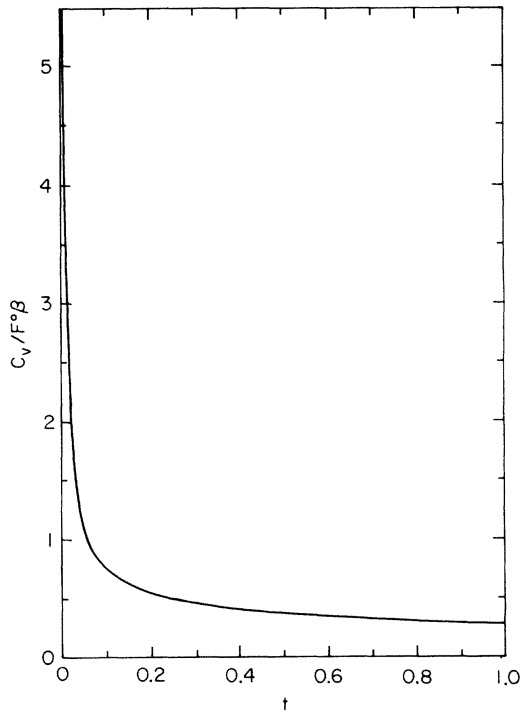

FIG. 2. Discommensuration heat capacity vs reduced temperature in the incommensurate phase.

III. THE DISCOMMENSURATION

We now calculate the properties of one DC in the commensurate state. We again assume $\phi(\vec{s}) = e^{-i\theta(x)}$ with θ going to zero for large negative x and to $\frac{2}{3}\pi$ for large positive x. Minimizing the free

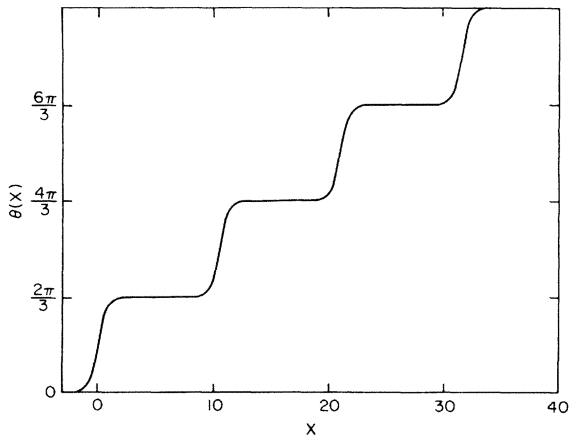

FIG. 3. Phase of incommensurate CDW relative to perfectly locked-in CDW vs distance for $\delta = 0.2$ near the lock-in temperature. The regions where θ is a multiple of $\frac{2}{3}\pi$ are locked in and the regions of rapidly varying phase in between are CDW defects called discommensurations.

energy (9) with respect to $\theta(x)$ we find the following nonlinear differential equation for $\theta(x)$:

$$+\tfrac{3}{2}Y \sin 3\theta - d^2\theta/dx^2 = 0. \tag{14}$$

For large negative x the asymptotic solution is

$$\theta(x) \sim \theta_0 e^{\alpha x}; \quad \alpha = (\tfrac{1}{2}9Y)^{1/2}. \tag{15}$$

With (15) as the starting function we integrate (14) numerically to find $\theta(x)$. $\theta(x)$ and $d\theta/dx$ for a DC at the transition temperature are shown in Fig. 4. The core thickness of the DC is roughly $2/\alpha$ (in dimensionless units). We define a new characteristic length $\xi_c \equiv 1/[(K_1/3 - q_1)(\frac{9}{2}Y_c)^{1/2}]$ which is of order 30 Å in $2H$-$TaSe_2$. This length is the healing length for phase distortions in the commensurate phase and establishes the core thickness of the DC. ξ_c does not diverge at the phase transition; it is a constant.

