One-dimensional charge-density wave in a random Gaussian potential

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The structure factor of a one-dimensional charge-density wave in a random potential is calculated in the Gaussian limit. The method of reduction to $N = 0$ fields and subsequent reduction to the Schrödinger equation is used.

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In a one-dimensional conducting system the electron-phonon interaction leads to a structural instability.[1] In the self-consistent field approximation a charge-density wave (CDW) with period $1/2p_F$, where p_F is the Fermi momentum, appears at a certain temperature T_{c0}. This wave is optically active and can carry current. Thermal and quantum fluctuations destroy the long-range order, but the contribution of the CDW to the conductivity remains large.[2]

A much stronger influence on the CDW is exerted by impurities. If the interaction between the conducting filaments is sufficiently strong, a three-dimensional CDW is formed. The effect of impurities in this case was studied in Ref. 3. It was shown that impurities destroy the long-range order and evidently lead to a finite dielectric permittivity. At sufficiently high temperatures or sufficiently large impurity concentrations the correlation between the CDWs of different filaments breaks down and we can consider each filament independently. In the one-dimensional case the result depends not only on the effective mean free path but also on the average distance between impurities in relation to the scattering amplitude at an individual impurity center. The contribution of the CDW to the conductivity in the limit of infrequent impurities was studied in Refs. 4 and 5. The limiting case of frequent impurities can be described by the model of a random potential with Gaussian distribution. Qualitative estimates for the dielectric permittivity at zero temperature in such a model have been given in Ref. 5.

Below we shall study the CDW in a random potential with a Gaussian distribution. The fundamental quantity to be determined is the structure factor. The structure factor is calculated in the limits of low and high temperatures (relative to the linkage energy). At high temperatures the correlation length is determined principally by the temperature, and the interaction with the impurities leads only to small corrections. The effect of impurities is much stronger at low temperatures. Even arbitrarily weak impurities destroy not only the long-range order but also the short-range order. The calculations are performed by reducing the problem to the solution of the Schrödinger equation.

1. REDUCTION OF THE PROBLEM TO THE SCHRÖDINGER EQUATION

We shall consider a one-dimensional electron-phonon system. In the self-consistent field approximation, at sufficiently low temperatures a CDW is formed, with amplitude Δ determined by the equation[1]

$$1 = \frac{g^2}{\pi v_F \omega^2 (2p_F)} \ln \frac{\varepsilon_F}{\Delta}, \tag{1}$$

where g is the electron-phonon interaction constant, v_F, p_F and ε_F are the Fermi velocity, momentum, and energy, and $\omega(2p_F)$ is the phonon energy at momentum $2p_F$. The formula (1) holds if the temperature is sufficiently low ($T \ll \Delta$) and the mean free path l determined by the impurities is sufficiently large ($l \gg v_F/\Delta$). These criteria will be assumed to be fulfilled below.

Of fundamental interest is the study of the slow phase fluctuations caused by the impurities. Fluctuations of the amplitude of the CDW will not be taken into account below. Then, following the results of Refs. 2 and 6, we can write the average $\langle M(\varphi)\rangle$ of any physical quantity over the states of the electron-phonon Hamiltonian by means of a continuous integral:

$$\langle M(\varphi)\rangle = \int M(\varphi) \exp(-F[\varphi]) D\varphi \Big/ \int \exp(-F[\varphi]) D\varphi. \tag{2}$$

The functional $F[\varphi]$ has the following form:

$$F[\varphi] = \int_0^L \int_0^{1/T} \Big[\frac{A\dot{\varphi}^2(x,\tau)}{2} + \frac{C}{2}\Big(\frac{\partial\varphi(x,\tau)}{\partial x}\Big)^2 + f(x)\sin(2p_F x + \varphi(x,\tau)) \Big] dx\, d\tau. \tag{3}$$

In this formula,

$$A = N_0 m^*/(2p_F)^2, \quad C = v_F/2\pi, \quad m^* = m(1 + \pi v_F \Delta^2/2g^2), \tag{4}$$

where N_0 is the electron density and m the electron mass. The quantity $f(x)$ describing the interaction with the impurities is equal to

$$f(x) = \sum_a \frac{\omega^2(2p_F)\Delta U(2p_F)}{g^2} \delta(x - x_a), \tag{5}$$

where $U(2p_F)$ is the scattering amplitude at momentum $2p_F$ for scattering by an impurity, and x_a are the coordinates of the impurity atoms.

