

One-dimensional periodic structure in a weak random potential

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A method is proposed for the investigation of the low-temperature properties of one-dimensional classical disordered system such as a charge density wave (CDW) in an impurity potential, or a chain of spins with random anisotropy. The energy and correlation radius in the ground state are calculated. A nonuniversal power-law behavior of the state density and of the conductivity of the CDW is observed at low frequencies, wherein the exponent is connected with the form of the static structural factor of the CDW.

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This paper deals with a theoretical investigation into the low-temperature properties of one-dimensional classical disordered systems, such as a charge-density wave,¹ in a random potential of weak impurities,² or a chain of XY spins with weak random anisotropy. The study of these systems is of interest both from the experimental³ and from the theoretical points of view, since they constitute the simplest forms of systems in which the "frustration" phenomenon, first observed in spin-glass theory,⁴ manifests itself. In its general formulation the gist of this phenomenon is that the presence of a substantial disorder causes the ground state of the system to be formed not locally, but at distances much larger than the lattice constants (in spin glasses these distances are of the order of the size of the system: in our problem they are determined by the microscopic parameters). The main problem in the theory of systems of this kind is indeed the determination of the properties of the ground state, and ordinary perturbation theory in terms of the disorder is not suitable for this purpose.

This paper makes use of a synthesis of the "transfer matrix" method⁵ and the method of the distribution function for systems with disorder.^{6,7} In principle, the employed method is suitable at all temperatures, but the concrete results of the paper pertain to $T=0$. The exposition in the main text is in the language of the charge-density wave (CDW). In Appendix A it is shown that the problem considered is identical with that of a ferromagnetic chain of classical XY spins with random anisotropy. The quantities determined in the paper (accurate to a number on the order of unity) are the energies of the ground state, the correlation radius, and the dielectric susceptibility of the CDW (these results confirm the dimensional estimate^{8,2}). The low-frequency behavior of the state density and of the CDW conductivity are established (with the same accuracy). These quantities turn out to have a power-law frequency dependence with an exponent that is a function of the form of the CDW structure factor.

1. FORMULATION OF PROBLEM

The phenomenological Hamiltonian of a CDW in an impurity field was obtained by Gor'kov⁹:

$$H = \int \left[\frac{1}{2} v_F (\nabla \varphi)^2 - V \sum_k \delta(x-x_k) \cos(\varphi + Qx) \right] dx; \quad (1)$$

here φ is the CDW phase shift, v_F is the Fermi velocity, $Q = 2p_F$ is the wave vector, x_k are the coordinate of the impurities, and V is proportional to the potential of the impurities (see Ref. 9); the impurities are assumed to be identical. The quantity Q/c (c is the impurity concentration) is assumed large, so that Qx_k are random uncorrelated quantities.

As noted by Fukuyama and Lee,² the behavior of the system depends essentially on the ratio of V and cv_F . At $V \gg cv_F$ the energy minimum is reached at $\varphi_k + Qx_k = 2\pi n$ for all points k ("strong pinning"). This case was investigated in detail by Gor'kov.⁹ At $V \ll cv_F$ ("weak pinning") the impurity phases $\varphi + Qx_k$ are almost random, and the pinning is effected by large regions with characteristic dimension $L_c \sim v_F (cv_F V^2)^{-1/3}$, and containing many impurities. The estimate presented for L_c was obtained^{2,8} from the following consideration: the energy of deformation of the CDW over the length L_c is of the order of $v_F L_c^{-1}$; the energy of binding to the impurities is $\sim V(cL_c)^{1/2}$; these energies are of the same order. In the present paper we consider the weak-pinning problem quantitatively.

The partition function corresponding to the Hamiltonian (1) is of the form

$$Z = \prod_k \frac{d\varphi_k}{2\pi} \exp \left\{ -\frac{1}{T} \sum_k \left[\frac{(\varphi_k - \varphi_{k+1})^2}{2(x_k - x_{k+1})} v_F - V \cos(\varphi_k + Qx_k) \right] \right\}. \quad (2)$$

On going from (1) to (2) we have carried out Gaussian integration with respect to $\varphi(x)$ at all points free of impurities. We shall use for the calculation a generalization of the transfer-matrix method known for regular systems.⁵