The free energy of one DC is found by substituting $\theta(x)$ into (9). Near the transition temperature we find for the energy per unit length of one DC

$$E_D = F^0\beta \times 1.698(Y - Y_c), \tag{16}$$

with $Y_c = 1.2337$ in agreement with Y_c determined in Sec. II. Since the density of DCs is $3\delta/2\pi$, the first term in the free energy of the incommensurate phase (11) is just the energy of the DCs present.

The energy of a DC is minimum if the line is in the $\hat{y}$ direction. If the DC lies at an angle Θ with respect to the $\hat{y}$ axis the energy per unit length (in the y direction) is

$$E_D(\theta) = F^0[\beta \times 1.698(Y - Y_c) + \gamma\theta^2 2.094]. \tag{17}$$

The DC strain falls off as $e^{-\alpha|x|}$ so one expects the interaction energy of two DCs to be proportional to $e^{-\alpha R}$ where R is the separation. Writing the interaction energy as

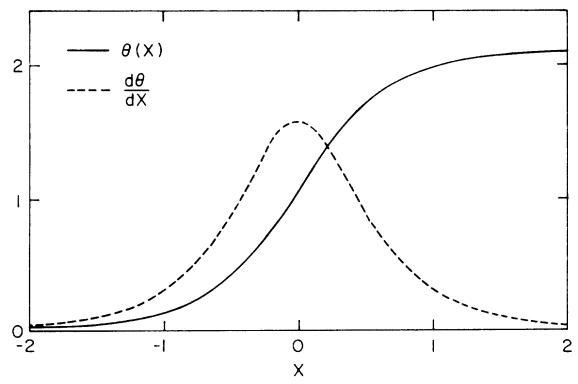

FIG. 4. Phase and gradient of the phase of the CDW relative to perfectly locked-in CDW for a single discommensuration at the lock-in temperature.

$$V_{DD} = V_0 e^{-\alpha R}, \tag{18}$$

the free energy in the incommensurate phase is

$$\Delta F = E_D(3\delta/2\pi) + V_0(3\delta/2\pi)e^{-2\pi\alpha/3\delta}. \tag{19}$$

From a fit to the free energy versus δ in the incommensurate phase at $Y = Y_c$ we find $V_0 = F^0\beta \times 16.8$ which fit yields (11). Thus the free energy and structure of the incommensurate phase near T_{CI} are interpreted in terms of a finite density of DCs. In the commensurate phase there are no DCs present in equilibrium. Thus we see that the natural physical interpretation of the commensurate-incommensurate (or lock-in) phase transition is as a defect melting transition with a finite number of defects in the high-temperature phase. The continuous phase transition cannot be described in the conventional Landau way using an order parameter which is finite in the ordered phase and vanishes in the disordered phase.

Let us now consider several effects which might change the character of the phase transition and make it first order. Recall that an approximate calculation, even in the weak-coupling case, yielded a first-order transition; it was only when the weak-coupling model was solved exactly that we found a second-order transition. When the coupling parameter β is not small there will be important amplitude modulation of the CDW as well as phase modulation. The amplitude of the CDW will be smaller in the core of the DC than it is between DCs. This will affect the quantitative behavior of the phase transition. However the interaction between DCs will still be repulsive and this is all that is necessary to ensure a continuous phase transition. The entropy of the DCs is unimportant and cannot affect the character of the phase transition. A weak dependence of lock-in temperature on lattice spacing can make the phase transition weakly first order but this effect may be small enough, in practice, to be negligible. We conclude that, at constant lattice parameter, the onset transition for a single CDW is truly continuous. For the triple CDW case there are DC crossings which may provide an attractive interaction. We cannot conclude that the triple CDW onset transition is continuous until these interactions have been studied in detail. Barmatz *et al.* observe a large hysteresis at the lock-in transition in $2H$-$TaSe_2$ indicating a first-order phase transition. They also observe a strong frequency dependence of the elastic anomaly which might arise from impurity pinning of the defects. Impurity pinning may give rise to extremely long equilibration times at this phase transition.

