Commensurability effects and collective excitations in systems with charge-density waves

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The spectrum of the collective excitations in the state of a noncommensurate charge-density wave (NCDW) is considered within the framework of a phenomenological approach, with account taken of commensurability effects. A model is investigated in which commensurability effects lead only to spatial changes of the CDW phase in the ground state of the system at a constant wave amplitude. In this model the NCDW superstructure consists of domains in which the CDW is almost commensurate with the host lattice, and which are separated by domain walls (solitons). It is shown that in such a phase there exist two branches of the collective CDW oscillations: an optical branch with a gap determined by the commensurability effects, and a zero-gap acoustic branch, which can be interpreted as the oscillations of the domain walls. The course of the transition to the commensurable case is traced. The conditions for the validity of the considered model are discussed.

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1. INTRODUCTION

Charge-density waves (CDW) have been observed recently in a large number of quasi-one-dimensional and layered compounds (see, e.g.,[1-3]). In the description of the properties of such systems, an important role is played by the characteristics of the collective excitations, principally oscillations of the CDW.[4] In the simplest case, without allowance for the scattering by the impurities and of commensurability effects, there exists in the system an optically active Fröhlich collective mode (FCM) with a spectrum that starts with zero; this mode makes a substantial contribution to the dielectric constant and to the conductivity of a system with CDW.[4,5]

In the commensurate phase a gap appears in the spectrum of the FCM that corresponds to small-amplitude oscillations of the CDW phase. In additions, among the excitations of the commensurate charge density wave (CCDW) there are large-amplitude changes of the CDW phase. Such excitations (solitons) are the consequence of the nonlinearity that appears in the system as a result of the commensurability effects.[6,7] Thus, in the commensurate phase the commensurability effects alter radically the spectrum of the phase oscillations, eliminating the acoustic character of the dispersion of the FCM as well as the Fröhlich dc conductivity.

The commensurability energy, however, may turn out to be significant also in the noncommensurate phase—it can alter the detailed structure of the ground state and the character of the oscillation spectrum of the CDW. For one-dimensional systems, the structure of the ground state of the noncommensurate CDW (NCDW) was investigated by Kotani,[8] near the doubling of the period, and by Moncton, Axe and Di Salvo[9] and by McMillan[10,11]1) for layered crystals near the tripling of the period. All these studies have shown that, owing to the commensurability effects, the ion displacement in the ground state of NCDW near the commensurate state is described by a period function of the coordinates that has not one but an infinite number of harmonics. We show in this article that this change of the ground state of the NCDW leads to a modification of the low-amplitude oscillation spectrum of the CDW.

2. FREE ENERGY OF A SYSTEM WITH CDW

We carry out the analysis within the framework of the phenomenological approach of [10,12], and confine ourselves to changes of only the phase of the order parameter, whose modulus is kept constant; just as in McMillan's paper,[10] we confine ourselves to an analysis of the situation wherein the order paremeter of one CDW changes in only one direction. The order parameter $\alpha(\mathbf{r})$ and the free energy of the Ginzburg-Landau type are written in the form[10,11]

$$\alpha(\mathbf{r})=\mathrm{Re}\,\Psi(\mathbf{r})=\mathrm{Re}\{\Psi_0\exp[i\mathbf{Qr}+\varphi(\mathbf{r})]\},$$
$$F=\int d\mathbf{r}\left\{a\alpha^2(\mathbf{r})-b\alpha^3(\mathbf{r})+c\alpha^4(\mathbf{r})+eQ^2\left|\left(\frac{\partial}{\partial\mathbf{r}}-i\mathbf{Q}\right)\Psi(\mathbf{r})\right|^2\right\},\qquad(1)$$

where a, b, c, and e are periodic functions and, for example, $b=b_0+2b_1\cos\mathbf{K}\cdot\mathbf{r}$, where K is the reciprocal vector of the initial lattice without the CDW. The term of third order in α with the coefficient b in (1) takes into account the commensurability effects in the case when $Q\approx K/3$, and we confine ourselves hereafter to this case only (in analogy with McMillan's work[10]). A free energy in the form (1) implies that the considered phases of the order parameters change quite slowly in space—over distances greatly exceeding the correlation length ξ_0 (otherwise the order-parameter amplitude cannot be regarded as constant). In the case when the lattice instability is due to singularities of the Fermi surface of the conduction electrons we have $\xi_0\approx\hbar v_F/\Delta$, where v_F is the electron Fermi velocity and Δ is the energy gap on the corresponding sections of the Fermi surface.