Let $\Psi_N(\varphi_N)$ be the partition function of the chain, normalized to unity and dependent on the phase φ_N at its last point x_N (integration was carried out over all the preceding φ_k ($k < N$)). We then have for $\Psi_{N+1}(\varphi_{N+1})$

$$\lambda_{N+1} \Psi_{N+1}(\varphi_{N+1}) = \exp \left[\frac{V}{T} \cos(\varphi_{N+1} + Qx_{N+1}) \right] \int \frac{d\varphi_N}{2\pi} \times \exp \left[-\frac{v_F}{2T} \frac{(\varphi_{N+1} - \varphi_N)^2}{l_{N+1}} \right] \Psi_N(\varphi_N) \quad (3)$$

(λ_{N+1} is a normalization constant, and $l_{N+1} = x_{N+1} - x_N$). In the absence of disorder, $\Psi_{N+1}(\varphi) = \Psi_N(\varphi)$ and (3) reduces to the Schrödinger eigenvalue problem.

The general formulation of the problem of the ther-

modynamics of a disordered system consists in the following: 1) the partition function of the system with disorder is calculated; 2) the logarithm of this function, i. e., the free energy, is determined; 3) averaging is carried out over the disorder.

To realize this program, we represent $\Psi_N(\varphi_N)$ in the form

$$\Psi_N(\varphi_N) = \text{const} \exp \left[-\frac{\varepsilon_N(\varphi_N)}{T} \right]. \quad (4)$$

The function $\varepsilon_N(\varphi_N)$ has the meaning of the free energy of the chain as a function of the phase φ_N at its last point. The integral with respect to φ_N is taken in (3) principally at $\varphi_N - \varphi_{N+1} \ll 1$ (under the nonrestrictive condition $T \ll cv_F$). Substituting (4), we get

$$\varepsilon_{N+1}(\varphi) - \varepsilon_N(\varphi) = -\frac{1}{2} \frac{l_{N+1}}{v_F} \left(\frac{\partial \varepsilon_N}{\partial \varphi} \right)^2 + \frac{T}{2} \frac{l_{N+1}}{v_F} \frac{\partial^2 \varepsilon_N}{\partial \varphi^2} - V \cos(\varphi + Qx_{N+1}). \quad (5)$$

Equation (5), which contains the random parameter x_{N+1} , is our fundamental relation. We note that in a regular system Eq. (5) would be a Riccati equation corresponding to the Schrödinger equation for $\Psi(\varphi)$. By virtue of the condition $V \ll cv_F$, all the terms in the right-hand side of (5) are much smaller than $\varepsilon_N(\varphi)$, so that the function $\varepsilon(\varphi)$ changes little following a shift by one step in the lattice. (We note that a similar statement for $\Psi_N(\varphi)$ would be utterly incorrect at low temperatures.)

We consider next the region of the lowest temperatures, and neglect therefore the second term in the right-hand side of (5). Equation (5) is then transformed into a Hamilton-Jacobi equation (with a discrete imaginary "time" N) corresponding to the "equation of motion"

$$v_F \varphi'' + V \delta(x - x_n) \sin(\varphi + Qx) = 0. \quad (6)$$

This equation is satisfied by the extrema of the Hamiltonian (1), including the configuration $\varphi(x)$ corresponding to the ground state. At first glance it seems that the ground state can be investigated by using Eq. (6) itself. This equation, however, is essentially nonlinear in φ and has therefore a tremendous number of solutions satisfying the boundary conditions, but located quite far in energy away from the ground state. Therefore the usual procedure of averaging over all the solutions of (6) with a single weight is physically unjustified.

The foregoing arguments pertain in principle to systems of all dimensionalities, but are particularly important for the consideration of one- and two-dimensional systems, where the use of the ordinary method leads to a physically meaningless result such as a zero correlation radius.¹⁰ The change to the Hamiltonian Jacobi equation separates from all the solutions of (6) those close to the ground state.

The use of the Hamiltonian-Jacobi equation means physically a definite method of solving Eq. (6): a solution is constructed that is necessarily a local minimum of the energy and has a definite value of the phase at the last point N . As already mentioned, the random phases Qx_k are independent, therefore (5) is a Markov process for the function $\varepsilon(\varphi)$. Our problem is now to calculate

the distribution functions of the various physical quantities, and primarily the Green's function $G(x, x)$ that is connected in obvious fashion with $\varepsilon(\varphi)$:

$$G^{-1}(x, x) = \frac{\partial^2 \varepsilon_x}{\partial \varphi_x^2} \Big|_{\partial x_z / \partial \varphi_x = 0} = \beta_x. \quad (7)$$