The weak-coupling model predicts δ as well as the amplitude of Fourier components of the CDW

(which can be measured by elastic neutron scattering). The magnitude of the Landau theory parameters are not known yet; however, both δ and the Fourier amplitudes are universal functions of reduced temperature in the weak coupling limit and we can compare our results directly with the neutron measurements. Moncton *et al.* observe a decrease of δ of a factor of 4 between $t=1$ and $t\approx 0.1$, whereas the weak-coupling model predicts a decrease of a factor of 1.5. Moncton *et al.* find the amplitude of the e^{2ix} Fourier component of about 0.3 relative to the primary e^{-ix} component at $t\approx 0.3$. We find that amplitude ($=\frac{1}{2}A_1$) equal to 0.1 at the same temperature. Obviously the weak coupling model is in poor quantitative agreement with the neutron measurements. One clear reason for the discrepancies is that the coupling parameter β is not weak in $2H$-$TaSe_2$. There is a rather large jump in the CDW amplitude at lock in which indicates a large value of β. The value of the weak coupling calculation is that it provides a simple qualitative picture of the lock-in transition with qualitatively new features.

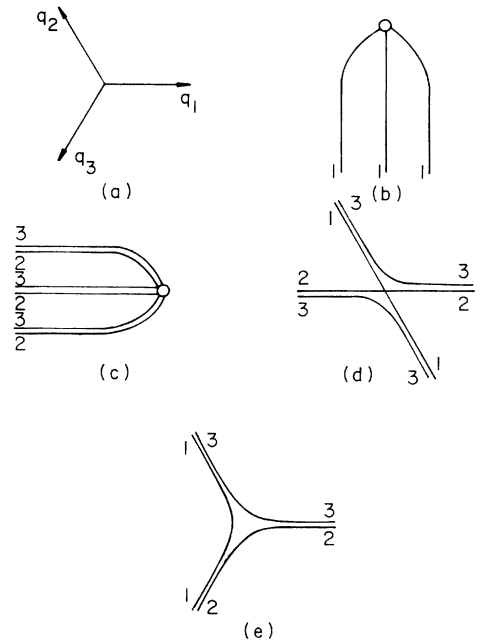

FIG. 5. (a) q vectors for the three CDWs in $2H$-$TaSe_2$. (b) Three DCs in the single CDW state terminating in a CDW dislocation (circle). (c) Three type-23 DCs in the triple CDW state terminating in a CDW dislocation (circle). (d) Type-13 DC crossing a type-23 DC with no point singularities in the CDWs. (e) Three DCs, one of each type, intersecting with no point singularities in the CDWs.

IV. RELATIONSHIP TO CDW DISLOCATIONS

We consider still the simple case of one layer (two-dimensional problem, line DCs) and only one CDW. As the temperature is lowered toward the lock-in phase transition the equilibrium density of DCs decreases and we wish to discuss the way in which DCs are removed from the system. In a large monodomain a modest amount of pinning at grain boundaries or impurities will prevent macroscopic motion of the CDW to push DCs out the ends of the sample. However there is a mechanism by which DCs can be terminated in a CDW dislocation and then removed by CDW dislocation motion. One DC involves a phase change of $\frac{2}{3}\pi$ of the CDW with respect to the lattice. With a perfect crystalline lattice there is no way to terminate one DC because of the nonintegral phase difference (a crystalline dislocation must terminate a DC since the dislocation removes one line of atoms which is equivalent to a $\frac{2}{3}\pi$ phase shift). However three similar DCs can be brought together at a point and give a total phase change of 2π along any path around that point. Such a point singularity is just a CDW dislocation [see Fig. 5(a)] and three DCs can be removed from the system by the traverse of one CDW dislocation. It must be emphasized that the CDW dislocation is a defect in the charge-density wave only and that the crystalline lattice is assumed to be perfect. Thus in order to approach equilibrium after a change in temperature there must be motion of dislocations across the sample to adjust the number of DCs. Near the phase transition the free-energy minimum (as a function of δ) is shallow, the forces driving the dislocations are weak, and the equilibrium times are correspondingly long.