The integration over x in formula (3) is performed over the length of the sample, τ is the "imaginary time," and T is the temperature. It is assumed that the phase φ satisfies the following boundary conditions:

$$\varphi(0,0)=\varphi(L,0)=\varphi(0,1/T)=\varphi(L,1/T). \tag{6}$$

To obtain physical quantities such as the structure factor or dielectric permittivity it is necessary to carry out averaging over the random potential $f(x)$. Averaging Eq. (2), we obtain

$$\langle\langle M(\varphi)\rangle\rangle_f=\left\langle\int M(\varphi)\exp(-F[\varphi])D\varphi\Big/\int\exp(-F[\varphi])D\varphi\right\rangle_f. \tag{7}$$

The angular brackets with the subscript f in formula (7) denote averaging over the random potential f. For the subsequent calculations it is convenient to transform Eq. (7) to the following form:

$$\langle\langle M(\varphi)\rangle\rangle_f=\left[\left\langle\int M(\varphi_1)\exp\left(-\sum_{\alpha=1}^{N}F[\varphi_\alpha]\right)\prod_{\alpha=1}^{N}D\varphi_\alpha\right\rangle\right.$$
$$\left.\times\left\{\left\langle\int\exp\left(-\sum_{\alpha=1}^{N}F[\varphi_\alpha]\right)\prod_{\alpha=1}^{N}D\varphi_\alpha\right\rangle_f\right\}^{-1}\right]_{N=0}. \tag{8}$$

It is necessary to calculate the right-hand side of this equation for arbitrary N, and then put $N=0$. In this case, the right-hand sides of (8) and (7) coincide.

We note that for $N=0$ the denominator in the right-hand side of formula (8) is equal to unity:

$$\left\langle\int\exp\left(-\sum_{\alpha=1}^{N}F[\varphi_\alpha]\right)\prod_{\alpha=1}^{N}D\varphi_\alpha\right\rangle_f=1. \tag{9}$$

In formula (8) it is convenient to average over the random potential f first, and only after this integrate over φ_α. We shall confine ourselves to the case of frequent but weak impurities. Then the averaging over the impurities is equivalent to averaging in a random Gaussian potential. In the notation of the present paper, this case obtains if the following inequality is fulfilled[4,5]:

$$n_0\gg\omega^2(2p_F)\Delta U(2p_F)/g^2v_F, \tag{10}$$

where n_0 is the impurity concentration.

Performing the averaging over the impurities in the Gaussian limit in the expression (8) and considering only slow variations of φ_α, we obtain

$$\langle\langle M(\varphi)\rangle\rangle_f=\left[\int M(\varphi_{1\omega})\exp(-F[\varphi_{1\omega}\ldots\varphi_{N\omega}])\right.$$
$$\left.\times\prod_{\alpha=1}^{N}D\varphi_{\alpha\omega}\left\{\int\exp(-F[\varphi_{1\omega}\ldots\varphi_{N\omega}])\prod_{\alpha=1}^{N}D\varphi_{\alpha\omega}\right\}^{-1}\right]_{N=0}. \tag{11}$$

In this formula,

$$F[\varphi_{1\omega}\ldots\varphi_{N\omega}]=\int_0^L\left[\frac{1}{2}\sum_{\alpha,\omega}A|\varphi_{\alpha\omega}|^2\omega^2+C\left|\frac{\partial\varphi_{\alpha\omega}}{\partial x}\right|^2\right.$$
$$\left.-\gamma\int_0^{1/T}\int_0^{1/T}d\tau\,d\tau'\sum_{\alpha,\alpha'}\cos T^{1/2}\sum_{\omega}(\varphi_{\alpha\omega}e^{i\omega\tau}-\varphi_{\alpha'\omega}e^{i\omega\tau'})\right]dx, \tag{12}$$

where

$$\gamma=n_0[\omega^2(2p_F)\Delta U(2p_F)/g^2]^2,$$
$$\varphi_\omega=T^{1/2}\int_0^{1/T}\varphi(\tau)e^{i\omega\tau}\,d\tau,\qquad\omega=2\pi nT. \tag{13}$$