2. THE DISTRIBUTION FUNCTION $W(\beta)$

The basic equation (5) specifies a Markov process for the 2π -periodic function $\varepsilon(\varphi)$, i. e., for an infinite set of parameters, where the "separation of the variables" in general form is impossible. To calculate many physical quantities, however, it suffices to determine the distribution function $W(\beta)$ of the quantity β given by Eq. (7). In this section we obtain the characteristic scale β_0 of the quantity β and the asymptotic forms of $W(\beta)$ at $\beta \gg \beta_0$ (with exponential accuracy) and $\beta \ll \beta_0$ (accurate to a number on the order of unity).

1. We expand the function $\varepsilon_N(\varphi)$ in a series near the minimum:

$$\varepsilon_N(\varphi) = \sum_{n=2}^{\infty} \frac{\beta_N^{(n)}}{n!} (\varphi - \gamma_N)^n + \varepsilon_N(\gamma_N); \quad \beta_N^{(2)} = \beta_N > 0$$

and obtain iteration equations of the type (5) for the parameters $\beta_N^{(n)}$ and γ_N . The function $\varepsilon(\varphi)$ has, generally speaking, more than one minimum in the period. Therefore the equations that we shall obtain, describe the parameters of one of the minima, not necessarily those of the absolute minimum. As a result, our formalism is subject to some inaccuracy, the consequences of which will be discussed at the end of the paper.

To find the connection between γ_N and γ_{N+1} , we differentiate (5) at the point $\varphi = \gamma_{N+1}$:

$$0 = \frac{\partial \varepsilon_{N+1}}{\partial \varphi} \Big|_{\gamma_{N+1}} = \frac{\partial \varepsilon_N}{\partial \varphi} \Big|_{\gamma_{N+1}} - \frac{\partial \varepsilon_N}{\partial \varphi} \Big|_{\gamma_{N+1}} \frac{\partial^2 \varepsilon_N}{\partial \varphi^2} \frac{l_{N+1}}{v_F} + V \sin(\gamma_{N+1} + Qx_{N+1}) \quad (8)$$

(we recall that here and below $T=0$),

$$\frac{\partial \varepsilon_N}{\partial \varphi} \Big|_{\gamma_{N+1}} = (\gamma_{N+1} - \gamma_N) \frac{\partial^2 \varepsilon_N}{\partial \varphi^2} = \beta_N (\gamma_{N+1} - \gamma_N). \quad (9)$$

It will be shown that the characteristic scale is $\beta \sim (cv_F V^2)^{1/3} \ll cv_F$. Therefore the second term in the right-hand side of (8) is small compared with the first. Substituting (9) in (8) we obtain

$$\gamma_{N+1} - \gamma_N = -\frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}). \quad (10)$$

We have neglected in the right-hand side of (10) the small difference $\gamma_{N+1} - \gamma_N \sim (V/cv_F)^{1/3} \ll 1$.

The equations for $\beta = \beta^{(2)}, \beta^{(4)}, \dots, \beta^{(2n)}$ are obtained similarly:

$$\beta_{N+1} - \beta_N = -\beta_N^2 \frac{l_{N+1}}{v_F} + V \cos \left(\gamma_N + Qx_{N+1} - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}) \right) + \beta^{(4)} \frac{V^2}{2\beta_N^2} \sin^2(\gamma_N + Qx_N), \quad (11a)$$

$$\beta_{N+1}^{(4)} - \beta_N^{(4)} = -4\beta_N \beta_N^{(4)} \frac{l_{N+1}}{v_F} - V \cos \left(\gamma_N + Qx_{N+1} - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}) \right) + \beta^{(6)} \frac{V^2}{2\beta_N^2} \sin^2(\gamma_N + Qx_{N+1}), \quad (11b)$$

$$\beta_{N+1}^{(e)} - \beta_N^{(e)} = -6\beta_N \beta_N^{(e)} \frac{l_{N+1}}{v_F} - 10(\beta_N^{(e)})^2 \frac{l_{N+1}}{v_F} + V \cos \left(\gamma_N + Qx_{N+1} - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}) \right) + \beta^{(e)} \frac{V^2}{2\beta_N^2} \sin^2(\gamma_N + Qx_{N+1}), \quad (11c)$$

etc. The reason why terms with odd derivatives $\beta^{(2n+1)}$, were discarded will be made clear below.

