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Structure factor of a charge-density wave

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The elastic structure factor of an unpinned charge-density wave (CDW) is derived. Both phase and amplitude excitations are studied. Phase modes cause a reduction of the intensity of CDW satellite peaks of any order. Amplitude modes, however, do not alter appreciably the intensity of the first-order CDW satellite. In fact, they enhance the intensity of peaks of higher order on account of their nonlinear nature. Neither phase nor amplitude excitations affect the usual Bragg reflections. The mean-square fluctuation of the CDW phase and the associated reduction of the satellite peaks are discussed for the case of potassium and are shown to depend critically on the phason spectrum.

I. INTRODUCTION

Systems containing incommensurate modulations of normal crystalline periodicity have recently attracted much interest. In particular incommensurate spin-density-wave[1] and charge-density-wave[2] (CDW) systems have been studied extensively since their observation in chromium[3] and in layered compounds.[4]

An interesting feature of these materials is the existence of a new branch of acoustic, collective modes named phasons[5] associated with fluctuations in space and time of the relative phase between the lattice and the incommensurate modulation. Such extra low-frequency modes, which coexist and merge with the normal acoustic phonons,[6] affect many physical properties. Examples are the low-temperature heat capacity,[7-9] electrical resistivity,[10] NMR spectrum,[11] lattice thermal conductivity, and diffraction pattern.[5,11] The latter phenomenon is the object of the present paper. Our emphasis will be on CDW systems but most of our results are directly applicable to any displacive, incommensurate modulated structure.[12]

The static structure factor of an incommensurate CDW has been thoroughly studied in Ref. 5, where it was shown that new collective modes associated with CDW phase modulation provide a peculiar contribution to the Debye-Waller factor of the CDW satellites in a diffraction pattern. In the present paper we extend the analysis of the structure factor to include the amplitude modes.[13] This is necessary for a complete and consistent treatment. The paper is organized as follows: In Sec. II we derive the general expression for the structure factor of an incommensurate CDW. In Sec. III we propose a theoretical model for the dispersion relation of the lowest-lying collective modes. In Sec. IV we discuss the temperature dependence of the CDW structure factor and the mean-square fluctuations of the phase and amplitude variables. Finally Sec. V contains further discussion and application, especially to some problems involving alkali metals.

II. DYNAMICAL STRUCTURE FACTOR FOR A CDW

The dynamical structure factor for an array of N ions is given by[14]

$$S_{\vec{k},\omega}=\frac{1}{N}\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{-i\omega t}\sum_{i,j}\langle e^{i\vec{k}\cdot\vec{R}_i(t)}e^{-i\vec{k}\cdot\vec{R}_j(0)}\rangle_T, \quad (1)$$

where $\vec{R}_i(t)$ represents the position of an ion i at time t. The subscript T denotes that a thermal average is taken over an equilibrium distribution of states. In a CDW system the ionic lattice undergoes a small distortion from the normal crystal situation.[2] The new equilibrium positions are given by

$$\vec{R}_i=\vec{R}_i^0+\vec{A}_0\sin(\vec{Q}'\cdot\vec{R}_i^0+\phi_0), \quad (2)$$

where $\vec{R}_i^0$ is the equilibrium position of the ion i in the undistorted lattice. $\vec{Q}'$, $\vec{A}_0$, and ϕ_0 are the wave vector, amplitude, and phase of the CDW in the ground state. $\vec{Q}'$ is the Brillouin-zone reduction of $\vec{Q}$, the wave vector of the corresponding electronic-charge-density modulation, which is assumed to be incommensurate with respect to the ionic lattice.

In a CDW system the vibrational modes of the lattice are strongly modified for wave vectors near the CDW wave vector $\vec{Q}'$. In this region the eigenstates of the distorted lattice are phasons[5] and amplitons.[13] These vibrational modes are associated with modulations of the phase ϕ and magnitude $|\vec{A}_0|$ of the CDW ionic displacements.