The calculation of the continuous integral of the form (11), (12) can be found in the book by Feynman and Hibbs.[7] The time has played the role of the coordinate x. Using the results expounded in Ref. 7, we reduce the calculation of the integral in (11) to the calculation of the following expression:

$$\langle\langle M(\varphi)\rangle\rangle=\left[\int M(\varphi_{1\omega})G(\varphi_{1\omega}\ldots\varphi_{N\omega})d\varphi_{1\omega}\ldots d\varphi_{N\omega}\Big/\right.$$
$$\left.\int G(\varphi_{1\omega}\ldots\varphi_{N\omega})d\varphi_{1\omega}\ldots d\varphi_{N\omega}\right]_{N=0}. \tag{14}$$

The function $G(\varphi_{1\omega}\ldots\varphi_{N\omega})$ in this formula is the Green function of the Schrödinger equation:

$$\frac{\partial G}{\partial x_0}-\frac{1}{2}\sum_{\alpha,\omega}\left(\frac{1}{C}\frac{\partial^2}{\partial\varphi^2_{\alpha,\omega}}-A\omega^2|\varphi_{\alpha\omega}|^2\right)G$$
$$-\gamma\int_0^{1/T}\int_0^{1/T}d\tau\,d\tau'\sum_{\alpha,\alpha'}\cos T^{1/2}\sum_{\omega}(\varphi_{\alpha\omega}e^{i\omega\tau}-\varphi_{\alpha'\omega}e^{i\omega\tau'})G$$
$$=\delta(x_0-x_0')\prod_{\alpha,\omega}\delta(\varphi_{\alpha\omega}-\varphi_{\alpha\omega}'), \tag{15}$$

taken at $x_0-x_0'=L$ and $\varphi_{\alpha\omega}=\varphi'_{\alpha\omega}$.

Thus, the problem of the calculation of the continuous integral (2), (3) and the subsequent averaging over the impurities has been reduced to the determination of the Green function of the Schrödinger equation (15) and to the calculation of certain integrals (14). The calculation of continuous integrals in another one-dimensional problem by the Feynman method was first carried out in Ref. 8.

2. THE STRUCTURE FACTOR

Using the method developed above, we can find the principal physical quantities. We shall consider the correlator $\Pi(x)$:

$$\Pi(x)=\Delta^2\exp(2ip_Fx)\langle\langle\exp(i\varphi(x)-i\varphi(0))\rangle\rangle_f. \tag{16}$$

The Fourier component $\Pi(q)$ of the correlator determines the scattering of neutrons and x-rays. The phases φ in (16) are taken at coincident times. The subsequent calculations will be performed with the assumption that the adiabaticity condition $m^*\gg m$ is fulfilled, where m^* is defined by formula (4). In this case we can neglect quantum fluctuations[2] and retain only the zeroth harmonics $\varphi_{\alpha 0}$ of the phases in (14) and (15). Using the expansion of the Green function in the eigenfunctions of the equation, we obtain a more convenient representation for the correlator $\Pi(x)$:

$$\Pi(x)=\Delta^2\exp(2ip_Fx)\sum_m\left|\int\psi_m^*(\mathbf{r})\exp(ir_1T^{1/2})\right.$$

$$\left.\times\psi_0(\mathbf{r})\,d\mathbf{r}\right|^2\exp\{-(E_m-E_0)x\}\Big/\int|\psi_0(\mathbf{r})|^2\,d\mathbf{r}\int|\psi_m(\mathbf{r})|^2\,d\mathbf{r}. \tag{17}$$