We note that in the arguments of the cosines in (11) it is necessary to retain the small differences $\gamma_{N+1} - \gamma_N$, therefore its presence leads to a nonzero result of the averaging of these terms over x_{N+1} . The averaging must be carried out with the distribution $P(l_N) = c \exp(-cl_N)$. By virtue of the condition $Q/c \gg 1$, the random phase Qx_N can be regarded as uniformly distributed over the circle $(0, 2\pi)$. The averaging of the terms containing l_{N+1} yields the factor $1/c$. Averaging Eq. (11), we obtain

$$0 = -\frac{1}{cv_F} \langle \beta^2 \rangle + \frac{V^2}{2} \left\langle \frac{1}{\beta} \right\rangle - \frac{V^2}{4} \left\langle \beta^{(4)} \frac{1}{\beta^2} \right\rangle, \quad (12a)$$

$$0 = -\frac{4}{cv_F} \langle \beta \beta^{(4)} \rangle + \frac{V^2}{2} \left\langle \frac{1}{\beta} \right\rangle - \frac{V^2}{4} \left\langle \beta^{(6)} \frac{1}{\beta^2} \right\rangle, \quad (12b)$$

$$0 = -\frac{1}{cv_F} (6 \langle \beta \beta^{(6)} \rangle + 10 \langle (\beta^{(4)})^2 \rangle) + \frac{V^2}{2} \left\langle \frac{1}{\beta} \right\rangle - \frac{V^2}{4} \left\langle \beta^{(8)} \frac{1}{\beta^2} \right\rangle, \quad (12c)$$

etc. In (12) are introduced the quantities $\beta^{(2n)} = (-1)^{n+1} \beta^{(2n)}$. As seen from Eqs. (12), all the quantities $\beta^{(2n)}$ are of the order of

$$\beta_0 = (cv_F V^2)^{1/3}. \quad (13)$$

Each equation in (12) contains one term with + sign, stemming from the averaging of the term

$$V \cos \left(\gamma_N + Qx_{N+1} - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}) \right).$$

In the equations for $\beta^{(2n+1)}$, the corresponding term contains the sine rather the cosine, its mean value is zero, so that the $\beta^{(2n+1)}$ are necessarily smaller in order of magnitude.

The estimate (13) of the order of magnitude of $\varepsilon(\varphi)$ shows that the term proportional to temperature, which we have discarded in (5), becomes of the same order as the remaining terms at $T \sim \beta_0$. Our results are thus valid at $T \ll (cv_F V^2)^{1/3}$.

2. We obtain now the asymptotic distribution function $W(\beta)$ at $\beta \gg \beta_0$. [$W(\beta)$ is the probability density of β , averaged over all the remaining $\beta^{(n)}$.] At $\beta \gg \beta_0$ the last term in (11a) is small, so that we can write for $W(\beta)$ an equation independent of the remaining parameters $\beta^{(n)}$. This is done in analogy with the derivation of the Fokker-Planck equation

$$W(\beta_{N+1}) d\beta_{N+1} = \langle W(\beta_N(\beta_{N+1}, x_{N+1})) d\beta_N \rangle_{x_{N+1}}, \quad (14)$$

$$\beta_N(\beta_{N+1}, x_{N+1}) = \beta_{N+1} + \beta_{N+1}^2 \frac{l_{N+1}}{v_F} - V \cos \left(\gamma_N + Qx_{N+1} - \frac{V}{\beta_{N+1}} \sin(\gamma_N + Qx_{N+1}) \right). \quad (15)$$

Substituting (15) in the general equation (14) we obtain for $W(\beta)$

$$\frac{\partial}{\partial \beta} \left(\frac{V^2}{4} \frac{\partial W}{\partial \beta} + \frac{1}{cv_F} \beta^2 W \right) = 0. \quad (16)$$

The solution of (16) is

$$W(\beta) = \text{const} \exp[-\gamma_3 (\beta/\beta_0)^3], \quad (17)$$

where β_0 is defined in (13). Equation (17) yields the asymptotic form of $W(\beta)$ at $\beta \gg \beta_0$ with exponential accuracy. To determine the pre-exponential factor it would be necessary to take into account the last term of (11a).

The quantity $W(\beta)$ determined in (17) us the distribution function of the quantity β at arbitrary values of the remaining $\beta^{(n)}$. It is easy to show that in the limit $\beta \gg \beta_0$ the remaining quantities $\beta^{(n)} \sim \beta$, so that averaging over them does not change the exponential form of (17).