Away from $\vec{Q}'$ these new modes merge with the phonon modes. The effects of phonons on the structure factor are well known. Moreover, pho-

nons are not relevant as far as the typical features of the distorted state are concerned. For instance, they do not affect appreciably the ratio of the CDW satellite intensities to the usual Bragg reflections in a diffraction analysis.[5,11,15] Accordingly we will disregard altogether these degrees of freedom in what follows. Allowance for phase and amplitude modulations in the CDW causes the positions of the ions, Eq. (2), to change in time and in space.

$$\vec{R}_i(t) = \vec{R}_i^0 + \vec{A}_0[1 + \delta A(\vec{R}_i^0, t)] \times \sin[\vec{Q}' \cdot \vec{R}_i^0 + \delta\phi(\vec{R}_i^0, t)] , \tag{3}$$

where $\delta\phi$ and δA are the magnitudes of the phase and amplitude modulations. For convenience ϕ_0 has been taken to be zero.

Inserting Eq. (3) into (1) we obtain

$$S_{\vec{k},\omega} = \frac{1}{N}\sum_{i,j}\sum_{n,m=-\infty}^{+\infty} e^{i\vec{k}\cdot(\vec{R}_i^0 - \vec{R}_j^0)} e^{i\vec{Q}'\cdot(n\vec{R}_i^0 - m\vec{R}_j^0)} J_n(\vec{k}\cdot\vec{A}_0) J_m(\vec{k}\cdot\vec{A}_0) \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{-i\omega t} \Phi_{nm,ij}(t) A_{nm,ij}(t) , \tag{4}$$

where n and m are integers and J_n is a Bessel function of the first kind. The functions $\Phi_{nm,ij}$ and $A_{nm,ij}$ are defined as follows:

$$\Phi_{nm,ij}(t) = \langle e^{in\delta\phi(\vec{R}_i^0, t)} e^{-im\delta\phi(\vec{R}_j^0, 0)} \rangle_T , \tag{5}$$

$$A_{nm,ij}(t) = \frac{\langle J_n\{\vec{k}\cdot\vec{A}_0[1 + \delta A(\vec{R}_i^0, t)]\} J_m\{\vec{k}\cdot\vec{A}_0[1 + \delta A(\vec{R}_j^0, 0)]\}\rangle_T}{J_n(\vec{k}\cdot\vec{A}_0) J_m(\vec{k}\cdot\vec{A}_0)} . \tag{6}$$

These quantities are correlation functions and contain the dynamics of the phase and amplitude modulations. In obtaining Eq. (4) extensive use has been made of the Jacobi-Anger generating function for the Bessel functions:

$$e^{iz\sin x} = \sum_{n=-\infty}^{+\infty} e^{inx} J_n(z) . \tag{7}$$

Finally since the eigenvectors of the amplitude and the phase modes are orthogonal, the average in Eq. (1) can be carried out independently for the two categories of fluctuation.

A. Phase excitations

We start with the quantization of the phase variable $\delta\phi$ of the CDW. Accordingly the phase field $\delta\hat{\phi}(\vec{R}_i^0, t)$ is defined as

$$\delta\hat{\phi}(\vec{R}_i, t) = \sum_{\vec{q}} \frac{\delta\phi_{\vec{q}}}{2i} (a_{\vec{q}} e^{i(\vec{q}\cdot\vec{R}_i^0 - \omega_{\vec{q}} t)} - a_{\vec{q}}^\dagger e^{-i(\vec{q}\cdot\vec{R}_i^0 - \omega_{\vec{q}} t)}) , \tag{8}$$

where $\vec{q}$, $\delta\phi_{\vec{q}}$, and $\omega_{\vec{q}}$ are the wave vector, amplitude, and frequency, respectively, of the phase mode created and destroyed by the operators $a_{\vec{q}}^\dagger$ and $a_{\vec{q}}$. These operators satisfy the usual commutation relations for bosons. From Eq. (8) it follows that

$$[\delta\hat{\phi}(\vec{R}_i^0, t), \delta\hat{\phi}(\vec{R}_j^0, 0)] = -2i\sum_{\vec{q}} \left|\frac{\delta\phi_{\vec{q}}}{2}\right|^2 \sin[\gamma_{ij}(\vec{q}, t)] , \tag{9}$$

where $\gamma_{ij}(\vec{q}, t)$ is an abbreviation for $\vec{q}\cdot(\vec{R}_i^0 - \vec{R}_j^0) - \omega_{\vec{q}} t$. This commutator is clearly a c number, and both $\delta\hat{\phi}(\vec{R}_i^0, t)$ and $\delta\hat{\phi}(\vec{R}_j^0, 0)$ commute with it. Now the function $\Phi_{nm,ij}$ of Eq. (5) can be expressed as