We discuss now the question whether the system with the free energy (1) is merely a model or whether it can describe in some cases a real situation.

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In quasi-one-dimensional systems with a fixed number of electrons on the chain (corresponding to a value $Q=2k_F$ that is not commensurate with K), an NCDW—CCDW transition with decreasing temperature leads inevitably to the appearance of electrons above the gap (see [8]). In this situation, the description of the system with the aid of the phase $\varphi(x)$ only may be insufficient. In addition the change of phase in space in connected with the change of the concentration ρ_e of the electrons located under the gap ($\rho_e \sim \partial\varphi/\partial x$), and the energy of the electric field must be taken into account in the free energy. One cannot therefore exclude the possibility that the free energy (1) is insufficient for the description of quasi-one-dimensional crystals, and at any rate we are unable at present to point to any real case for which the description (1) can be regarded as fully satisfactory.

In layered compounds, the state with CDW is metallic and the change of phase in space does not change the electron density (in the model with saddle points or congruent sections of the Fermi surface, variation of the phase with the coordinate leads only to a change of the electron distribution function with respect to the electron momentum in momentum space). Layered systems therefore do not pose those difficulties which were noted above for quasi-one-dimensional systems (their FCM is optically inactive). But layered crystals do have a hexagonal lattice structure and three CDW that interact with one another appear in such crystals. This factor is not taken into account in (1), yet the interaction of the three CDW can significantly alter the behavior of the system (see [13]) and in this case we must consider the free energy for the three CDW in two-dimensional space. We shall return to the question of the applicability of (1) to real layered crystals at the end of the article, and note for the present only that the system considered by us is the simplest one and admits of a complete analytic solution of the spectrum of the small-amplitude phase oscillations. This solution explains, at least qualitatively, how the FCM spectrum is transformed into CCDW under the influence of the commensurability effect.

Following McMillan,[10] we express that part of the free energy (1) which depends on the phase $\varphi(x)$ in the form

$$F=F_0\int dx\left[\left(\frac{\partial\varphi}{\partial x}-1\right)^2-Y(\cos M\varphi-1)\right]. \tag{2}$$

In the derivation of (2) from (1) we have introduced the dimensionless length $x=r|Q-K/3|$ and have introduced the notation $F_0=e_0Q^2\Psi_0^2/2$, $Y=b_1\Psi_0/e_0Q^2(Q-K/3)^2$ and put $M=3$ in (2), even though the case of arbitrary commensurability can be treated within the framework of the approach with the free energy (2).

3. GROUND STATE

Starting with the free energy (2), McMillan investigated the properties of the system in a variational approach by numerically minimizing F. Dzyaloshinskiĭ[12] obtained an analytic solution of a similar problem. We present here briefly the analytic results that will be needed subsequently.

Making of change of variable $M\varphi=\theta$, we rewrite (2) in the form

$$F=M^{-2}F_0\int dx\left[\left(\frac{\partial\theta}{\partial x}-M\right)^2-2\zeta(\cos\theta-1)\right], \tag{3}$$

where $2\zeta=YM^2$. The extremum condition takes the form of the sine-Gordon equation for θ,

$$d^2\theta/dx^2-\zeta\sin\theta=0. \tag{4}$$

This is the equation of a physical pendulum; its solution is well known, namely,

$$x-x_0=\int_0^\theta\frac{d\theta}{(C-2\zeta\cos\theta)^{1/2}}, \tag{5}$$

where $C\geq 2\zeta$ is the integration constant, and the origin is arbitrary, since the system is isotropic.