3. We determine now the asymptotic form of $W(\beta)$ at $V \gg \beta \ll \beta_0$. In this region all $\beta^{(2n)} \sim \beta \ll \beta_0$, therefore we can leave out of (5) the nonlinear term $(\partial \varepsilon / \partial \varphi)^2$, and the condition $V \ll \beta$ ensures smallness of all the parameters, which is needed for the validity of the method, on going from N to $N+1$. The potential $V \cos(\varphi + Qx_N)$ contains only one harmonic, so that in the absence of nonlinear terms it is natural to seek $\varepsilon(\varphi)$ in the form

$$\varepsilon_N(\varphi) = -\beta_N \cos(\varphi - \gamma_N). \quad (18)$$

By regarding the term $(\partial \varepsilon / \partial \varphi)^2$ as a perturbation, it can be shown that the amplitudes of the higher harmonics $a^{(n)} (n \geq 2)$ are small compared with β like $\beta/\beta_0 (a^{(2)} \sim \beta(\beta/\beta_0)^3)$. Therefore in the region $\beta \ll \beta_0$ the amplitude of the first harmonic of β coincides with the value $\beta = \partial^2 \varepsilon / \partial \varphi^2 |_{\tau}$, determined in the preceding section; it is this which justifies the notation used.

We obtain for β the equation

$$\beta_{N+1} = \beta_N \left[1 - \frac{V^2}{2\beta_N^2} \sin^2(\gamma_N + Qx_{N+1}) \right] + V \cos \left(\gamma_N + Qx_{N+1} - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}) \right). \quad (19)$$

The corresponding equation for the distribution function is

$$\frac{\partial}{\partial \beta} \left(\frac{\partial W}{\partial \beta} - \frac{W}{\beta} \right) = 0. \quad (20)$$

Its solution is

$$W(\beta) = A \frac{\beta}{\beta_0^2}; \quad A \sim 1. \quad (21)$$

[The factor β_0^{-2} stems from the normalization $\int_0^{\beta_0} W(\beta) d\beta \sim 1$.]

We note that the linear asymptotic form (21) in contrast to the universal result (13) and (17) is valid only for the concrete form $V(\varphi) = V \cos(\varphi + Qx)$ of the potential: if the potential has several harmonics, Eq. (21) is replaced by

$$W(\beta) = A' (\beta/\beta_0)^{\eta/\beta_0}. \quad (22)$$

For the potential

$$V(\varphi) = -V [\cos(\varphi + Qx) + a \cos 2(\varphi + Qx)]; \quad a \ll 1, \quad (23a)$$

which has a small second-harmonic component, the exponent η is calculated in Appendix B:

$$\eta = 1 - 100/\beta a^2. \quad (23)$$

We emphasize that (22) is an intermediate asymptotic value in the region $V \ll \beta \ll \beta_0$, the so-called "Gaussian tail" of the distribution function. The region $\beta \ll V$ corresponds to the "Poisson tail," in which $W(\beta) \sim \exp(-\text{const}/\beta)$.

3. STATISTICAL CHARACTERISTICS OF CDW

We obtain in this section expressions for the energy of the ground state E_p and for the correlation radius R_c in terms of the distribution function $W(\beta)$.

1. The total ground-state energy of a chain with N impurities is, by definition, $\varepsilon_N(\gamma_N)$. The average energy density per lattice site is

$$E_p = c \langle \varepsilon_N(\gamma_N) \rangle / N = c \langle \varepsilon_{N+1}(\gamma_{N+1}) - \varepsilon_N(\gamma_N) \rangle. \quad (24)$$

Using (5) and (9) we obtain

$$\begin{aligned} \varepsilon_{N+1}(\gamma_{N+1}) - \varepsilon_N(\gamma_N) &= -V \cos(\gamma_{N+1} + Qx_{N+1}) + \frac{1}{2}(\gamma_{N+1} - \gamma_N)^2 \frac{\partial^2 \varepsilon_N}{\partial \varphi^2} \\ &= -V \cos(\gamma_N + Qx_{N+1} - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1})) + \frac{V^2}{2\beta_N^2} \sin^2(\gamma_N + Qx_{N+1}). \end{aligned} \quad (25)$$

Expression (25) must be averaged over x_{N+1} , and then over the distribution $W(\beta)$. Thus,

$$E_p = -\frac{cV^2}{4} \int_0^\infty W(\beta) \frac{d\beta}{\beta}. \quad (26)$$