The DC dislocation picture of the lock-in phase transition provides a natural explanation for the Young's modulus experiments of Barmatz *et al.* These authors observe a sharp decrease of Young's modulus of $2H$-$TaSe_2$ near the lock-in phase transition as well as low-frequency loss. In the experiment the crystal is bent in such a way that the crystalline lattice of one layer is expanded in one direction and contracted in the orthogonal direction to maintain constant volume. We assume a triple CDW with the lattice expansion in the direction of one CDW. Since the incommensurate CDW wavelength is somewhat longer than the commensurate CDW wavelength $\frac{1}{2}(3\sqrt{3}\,a)$ (a is the lattice spacing), expanding the lattice will bring these wavelengths closer together and will cause the CDW to lock in at a higher temperature. Thus modulation of the strain modulates T_{CI} as well as the equilibrium number of DCs. The linear term in the free energy is then

$$\epsilon \left(\frac{\partial T_{CI}}{\partial \epsilon}\right) \frac{\partial F_D}{\partial T}, \tag{20}$$

where ϵ is the strain and F_D is the DC free energy computed in Sec. II. The other two CDWs feel a contraction of the lattice of $\frac{1}{2}\epsilon$ and the linear contributions to the free energy from the three CDW's cancel. The second-order term is

$$\tfrac{3}{2}\epsilon^2 \left(\frac{\partial T_{CI}}{\partial \epsilon}\right) \frac{\partial^2 F_D}{\partial T^2}. \tag{21}$$

The rapidly varying part of $\partial^2 F_D/\partial T^2$ is just the heat capacity so that Young's modulus is predicted to behave as

$$Y = Y_0 - \tfrac{3}{2}\left(\frac{\partial T_{CI}}{\partial \epsilon}\right)^2 C_V^D, \tag{22}$$

where C_V^D is the DC heat capacity of one CDW (the heat capacity of Fig. 2). The theory explains why only a small anomaly is observed in Y at the onset transition and predicts a large negative anomaly above the lock-in transition. Barmatz *et al.* observe a strong negative anomaly at the lock-in transition but the anomaly appears to be as large or larger in the commensurate phase where the theoretical model predicts a constant heat capacity (near the lock-in transition). Heat-capacity measurements are not yet available to check the heat-capacity predictions of the model. The weak coupling model provides at least a qualitative explanation for the Young's modulus anomaly. The losses observed near the lock-in transition may be due to the CDW dislocation motion involved in removing discommensurations from the sample. Barmatz *et al.* have suggested CDW dislocation motion as a possible loss mechanism near the onset transition.

V. THREE-DIMENSIONAL ASPECTS

We digress to discuss the phasing of CDWs on neighboring layers in a three-dimensional crystal. We consider the triple CDW case in the incommensurate phase. There is a cubic term (proportional to b_0) in the free energy which is optimized if the relative phases of the three CDWs in one layer are zero with respect to a particular origin in space. This phasing piles up the charge density from the three CDWs at lattice sites of a two-dimensional hexagonal lattice. The interlayer Coulomb interaction, on the other hand, is optimized when the CDWs with the same $\vec{q}$ vector on neighboring planes are out of phase. This phasing is inconsistent with that required to optimize the cubic term and the CDWs adopt an intermediate phase relationship which we now calculate.