The solution (5) at $C>2\zeta$ takes the form shown schematically in Fig. 1, i.e., it describes the change of the phase (oscillations) with period l that depends on C; $C\to 2\zeta+0$ we have $l\to\infty$ and $\theta\to 0$, corresponding to a transition to the commensurate phase.

The free energy (3) is a function of the parameter C on the class of solutions (5). This parameter is determined not from the boundary conditions, but from the condition that the free energy be a minimum. (The same situation was encountered in the analysis of the vortex structure in type-II superconductors[14] and in Josephson junctions.[15])

Substituting the solution (5) in (3) and taking into account the relation $d\theta/dx=(C-2\zeta\cos\theta)^{1/2}$, we can reduce the free energy to the form

$$\frac{FM^2}{F_0}=\int dx\left[C-2M\frac{d\theta}{dx}-4\zeta\cos\theta\right]+\text{const}. \tag{6}$$

It is convenient to rewrite this expression in the form

$$\frac{M^2F}{F_0}=\frac{L}{l}\int_0^l dx\left[C-2M\frac{d\theta}{dx}-4\zeta\cos\theta\right]$$
$$=\frac{L}{l}\left[Cl-4\pi M-4\zeta\int_0^{2\pi}\frac{d\theta\cos\theta}{(C-2\zeta\cos\theta)^{1/2}}\right], \tag{7}$$

where L is the dimension of the system, and the period l is expressed in terms of elliptic functions

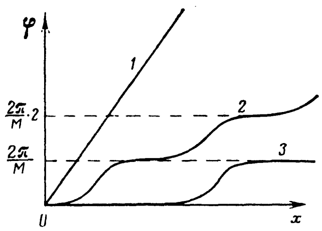

FIG. 1. Schematic dependence of the phase of the order parameter on the coordinate in the quasi-commensurate state. Curves 1, 2, and 3 correspond to different (increasing) values of the commensurability constant ξ.

$$l=\int_0^{2\pi}\frac{d\theta}{(C-2\zeta\cos\theta)^{1/2}}=\frac{4\gamma}{\zeta^{1/2}}K(\gamma),\qquad \gamma^2=\frac{4\zeta}{C+2\zeta}. \tag{8}$$

We can express in same fashion the free energy (7) itself, which takes, with allowance for (8), the form

$$\frac{M^2F}{LF_0}=C-\frac{2\pi M\sqrt{\zeta}}{\gamma K(\gamma)}+4\zeta\left[1-\frac{2}{\gamma^2}+\frac{2}{\gamma^2}\frac{E(\gamma)}{K(\gamma)}\right]. \tag{9}$$

Taking into account the properties of the functions $E(\gamma)$ and $K(\gamma)$, and in particular their asymptotic forms as $\gamma\to 1 (C\to 2\zeta): E(\gamma)\to 1, K(\gamma)\to \ln(4/\gamma')$, where $\gamma'^2=1-\gamma^2\to 0$, we find that the free energy (9) has a minimum at $C>2\zeta$ (noncommensurate phase) if the following condition is satisfied:

$$\zeta<\zeta_c=\pi^2M^2/16, \tag{10}$$

and in the opposite case the minimum is reached at $C=2\zeta$, corresponding to the commensurate phase. The transition between them is continuous and proceeds via an increase of the period l of the "commensurate domains" (see Fig. 1).[2)]

In the original notation, the critical value of the constant in the commensurability term in (2) is $Y_c=\pi^2/8$, which agrees with the value $Y_c=1.2337$ obtained by McMillan[10]. We note that when the constant Y_c corresponding to expression (2) is determined, the critical value Y_c is independent of the commensurability index M.

The qualitative picture is thus that even in the noncommensurate phase the commensurability energy deformation of the CDW, so that the system consists of domains where the CDW is practically commensurate with the initial lattice (phases $\theta(x)=2\pi n$ or $\varphi(x)=2\pi n/M$) separated by relatively narrow domain walls (called "discommensurations" by McMillan); in fact, as seen from (5), they coincide with static solitons). It is important to us that these domain walls do not act now as elementary excitations in the system[6]; the commensurability effects have the very structure of the ground state of the NCDW, in which a periodic lattice of static solitons and domain walls exists.