$$\Phi_{nm,ij}(t) = \exp\left(nm\sum_{\vec{q}} \left|\frac{\delta\phi_{\vec{q}}}{2}\right|^2 \sin[\gamma_{ij}(\vec{q}, t)]\right) \langle \exp\{i[n\delta\hat{\phi}(\vec{R}_i^0, t) - m\delta\phi(\vec{R}_j^0, 0)]\}\rangle_T . \tag{10}$$

Since the exponent in the last factor is a linear form in the boson operators $a_{\vec{q}}$, the thermal average in Eq. (10) reduces to a simpler result when we take the phasons to be harmonic oscillators.

$$\langle \exp i[n\delta\hat{\phi}(\vec{R}_i^0, t) - m\delta\hat{\phi}(\vec{R}_j, 0)]\rangle_T = \exp -\tfrac{1}{2}\langle |n\delta\phi(\vec{R}_i^0, t) - m\delta\phi(\vec{R}_j^0, 0)|^2\rangle_T . \tag{11}$$

The remaining thermal average is then computed in a straightforward manner with the aid of Eq. (8), i.e.,

$$\langle |n\delta\hat{\phi}(\vec{R}_i^0, t) - m\delta\hat{\phi}(\vec{R}_j, 0)|^2\rangle_T = \sum_{\vec{q}} \left|\frac{\delta\phi_{\vec{q}}}{2}\right|^2 (2N_{\vec{q}} + 1)\{n^2 + m^2 - 2nm\cos[\gamma_{ij}(\vec{q}, t)]\} . \tag{12}$$

$N_{\vec{q}}$ is the temperature-dependent mean occupation number of the phason mode of $\vec{q}$, $\langle a^{\dagger}_{\vec{q}} a_{\vec{q}} \rangle_T$, and is given by the usual expression $[\exp(\hbar\omega_{\vec{q}}/k_B T) - 1]^{-1}$.

The mean-square fluctuation of the phase at a given lattice site is defined by

$$\langle \delta\phi^2 \rangle = \langle | \delta\phi(\vec{R}^0_i, t) |^2 \rangle_T . \tag{13}$$

By means of Eq. (8) one can readily show that

$$\langle \delta\phi^2 \rangle = \sum_{\vec{q}} \left| \frac{\delta\phi_{\vec{q}}}{2} \right|^2 (2N_{\vec{q}} + 1) \tag{14}$$

Then with the use of Eqs. (10), (11), (12), and (14) the function $\Phi_{nm,ij}$ can be finally written as

$$\Phi_{nm,ij}(t) = \exp[-\tfrac{1}{2}(n^2 + m^2)\langle \delta\phi^2 \rangle] \exp nm \sum_{\vec{q}} \left| \frac{\delta\phi_{\vec{q}}}{2} \right|^2 \{(2N_{\vec{q}} + 1)\cos[\gamma_{ij}(\vec{q}, t)] + i \sin[\gamma_{ij}(\vec{q}, t)]\} . \tag{15}$$

If we define Φ_{nm} as the time-independent component of the function $\Phi_{nm,ij}(t)$ we have

$$\Phi_{nm} = e^{-1/2(n^2+m^2)\langle \delta\phi^2 \rangle} . \tag{16}$$

B. Amplitude excitations

Consider the function $J_n[\vec{k} \cdot \vec{A}_0(1 + \delta A)]$ entering Eq. (6). For small amplitude modulations we can expand this quantity to second order in δA. In the limit of small CDW amplitude, $(\vec{k} \cdot \vec{A}_0 \ll 1)$, we use standard recursion relations for the Bessel functions and write

$$J_n\{\vec{k} \cdot \vec{A}_0[1 + \delta A(\vec{R}^0_i, t)]\} \simeq J_n(\vec{k} \cdot \vec{A}_0) \left(1 + |n| \delta A(\vec{R}^0_i, t) + \frac{|n|(|n| - 1)}{2} \delta A^2(\vec{R}^0_i, t)\right) . \tag{17}$$