In this formula, $\psi_m(\mathrm{r})$ and E_m are the wavefunction and energy of the m-th state of the Schrödinger equation $\hat{H}\psi=E\psi$, where

$$\hat{H}=-\frac{1}{2C}\sum_{\alpha=1}^{N}\frac{\partial^2}{\partial r_\alpha^2}-\frac{\gamma}{T^2}\sum_{\alpha,\alpha'=1}^{N}\cos(T^{1/2}\mathbf{r}(\mathbf{e}_\alpha-\mathbf{e}_{\alpha'})), \tag{18}$$

$$\mathbf{r}=(r_1,r_2\ldots r_N),\quad \mathbf{e}_1=(1,0\ldots0),\quad \mathbf{e}_2=(0,1\ldots0),\ldots,\mathbf{e}_N=(0,0\ldots1).$$

We shall consider the high-temperature case. In this limit the second term in the Hamiltonian (18) can be taken into account as a perturbation. In the zeroth approximation the ground-state eigenfunction is equal to unity and the ground-state energy is zero: $\psi_0^{(0)}=1, E_0^{(0)}=0$. The correction to the energy for $N=0$ is equal to zero. The wavefunctions of the excited states are plane waves:

$$\psi_m^{(0)}=\exp(i\mathbf{p}_m\mathbf{r}). \tag{19}$$

The matrix element in (17) is nonzero for $\mathrm{p}_1=T^{1/2}(-1,\ldots,0)$. States with momentum are degenerate with respect to the direction of the momentum. In the zeroth approximation the energy of the state with momentum p_1 is equal to

$$E_1^{(0)}=T/2C. \tag{20}$$

To determine the correction it is necessary to solve the secular equation, which, in the case under consideration, has the form

$$\mathrm{Det}\left(E_1^{(1)}\delta_{nn'}+\frac{\gamma}{2T^2}(1-\delta_{nn'})\right)=0. \tag{21}$$

Calculating the determinant in (21), we obtain

$$\left(E_1^{(1)}-\frac{\gamma}{2T^2}\right)^{N-1}\left(E^{(1)}+(N-1)\frac{\gamma}{2T^2}\right)=0. \tag{22}$$

Substituting the expressions (19), (20), and (22) for the eigenfunctions and energy into (17) and putting $N=0$, we find $\Pi(x)$:

$$\Pi(x)=\Delta^2\exp(2ip_Fx)\exp[(-T/2C-\gamma/2T^2)x]. \tag{23}$$

Considering the perturbation-theory terms of higher order, we can convince ourselves that the formula (23) is applicable for $T\gg(\gamma C)^{1/3}$. The expression (23) shows that at high temperatures the correlation length in the exponential-decay law for $\Pi(x)$ is determined principally by thermal fluctuations. The impurities only slightly decrease the distance over which short-range order exists.

The analysis at low temperatures is more complicated. We shall transform the coordinates by the following formula:

$$r_\alpha'=r_\alpha-r_1,\quad \alpha\neq1,\quad r_1'=r_1. \tag{24}$$

The potential energy in (18) does not depend on r_1', and therefore the variable r_1' can be eliminated from the expressions (17) and (18). As a result, we obtain

$$\Pi(x)=\Delta^2\exp(2ip_Fx)\sum_m\left|\int\psi_m^*(\mathbf{r}')\exp\{i\mathbf{r}'\mathbf{n}(T(N-1))^{1/2}/N\}\psi_0(\mathbf{r}')\,d\mathbf{r}'\right|^2$$

$$\times\left\{\int|\psi_0(\mathbf{r}')|^2\,d\mathbf{r}'\left|\int\psi_m(\mathbf{r}')\right|^2d\mathbf{r}'\right\}^{-1}\exp\{-(E_m'-E_0')x-Tx/2CN\}. \tag{25}$$

The wavefunctions and energies in (25) are determined from the equation

$$\hat{H}\psi=\left\{\frac{\hat{\mathbf{p}}'^2}{2C}+\frac{(\hat{\mathbf{p}}'\mathbf{n})^2(N-1)}{2C}-\frac{\gamma}{2T^2}\sum_{\alpha=2}^{N}\cos(T^{1/2}\mathbf{r}'\mathbf{e}_\alpha)\right.$$

$$\left.-\frac{\gamma}{2T^2}\sum_{\alpha,\alpha'=2}^{N}\cos(T^{1/2}\mathbf{r}'(\mathbf{e}_\alpha-\mathbf{e}_{\alpha'}))\right\}\psi=E\psi, \tag{26}$$

where

$$\mathbf{n}=\frac{1}{(N-1)^{1/2}}(1,1\ldots1),\quad \mathbf{r}'=(r_2'\ldots r_N'),\quad p_i'=-i\frac{\partial}{\partial r'}.$$