4. COLLECTIVE EXCITATIONS

We consider now the collective excitations (phasons) in a system described by the free energy (2), with account taken of the ground-state restructuring considered above. To this end it is necessary to add to the integrand of (3) a term $-s^{-2}\partial^2\theta/\partial t^2$ (s is the speed of the phason in the absence of commensurability effects).

The classical equation for the phase $\theta(x,t)$ takes now the form[3)]

$$\frac{\partial^2\theta}{\partial x^2}-\frac{1}{s^2}\frac{\partial^2\theta}{\partial t^2}-\zeta\sin\theta=0. \tag{11}$$

We seek a solution of (11) in the form $\theta(x,t)=\theta_0(x)+\psi(x)e^{i\omega t}$, where $\theta_0(x)$ is the solution of the static equation (4) and $\psi(x)e^{i\omega t}$ is a small increment. Linearizing with respect to ψ, we find that this quantity satisfies the "Schrödinger equation"

$$-\frac{\partial^2\psi}{\partial x^2}-\zeta\cos\theta_0(x)\psi=\omega^2\psi, \tag{12}$$

where the role of the potential is assumed by $V(x)=\zeta\cos\theta_0(x)$. An identical problem was encountered earlier in an investigations of small oscillations of the vortex lattice in a Josephson junction.[15,17] It was shown there that the spectrum of the collective oscillations consists of two branches, acoustic and optical: in the broadened-band scheme this spectrum takes the form shown schematically in Fig. 2.[17] Here $q_m=\pm\pi/l$ is the vector of the new reciprocal lattice and l is given by (8). The spectrum itself was investigated by Fetter and Stephen[17]; they have shown that the dispersion law of the acoustic branch is given by

$$\omega_{ac}^2(q\ll q_m)=s^2F^2(\gamma)q^2,\quad F(\gamma)=(1-\gamma^2)^{1/2}K(\gamma)/E(\gamma),$$
$$\omega_{ac}^2(q=q_m)=s^2(1-\gamma^2)\zeta/\gamma^2, \tag{13}$$

and the optical spectrum is of the form

$$\omega_{opt}^2(q-q_m\ll q_m)=s^2\left[\frac{\zeta}{\gamma^2}+G^2(\gamma)(q-q_m)^2\right],$$
$$G(\gamma)=\frac{\gamma K(\gamma)}{K(\gamma)-E(\gamma)},\quad \omega_{opt}(q\gg q_m)=s^2q^2. \tag{14}$$

The gap in the spectrum at $q=q_m$

$$\omega_{opt}^2(q_m)-\omega_{ac}^2(q_m)=s^2\zeta={}^1/_2 s^2YM^2 \tag{15}$$

coincides with the gap in the commensurate phase, in which the phason spectrum is

$$\omega^2(q)=s^2(\zeta+q^2). \tag{16}$$

The physical meaning of the appearance of two branches in the spectrum of the noncommensurate phase is quite clear. The optical branch can be treated as phase oscillations within the commensurate domains. In the limit as $\zeta\to\zeta_c$ ($l\to\infty$ and $q_m\to 0$) only this mode remains in the system. On the other hand the acoustical mode corresponds to oscillations of the domain-wall system. The validity of this interpretation can be verified directly by examining the solution of Eqs. (4) and (12) at when only one domain wall remains in the system in the limit. The explicit solution of Eq. (4) is then (see, e.g., [15])

$$\theta_0(x)=4\,\mathrm{arctg}\,e^{-\zeta^{1/2}x}$$

and the "potential" $V(x)=\zeta\cos\theta_0(x)$ in (12) turns out to be $V(x)=[1-2\cosh^{-2}(x\sqrt{\zeta})]$. The corresponding equa-

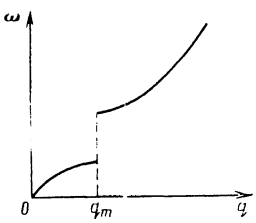

FIG. 2. Spectrum of collective oscillations of CDW (phasons) in quasicommensurate states.

tion can be solved exactly and has an eigenvalue $\omega^2=0$, while the "wave function" $\psi(x)$ is localized near the domain wall (taken here to be at the origin).