In analogy with Eq. (8) we introduce the field $\delta\hat{A}(\vec{R}^0_i, t)$ defined as

$$\delta\hat{A}(\vec{R}^0_i, t) = \sum_{\vec{q}} \frac{\delta A_{\vec{q}}}{2i} \left(b_{\vec{q}} e^{i(\vec{q} \cdot \vec{R}^0_i - \Omega_{\vec{q}} t)} - b^{\dagger}_{\vec{q}} e^{-i(\vec{q} \cdot \vec{R}^0_i - \Omega_{\vec{q}} t)}\right) , \tag{18}$$

where $\vec{q}$, $\delta A_{\vec{q}}$, and $\Omega_{\vec{q}}$ are the wave vector, amplitude, and frequency, respectively, of the amplitons created or destroyed by the operators $b^{\dagger}_{\vec{q}}$ and $b_{\vec{q}}$. These also satisfy the usual commutation rules for bosons. The function $A_{nm,ij}(t)$ can be evaluated explicitly. With the use of Eqs. (17) and (16) in (6), we get

$$A_{nm,ij}(t) \simeq 1 + \tfrac{1}{2}[|n|(|n| - 1) + |m|(|m| - 1)]\langle \delta A^2 \rangle + |nm| \sum_{\vec{q}} \left| \frac{\delta A_{\vec{q}}}{2} \right|^2 \{(2\tilde{N}_{\vec{q}} + 1)\cos[\tilde{\gamma}_{ij}(\vec{q}, t)] + i \sin[\tilde{\gamma}_{ij}(\vec{q}, t)]\} . \tag{19}$$

The functions $\tilde{N}_{\vec{q}}$ and $\tilde{\gamma}_{ij}(\vec{q}, t)$ differ from $N_{\vec{q}}$ and $\gamma_{ij}(\vec{q}, t)$ only by the substitution of $\Omega_{\vec{q}}$ for $\omega_{\vec{q}}$. In complete analogy with $\langle \delta\phi^2 \rangle$, Eq. (13), the CDW fractional amplitude fluctuation $\langle \delta A^2 \rangle$ appearing in Eq. (19) is defined as

$$\langle \delta A^2 \rangle = \langle | A(\vec{R}^0_i, t) |^2 \rangle_T = \sum_{\vec{q}} \left| \frac{\delta A_{\vec{q}}}{2} \right|^2 (2\tilde{N}_{\vec{q}} + 1) . \tag{20}$$

With the use of Eqs. (15) and (18) in (4) the dynamical structure factor of the CDW system can be obtained. Finally notice we use our approximations, $\delta A \ll 1$ and $\vec{k} \cdot \vec{A}_0 \ll 1$, to calculate A_{nm}, the time-independent part of $A_{nm,ij}(t)$. It can be written in the following suggestive way:

$$A_{nm} \simeq \exp\tfrac{1}{2}[|n|(|n| - 1) + |m|(|m| - 1)]\langle \delta A^2 \rangle . \tag{21}$$

The exponent of Eq. (21) is positive definite.

C. Elastic structure factor

We focus our attention now on $S^0_{\vec{k}}$ the elastic part of the dynamic structure factor, Eq. (1). From Eq. (4) it is clear that the elastic contributions to $S_{\vec{k},\omega}$ come only from the time-independent components of both $\Phi_{nm,ij}(t)$, Eq. (5), and $A_{nm,ij}(t)$, Eq. (6). By means of the results (16) and (21) in (4), the elastic structure factor of an incommen-

surate CDW can be expressed as

$$S^0_{\vec{k}} = \sum_{\vec{G}} \sum_{n=-\infty}^{\infty} \delta[\vec{k} - (\vec{G} + n\vec{Q})] J_n^2(\vec{k}\cdot\vec{A}_0) F_n^{\phi}(T) F_n^{A}(T), \tag{22}$$

where $\vec{G}$ is a vector in the reciprocal lattice. The temperature dependence of this quantity is contained in the functions F_n^{ϕ} and F_n^{A} defined as follows:

$$F_n^{\phi}(T) = e^{-2n^2 W_{\phi}(T)}, \tag{23}$$

with

$$W_{\phi}(T) = \tfrac{1}{2}\langle \delta\phi^2 \rangle \tag{24}$$

and

$$F_n^{A}(T) = e^{2|n|(|n|-1)W_A(T)}, \tag{25}$$

with

$$W_A(T) = \tfrac{1}{2}\langle \delta A^2 \rangle . \tag{26}$$

The functions F_n^{ϕ} and F_n^{A} are, respectively, the phason[11] and ampliton temperature factors.