Using the free energy (5) we assume

$$\psi_{1j}(\vec{r}) = \psi_0 \exp[i\vec{q}_j \cdot \vec{r} + i(-1)^l \epsilon], \tag{23}$$

with $\psi_0^2 = -2a_0/(15c_0 - 8d_0)$ and find for the free energy per layer per unit area

$$F = \text{const.} - \tfrac{3}{2}b_0\psi_0^3 \cos(3\epsilon) + g\psi_0^2 \cos(2\epsilon). \tag{24}$$

Minimizing F with respect to ϵ, we find

$$z \sin(3\epsilon) = \sin(2\epsilon), \tag{25}$$

with $z = 27b_0\psi_0/4g$. Near the normal-incommensurate transition z is small and $\epsilon \approx \frac{1}{2}\pi$ optimizing the Coulomb term. The cubic term is unimportant at the onset transition and this phase transition is second order (in agreement with experiment[1]). In an earlier treatment neglecting the interlayer Coulomb interaction the cubic term made the onset transition weakly first order. At lower temperature and providing b_0 is large enough z can become large and ϵ approaches $\frac{2}{3}\pi$ optimizing the cubic term. For intermediate values of z, ϵ varies continuously from $\frac{1}{2}\pi$ to $\frac{2}{3}\pi$. Both the relative phasing of the three CDWs in one layer and the relative phasing of CDWs on neighboring layers are fixed by these two terms in the free energy.

We can now discuss qualitatively DCs in the triple CDW commensurate state in three dimensions. A DC in one CDW introduces a phase change of $\frac{2}{3}\pi$ and throws the three CDWs out of phase. It is necessary to introduce a DC into one of the other two CDWs in order to restore the proper phasing of the CDWs. We label the CDWs 1, 2, or 3 according to whether the q vector is $\vec{q}_1$, $\vec{q}_2$, or $\vec{q}_3$. A DC in CDW_1 and CDW_2 we will call a type 12 DC. There are three types, 12, 23, and 13. Recall[4] that in the CDW dislocation the 2π phase change occurred in two of the three CDWs. Thus three DCs of the same type can terminate in a CDW dislocation as shown in Fig. 5(c). In addition it is possible for three DCs, one of each type, to intersect without a point singularity in any of the three CDWs [see Fig. 5(e)].

In a three-dimensional system the interlayer Coulomb interaction forces a phase relationship between CDWs on successive layers. Therefore a phase slip of $\frac{2}{3}\pi$ in a CDW in one layer must be near a phase slip of $\frac{2}{3}\pi$ in the corresponding CDW in a neighboring layer. The DC therefore extends from one layer to another and the defect is a planar (two-dimensional) object in the three-dimensional system. The minimum energy configuration for a type-12 DC is a flat plane perpendicular to the $\vec{q}_3$ direction. The DC plane may be curved but it costs elastic energy to do so. We can describe a general type-12 DC by specifying the y coordinate $y(x,z)$ as a function of x and z, with $\hat{x}$ lying in the $\vec{q}_3$ direction and $\hat{z}$ being normal to the layers. The elastic energy is then

$$E_D = \int dxdz \left[A(T_{CI} - T) + B\left(\frac{\partial y}{\partial x}\right)^2 + C\left(\frac{\partial y}{\partial z}\right)^2 \right], \tag{26}$$

where the first term is the energy to create the DC, the second is the orientational energy to rotate it from the preferred direction, and the third term is the Coulomb energy necessary to slip the DC in one layer relative to the neighboring layer. DCs interact via (18).

VI. CONCLUSIONS

We have presented a new physical picture of the lock-in transition in $2H$-$TaSe_2$ based on an exact solution of the free energy optimization problem in the weak coupling limit. We have introduced a new CDW defect, the discommensuration, and have shown that the phase transition is continuous and can be viewed as a defect melting transition. The theory is in qualitative agreement with available neutron diffraction data and provides a qualitative explanation of the Young's modulus anomaly at the lock-in transition. The discommensuration should be directly observable in the electron microscope. There is a pressing need for quality heat-capacity work to determine the nature of the phase transition experimentally.

This work began as an attempt to explain the Young's modulus anomaly. I would like to thank M. Barmatz, L. R. Testardi, and F. J. DiSalvo for several stimulating discussions and for a preprint of Ref. 3.

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