It is also clear from this how the transition to the commensurate phase takes place as $\zeta\to\zeta_c$ (the phenomenological parameter Y or ζ, introduced in the Ginzburg-Landau functional, changes, for example, with temperature). In the foregoing analysis (neglecting pinning by the impurities), the acoustic mode is preserved in the noncommensurate phase at all $\zeta<\zeta_c$, which is in fact again a reflection of the noncommensurability, since the positions of the domain walls themselves are not fixed in the lattice and can vary continuously in the assumed model. The weight of this mode (its phase volume), however, decreases as $\zeta\to\zeta_c$ like $q_m\sim l^{-1}$, and in the limit as $\zeta\to\zeta_c$ this mode vanishes, so that only the mode with the spectrum (16) remains in the system.

5. DISCUSSION OF RESULTS

We discuss now some consequences of the results, as well as the limits of their applicability.

We see that owing to the commensurability effects the CDW structure in the noncommensurate phase changes, so that domains commensurate with the initial lattice appear and are separated by domain walls in which the CDW phase undergoes relatively fast changes. (In different language, this corresponds to the appearance of harmonics of the fundamentals CDS.[8,10]) In such a phase, the spectrum of the collective excitations (oscillations of the CDW phase) consists of two branches: acoustic, but extending only to $q=q_m=\pi/l$, where l is the period of the produced domain structure, and optical, which in fact is very close to the corresponding mode in the commensurate phase. The relative weight of the acoustic (zero-gap) mode can in this case be substantially decreased in comparison with the case when there are no commensurability effects.

Starting from the interpretation wherein the acoustic branch of the spectrum is regarded as oscillations of the domain walls, we can assume that when account is taken of impurities, defects, etc., a gap, appears in this branch and the conditions for this appearance are easier than the usual ones[4,18], since such walls can apparently be easily pinned even by weak inhomogeneities. In this case, two gaps can appear in the spectrum: the gap due to the commensurability effects and discussed in Sec. 3, and the gap produced in the spectrum of the domain-wall oscillations by pinning on impurities. It can thus be assumed that the joint action of these two pinning mechanisms greatly facilitates the conditions for the appearance of phasons in the spectrum.

We turn now to the question of the applicability of these results to layered compounds. Inside the domain walls, the phase changes over a characteristic length $\xi_0^{-1}=|9Y_c(K/3-Q)^2/2|^{1/2}$ at $Y\approx Y_c$. The theory is valid if $\xi_c\gg\xi_0$, and in the case of instability due to singularities of the Fermi surface we get the condition $|K/3-Q|/Q\ll\Delta/\epsilon_F$. According to the data of Barker, Ditzenberger, and Di Salvo we have $\Delta\approx0.25$ eV in $2H$-$TaSe_2$ (see [19]), from which we get $\xi_0\approx3$Å at $\xi_c\approx30$Å.[10] The condition $\xi_c\gg\xi_0$ is therefore satisfied in $2H$-$TaSe_2$. In fact, however, the NCDW—CCDW transition in this compound is of first order. This may be due to a three-wave interaction that causes changes in the modulus of the order parameter (see [13]) or to the substantial influence of the phonons in the region of the NCDW—CCDW transition.[19]

Thus, the simple model considered above can at present not be applied directly to any of the compounds known to us. There is no doubt, however, that in layered compounds the commensurability effects near the commensurate phase actually lead to the appearance of a CDW structure of the domain type (but apparently with an additional change of the order-parameter modulus in the domain wall). Solutions of this type were obtained in [13] for the partially commensurate phase in $1T$-TaS_2 between 200 and 352 K; it appears that the NCDW in the $2H$-$TaSe_2$ phase is of similar character near the transition to the commensurate phase.[9] In this case the CDW oscillation spectrum should have the same qualitative singularities that are inherent in the McMillan model: the mode with dispersion of the acoustic type should be concentrated mainly in the domain walls, and the dispersion curve has a discontinuity at the momentum q_m. The last effect can be observed in principle in experiments via inelastic scattering of neutrons in $2H$-$TaSe_2$ or $1T$-TaS_2.