The pattern associated with the elastic structure factor $S^0_{\vec{k}}$, Eq. (22), has been thoroughly discussed in Refs. 5 and 15. We add here just a few remarks. The phason and ampliton temperature factors do not affect the normal Bragg reflections, $(n=0)$. As is apparent from Eq. (23), F_n^{ϕ} plays for the phase modes a role similar to that of the usual Debye-Waller factor. The phase oscillations of a CDW reduce the intensity of the satellite peaks.

The amplitude fluctuations, on the other hand, do not have any significant effect on the intensities of both the Bragg reflections and their first, $(n=1)$, satellites, which are the most relevant features of the diffraction pattern. Finally a noteworthy result is that the intensity of higher-order satellites, $|n| \gtrsim 2$, is enhanced by amplitude fluctuations.[16]

III. EXCITATION SPECTRUM

The strong coupling of phonons with wave vector $\pm\vec{Q}'$ induced by the presence of the electronic CDW gives rise to a qualitative modification of the vibrational dispersion relation. As already pointed out, the regions of the spectrum most strikingly modified are those assigned to phase[5] and amplitude modes.[13] The dispersion relation of the lowest-lying modes is shown schematically in Fig. 1, where the wave vector $\vec{q}$ of a phason (or an ampliton) is also defined. The situation can be described by the following simple model.[9] We start with the assumption that only the lowest acoustic branch of the phonon spectrum of the undistorted lattice is relevant. That is, for $\vec{k} = \pm\vec{Q}'$ the other branchs have much higher frequencies. In this case, for small $\vec{q}$ (i.e., for $\vec{k} \simeq \pm\vec{Q}'$) the vibrational modes of the system can be described by a 2×2 dynamical matrix

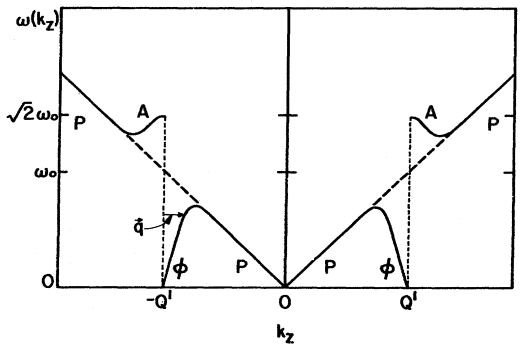

FIG. 1. Schematic dispersion relation for the low-lying excitations of a CDW (in a three-dimensional metal). The phonon, phason, and ampliton regions are denoted by P, ϕ, and A. ω_0 is the frequency of the lowest-energy phonon (of the normal state) at $\vec{k} = \pm\vec{Q}'$. The phason (or ampliton) wave vector $\vec{q}$ is the deviation of $\vec{k}$ from $\pm\vec{Q}'$.

$$D_{ij} = \begin{pmatrix} \omega_0^2 & \omega_0^2 F(\vec{q}) \\ \omega_0^2 F(\vec{q}) & \omega_0^2 \end{pmatrix}, \tag{27}$$

where ω_0 is the frequency of the unperturbed phonons with $\vec{k} = \pm\vec{Q}'$ (see also Fig. 1). These phonons are assumed to be dispersionless in the vicinity of $\pm\vec{Q}'$. The off-diagonal coupling $F(\vec{q})$ is associated with new terms appearing in the electronic dielectric-response matrix and caused by the CDW.[6,13] The spectrum of collective modes described by (27) is given by

$$\omega_{\pm}(\vec{q}) = \omega_0[1 \pm F(\vec{q})]^{1/2}. \tag{28}$$

The frequency ω_+ is Ω (the ampliton frequency), Eq. (18), whereas ω_- is $\omega_{\vec{q}}$ (the phason frequency), Eq. (8). The situation here differs significantly from that of a one-dimensional CDW system. In that case the Peierls mechanism[17] is related to a giant Khon anomaly[13,18] in the phonon spectrum. Such an effect need not occur in the diagonal part of the dynamical matrix, Eq. (27).