Representing $\mathbf{r}'$ in the form

$$\mathbf{r}'=N^{1/2}\mathbf{n}r_\parallel+\mathbf{r}_\perp, \tag{27}$$

where the vector $\mathbf{r}_\perp$ lies in the hyperplane perpendicular to n, we rewrite the Hamiltonian $\hat{H}$ (26) as follows:

$$\hat{H}=\frac{\hat{p}_\parallel^2}{2C}+\frac{\hat{\mathbf{p}}_\perp^2}{2C}-\frac{\gamma}{2T^2}\sum_{\alpha=2}^{N}\cos\left\{T^{1/2}\left(r_\parallel\left(\frac{N}{N-1}\right)^{1/2}+\mathbf{r}_\perp\mathbf{e}_\alpha\right)\right\}$$

$$-\frac{\gamma}{2T^2}\sum_{\alpha,\alpha'=2}^{N}\cos\{T^{1/2}(\mathbf{e}_\alpha-\mathbf{e}_{\alpha'})\mathbf{r}_\perp\}. \tag{28}$$

In the new notation, the exponent in the matrix element in (25) is equal to $ir_\parallel(T(N-1)/N)^{1/2}$. At low temperatures the not very high-lying states can be found by expanding the cosines in the Hamiltonian to the second-order terms. In this approximation the Hamiltonian (28) takes the form

$$\hat{H}=\frac{\hat{p}_\parallel^2}{2C}+\frac{\gamma N}{4T}r_\parallel^2+\hat{H}_\perp; \tag{29}$$

$\hat{H}_\perp$ contains only $\hat{\mathbf{p}}_\perp$ and $\hat{\mathbf{r}}_\perp$. In deriving (29) we used the equality

$$\sum_{\alpha=2}^{N}\mathbf{r}_\perp\mathbf{e}_\alpha=0.$$

This equality is understandable from symmetry considerations.

Solving the Schrödinger equation with the Hamiltonian (29), substituting the wavefunctions and energies found into (25), and calculating the sum over states in (25), we obtain

$$\Pi(x)=\Delta^2\exp(2ip_Fx)\exp\left[-\frac{xT}{2NC}+\frac{N-1}{2N}\frac{1-\exp\{-(\gamma N/2TC)^{1/2}x\}}{(\gamma NC/2T^3)^{1/2}}\right]. \tag{30}$$

For $N=0$ the expression (30) vanishes for all x. For $N=0$, taking into account the possibility of tunneling from one minimum of the cosine to another does not change the result. Expanding the Hamiltonian (28) to terms of higher order cannot change the result either, if the condition $T \ll (\gamma C)^{1/3}$ is fulfilled.

However, the contribution of states with energies of the order of γ/T^2 has not yet been taken into account. It remains unclear whether taking these states into account will lead to the appearance of a finite correlation length at $T \neq 0$ or not. In any case, at $T=0$ this length should vanish.

The results obtained above show that, in the Gaussian limit at low temperatures, impurities destroy not only the long-range order but also the short-range order. Evidently, this strong violation of the order is a specific property of the Gaussian limit, when the average distance between impurities tends to zero.

Above, we did not take into account the long-range part of the Coulomb interaction, which was extremely important in the presence of transverse gradients in the free energy.[3] However, if these gradients are absent, the Coulomb long-range interaction leads only to a renormalization of the interaction constant.

The model considered above can be applied to describe the behavior of the KCP salts ($K_2[Pt(CN)_4]Br_{0.3}\cdot 3H_2O$) at temperatures in the range 100 K< T < 500 K. In this range there is no correlation between the CDWs of different chains and, therefore, we can consider each chain independently. The Br atoms are randomly located, but they are strongly screened by the water molecules.[9] For this reason, the scattering amplitude at an individual Br atom is small. This makes it highly probable that the Gaussian situation is realized.

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