As to quasi-one-dimensional compounds, the foregoing analysis cannot be applied to them directly, because of the factors noted in Sec. 2. The most substantial factor is that on going over to the described quasi-commensurate state the "extra" electrons must occupy positions above the gap. When these extra electrons are taken into account, in an approximation in which the modulus of the order parameter is constant in space, there is added to the free energy (2) a term

$$\alpha\int dx\left(\frac{\partial\varphi}{\partial x}-1\right)$$

with a large coefficient $\alpha\gg1(\alpha\approx\epsilon_F/\Delta)^{M-2}$. As a result, the form of the equation for $\varphi(x)$ remains unchanged (see (4)), nor does the solution (5) change. However, the minimum of the free energy (6), (7) will be reached when the constant $C\gg1$, i.e., the solution is in fact always close, with high accuracy, to the function $\varphi(x)=x$ (simple noncommensurate wave).

The situation becomes different in systems of the TIF-TCNQ type, in which the electrons can become redistributed among the donor and acceptor chains and there is no need to locate them above the gap when the period of the superstructure changes. The NCDW structures and the NCDW—CCDW transitions are possible in principle if the noncommensurate structure is close to the commensurate one. In experiment, however, no such transitions have been observed as yet, apparently because of the strong difference between real CDW and commensurate ones.

We note that all our results were obtained in the self-consistent field approximation and we did not take phase fluctuations into account. In a purely one-dimensional system, such fluctuations are important; allowance for them jointly with consideration of commensurability effect is reported by Brazovskiĭ *et al.*[20] In quasi-one-dimensional compounds with sufficiently strong interaction of the CDW on different chains or in layered compounds, the phase fluctuations are not so important, especially far from the temperature at which the three-dimensional CDW structure appears.

We note in conclusion that our results can apparently be used not only for compounds with CDW, but also to other systems in which structural transitions to a non-commensurate phase are observed.[21]

In conclusion, we are deeply grateful to L. V. Keldysh, as well as to V. L. Ginzburg and to the participants of his seminar, for useful discussions.

1) Macmillan's analysis is in fact fully equivalent to Dzyaloshinskiĭ's earlier investigation of helicoidal magnetic structures.[12]

2) We note that a relation similar to that in Fig. 1 was observed numerous times in different systems; e.g.,[6].

3) Similar results are arrived at also by a consistent quantization procedure.[17]

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Continual theory of tunnel self-trapping

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A theory is developed for tunnel self-trapping of electrons (or of Frenkel excitons) as they interact with acoustic and nonpolar optical phonons. It is assumed that the electron-phonon interaction is strong enough, so that the size of the self-trapping barrier exceeds greatly the lattice constant and the continual theory can be used. It is shown that in these two cases the tunneling picture is entirely different. In the interaction with the optical phonons, the decisive contribution is made by quasiclassical trajectories with a spatial scale on the order of the barrier size. In interaction with acoustic phonons, on the contrary, the optimal trajectories have a scale much smaller than the barrier size. Explicit expressions for the transparency of the self-trapping barrier are obtained for both cases.

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A sufficiently strong electron-photon interaction produces in a crystal self-trapping of electrons (excitons) into states with scale dimensions equal to the lattice constant. They are called small-radius polarons, condensons, and polarizing or deforming excitons. The character of the resultant final states (for example, single-site or quasimolecular formation) are determined mainly by quantum-chemical considerations and is practically independent of the type of the phonons with which the dominant interaction takes place. On the contrary, the process of formation of a self-trapped state from a band state is decisively affected by the type of the electron-phonon interaction. Thus, for example, in a polarization interaction with optical phonons the self-trapping, i.e., the transition to the polaron state, always takes place without a barrier.[1] On the contrary, if

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