The function $F(\vec{q})$ dictates the crossover region where phase and amplitude mode merge into normal phonons (as $|\vec{q}|$ increases). The knowledge of this function is crucial in the present context since (as discussed above) the two different sets of collective modes contribute in a completely different way to the Debye-Waller factor of the system. At present a theory for $F(\vec{q})$ is not at hand. Nevertheless the problem can be easily solved in the limit of long wavelength $(\vec{q} \to 0)$ by taking advantage of the phason dispersion relation which is known in this regime.

As was first shown in Ref. 5, the phason frequency goes to zero linearly with $|\vec{q}|$ and can be expressed as

$$\omega_{\vec{q}} = (c_x^2 q_x^2 + c_y^2 q_y^2 + c_z^2 q_z^2)^{1/2}, \vec{q} \to 0 . \tag{29}$$

c_x, c_y, and c_z are the phason velocities along orthogonal principal axes $\hat{x}$, $\hat{y}$, and $\hat{z}$. Usually $\hat{z}$ can be taken along $\vec{Q}$. $\omega_{\vec{q}}$ is in general very anisotropic. In jellium, for instance, the spatial isotropy causes c_x and c_y, the transverse-phason velocities, to be zero. (The longitudinal-phason velocity c_z is finite.) For a CDW in simple metals c_x and c_y are expected to be of the order of magnitude as the sound velocity,[19] whereas c_z is thought to be larger by one order of magnitude.[9,20]

If we substitute $\omega_{\vec{q}}$, Eq. (29), for ω_- in Eq. (28), we obtain

$$F(\vec{q}) = 1 - \frac{(c_x^2 q_x^2 + c_y^2 q_y^2 + c_z^2 q_z^2)}{\omega_0^2}, \vec{q} \to 0 . \tag{30}$$

The corresponding expression for $\Omega_{\vec{q}}$, the ampliton frequency, is obtained from (28).

$$\Omega_{\vec{q}} = [2\omega_0^2 - (c_x^2 q_x^2 + c_y^2 q_y^2 + c_z^2 q_z^2)]^{1/2}, \vec{q} \to 0 . \tag{31}$$

Expressions (29), (30), and (31) provide a correct description of the excitation spectrum only for small $|\vec{q}|$, but fail to account for the details of the dispersion relation when $\omega_{\vec{q}}$, Eq. (29), becomes comparable to ω_0. A model for $F(\vec{q})$ can be postulated when such details are needed.[9]

IV. PHASON AND AMPLITON TEMPERATURE FACTORS

This section is devoted to the study of the temperature dependence of both the phason and ampliton temperature factors F_n^ϕ and F_n^A.

A. Phasons: W_ϕ

The quantity W_ϕ is proportional to the mean-square fluctuation of the CDW phase and is defined in Eq. (23). With the use of Eq. (14) we can write

$$W_\phi = \tfrac{1}{8} \sum_{\vec{q}} |\delta\phi_{\vec{q}}|^2 \coth\left(\frac{\hbar\omega_{\vec{q}}}{2k_B T}\right) , \tag{32}$$

where the sum runs over all the N_ϕ phason modes of the system. The virial theorem allows us to obtain the amplitude coefficient of a single phase mode, defined by Eq. (8).

$$\delta\phi_{\vec{q}} = \left(\frac{4\hbar}{\rho V A_0^2 \omega_{\vec{q}}}\right)^{1/2} , \tag{33}$$

where ρ and V are the mass density and the total volume of the ionic lattice. As discussed in Refs. 5 and 11, W_ϕ does not depend explicitly upon the magnitude of the CDW wave vector $\vec{Q}'$. Notice also that the contribution to W_ϕ of a phason compared to an equivalent phonon's contribution to the Debye-Waller factor is a ratio (in the exponent) of $(|\vec{G}|A_0)^{-2}$, typically of the order of 10^3. Of course this factor does not carry through to the total sum (32) when compared to the total Debye-Waller factor, since N_ϕ is much smaller than $3N$, the total number of vibrational modes of a monatomic lattice.

The qualitative behavior of W_ϕ as a function of temperature can be readily obtained by an explicit evaluation of the sum (32). We approximate $\omega_{\vec{q}}$ by Eq. (29). The phason wave-vector space is then taken as the volume in $\vec{q}$ space contained in a surface of constant frequency ω_0, the frequency at $\vec{Q}'$ of the lowest-energy phonon of the normal lattice.[21] Due to the strong anisotropy of the phason spectrum, such a region of the Brillouin zone has the shape of a pancake with the short axis along $\vec{Q}$. Within this model the quantity $W_\phi(T)$ can be expressed as

$$W_\phi(T) = W_\phi^0 f_\phi(T) , \tag{34}$$

where the temperature-dependent function of $f_\phi(T)$ is

$$f_\phi(T) = 8\left(\frac{T}{\Theta_\phi}\right)^2 \int_0^{\Theta_\phi/2T} dx\, x \coth x . \tag{35}$$

Θ_ϕ is the phason characteristic temperature defined as $\Theta_\phi = \hbar\omega_0/k_B$. The constant factor W_ϕ^0 in Eq. (34) is

$$W_\phi^0 = \frac{\eta(k_B\Theta_\phi)^2}{8\pi^2\hbar\rho A_0^2 C_\perp^3} . \tag{36}$$

An average transverse-phason velocity $c_\perp \equiv \sqrt{c_x c_y}$ has been introduced together with the quantity η, the phason anisotropy ratio, defined as

$$\eta = \frac{c_\perp}{c_z} . \tag{37}$$

If the temperature is much smaller than the cutoff Θ_ϕ, $f_\phi(T) \simeq 1$, i.e.,

$$\lim_{T/\Theta_\phi \to 0} W_\phi(T) = W_\phi^0 . \tag{38}$$

W_ϕ^0 represents the contribution of zero-point phase fluctuations of the CDW. In the high-temperature limit, when T is greater than Θ_ϕ, W_ϕ is proportional to T. In this regime we can write

$$W_\phi(T) \simeq 4\,\frac{T}{\Theta_\phi} W_\phi^0, \quad T > \Theta_\phi . \tag{39}$$

The temperature dependence of F_n^ϕ, Eq. (23), is readily deduced with the use of Eqs. (35), (38), and (39). As the temperature increases F_n^ϕ goes

to zero exponentially with T from its zero-temperature value $\exp(-n^2W_\phi^0)$.

B. Amplitons: W_A

The mean-square fluctuation of the fractional amplitude of the CDW, $2W_A$, Eq. (26), can be rewritten by means of Eq. (20) as

$$W_A = \frac{1}{8}\sum_{\vec{q}} |\delta A_{\vec{q}}|^2 \coth(\hbar\Omega_{\vec{q}}/2k_BT). \tag{40}$$

The sum in Eq. (40) runs over the same range of $\vec{q}$ as in Eq. (32). Then the analysis can be carried out with the use of Eq. (31) and follows the same procedure outlined in the discussion of W_ϕ. For the sake of brevity, we report here just the most relevant steps and results.

The virial theorem allows us to show that $\delta A_{\vec{q}}$ is also given by Eq. (33), with $\Omega_{\vec{q}}$ replacing $\omega_{\vec{q}}$. The final result can be cast in the following form:

$$W_A(T) = W_A^0 f_A(T), \tag{41}$$

with

$$W_A^0 = \frac{\pi - 2}{2} W_\phi^0 \simeq 0.57 W_\phi^0 \tag{42}$$

and

$$f_A(T) = \frac{4}{\pi - 2}\int_0^1 dx \frac{x^2}{(2-x^2)^{1/2}} \coth\left(\frac{\Theta_\phi}{2T}(2-x^2)^{1/2}\right). \tag{43}$$

Notice that the zero-point, fractional-amplitude fluctuations, Eq. (42), are roughly half of the corresponding phase fluctuations. In the high-temperature limit $W_A(T)$ increases also linearly with T, with a slope which is approximately one-quarter of the corresponding slope of $W_\phi(T)$, Eq. (39). The behavior of $F_n^A(T)$, $|n| \geq 2$, is obtained via Eq. (25) and is of course the inverse of that of $F_n^\phi(T)$, as the signs of the exponents in Eq. (23) and (25) differ. From its zero-temperature value, $\exp[|n|(|n|-1)W_A^0]$, $F_n^A(T)$ grows exponentially with T. Nevertheless the product $F_n^A(T)F_n^\phi(T)$, entering the expression for the CDW structure factor, Eq. (22), goes to zero exponentially as the temperature is increased.

V. DISCUSSION

In the previous sections we have discussed the theory of the dynamical structure factor in a CDW system. The elastic part of this quantity can be directly analyzed by a neutron-diffraction experiment. The typical signature of a CDW is the presence of extra spots, the satellite reflections, in the diffraction pattern.[2] The ratio of the intensity of a satellite peak $\vec{k} = \vec{G} + n\vec{Q}$ to that of a normal Bragg reflection $\vec{k} = \vec{G}$, can be readily expressed with the use of Eq. (22):

$$\frac{I_{\vec{G}+n\vec{Q}}}{I_{\vec{G}}} = \left(\frac{J_n[(\vec{G}+n\vec{Q})\cdot\vec{A}_0]}{J_0(\vec{G}\cdot\vec{A}_0)}\right)^2 F_n^\phi(T)F_n^A(T). \tag{44}$$

F_n^ϕ and F_n^A are given in Eqs. (23) and (25). In particular, for the first-order satellite this ratio is[23]

$$\frac{I_{\vec{G}+\vec{Q}}}{I_{\vec{G}}} \simeq \left(\frac{(\vec{G}+\vec{Q})\cdot\vec{A}_0}{2}\right)^2 e^{-2W_\phi(T)}. \tag{45}$$

This quantity is explicitly evaluated in Ref. 15 for the case of a CDW state in metallic potassium. Equation (45) gives also a satisfactory description of the temperature dependence of the satellite spots in the quasi-one-dimensional conductor KCP.[11] Notice that for *higher-order* satellites the amplitude fluctuations tend to oppose the reduction of intensity caused by phase fluctuations. This phenomenon may be relevant in the explanation of the anomalously intense high-order satellites observed in modulated structures such as Na_2CO_3.[24]

Recently the authors discussed some aspects of lattice dynamics in alkali metals assumed to have a CDW ground state.[15,19,25] In particular the CDW amplitude $|\vec{A}_0|$ and the average transverse-phason velocity $c_\perp$ were calculated. The specific values for potassium are $|\vec{A}_0| \simeq 0.03$ Å (Ref. 15) and $c_\perp \simeq 1.4\times10^5$ cm/sec.[19] As far as the phason anisotropy ratio η [Eq. (37)] is concerned, no theory is currently at hand. However an estimate for this quantity can be obtained in an indirect way by fitting experimental data.[9,20] According to those analyses, η is thought to be roughly 0.1. Furthermore if ω_0, the frequency cutoff for phasons, is chosen as in Sec. IV, its value for potassium is $\omega_0 \simeq 1.2\times10^{12}$ Hz. Accordingly $\Theta_\phi \simeq 9$ K. With the use of Eq. (36) we can now evaluate the zero-point, mean-square phase fluctuation for this CDW model. The result is $W_\phi^0 \simeq 0.85\times10^{-2}$, corresponding to a temperature factor which is practically unity at zero temperature. At $T \sim 10$ K, $W_\phi(T) \simeq 0.37$. The reduction of the satellite intensity would be given by $F_1^\phi = \exp[-2W_\phi(T)] \simeq 0.93$.

This indicates that at low temperatures ($T \leq 10$ K), the phase fluctuations in the system are small and do not seriously reduce the satellite intensity. It should be noticed, however, that W_ϕ^0 is extremely sensitive to the value of $c_\perp$: a change of a factor of three in $c_\perp$, for instance, would completely reverse these conclusions.

The phase fluctuations in a CDW are also relevant in the NMR spectrum. A static CDW theory for the NMR spectrum in potassium[11,26] leads to an inhomogeneous shift having a full width of ~40 G.[27] What is observed[26] is a single narrow line with a full width of ~0.2 G. This result could be explained

within a CDW model if motional narrowing of the Knight shift by thermal phase fluctuations[11] were large. The results obtained above seem to make this explanation unlikely. The discrepant NMR linewidth is an important challenge for the CDW theory of alkali metals.

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