Equation (26) yields a correct expression for the ground-state energy of the CDW in the field of the impurities (the so-called pinning energy) in terms of the distribution function $W(\beta)$. Not knowing the exact form of $W(\beta)$, we can only estimate E_p :

$$E_p = -\frac{1}{4v_F} (cv_F V^2)^{3/2} B; \quad B \sim 1. \quad (27)$$

Of course, the estimate (27) coincides with the previously obtained one.²

2. The correlation function of the CDW

$$K(x) = \langle \delta\rho(x) \delta\rho(0) \rangle = \text{const} \langle \cos(\varphi(x) - \varphi(0)) \rangle \sim \exp(-|x|/R_c),$$

where $\varphi(x)$ and $\varphi(0)$ are the phases in the ground state. In the calculation of the correlation radius R_c the point can be placed at the end of the chain: $\varphi(x) = \gamma_N$. This can change the pre-exponential factor in $K(x)$, but not the value of R_c . We obtain now the change of $\cos(\gamma_N - \varphi_0)$ following addition of one more impurity (we note that at $N \gg R_c$ the change of φ_0 is exponentially small):

$$\begin{aligned} \cos(\gamma_{N+1} - \varphi_0) &= \cos\left(\gamma_N - \varphi_0 - \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1})\right) \\ &= \cos(\gamma_N - \varphi_0) \left[1 - \frac{V^2}{2\beta_N^2} \sin^2(\gamma_N + Qx_{N+1}) \right] \\ &\quad + \sin(\gamma_N - \varphi_0) \frac{V}{\beta_N} \sin(\gamma_N + Qx_{N+1}). \end{aligned} \quad (28)$$

Averaging (28) and bearing in mind the independence of γ_N of x_{N+1} , we obtain

$$\langle \cos(\gamma_{N+1} - \varphi_0) \rangle = \langle \cos(\gamma_N - \varphi_0) \rangle \left[1 - \frac{V^2}{4} \int_0^\infty W(\beta) \frac{d\beta}{\beta^2} \right]. \quad (29)$$

From (29) we obtain the asymptotic form

$$\langle \cos(\gamma_N - \varphi_0) \rangle \sim \exp\left[-\frac{NV^2}{4} \int_0^\infty W(\beta) \frac{d\beta}{\beta^2}\right]. \quad (30)$$

Recognizing that $N = cx$, we obtain ultimately

$$R_c^{-1} = \frac{cV^2}{4} \int_0^\infty W(\beta) \frac{d\beta}{\beta^2}. \quad (31)$$

The logarithmic integral on (31) is cut off at $\beta \sim V$. As a result,

$$R_c^{-1} = \frac{1}{4v_F} (cv_F V^2)^{3/2} A_1; \quad A_1 \sim 1. \quad (32)$$

Under the condition $\ln(\beta_0/V) \gg 1$, the quantity A_1 is expressed in terms of A from (21):

$$A_1 = A \ln \frac{\beta_0}{V} = \frac{A}{3} \ln \frac{cv_F}{V}. \quad (33)$$

3. The dielectric susceptibility χ cannot be expressed in terms of $W(\beta)$. To calculate it we must find the joint distribution function $W(\beta, p)$, where p is the local polarization. We shall not perform the corresponding calculations, since it has not been possible to determine χ exactly. The estimate of χ agrees with that obtained earlier.²

4. STATE DENSITY AND CONDUCTIVITY OF CDW AT LOW FREQUENCIES

The equation for small oscillations of CDW about the ground state is^{3,9}

$$\frac{v_F}{u^2} \omega^2 \theta = -v_F \theta'' + V \cos(\varphi(x) + Qx) \theta; \quad (34)$$

here $\varphi(x)$ is the distribution of the phases in the ground state, and u is the phase velocity of the CDW.

We obtain now the state density $\rho(\omega)$ for the Schrödinger equation with the random potential (34) in the region of the "Gaussian tail" $uV/v_F \ll \omega \ll u\beta_0/v_F$. The existing exact methods of investigating the Schrödinger equation with a random potential^{6,7} are valid if the correlation radius of the potential is small compared with the characteristic length encountered in the problem. In our case this condition is not satisfied, and we therefore proceed differently and express $\rho(\omega)$ directly in terms of the distribution function $W(\beta)$ (accurate to a number of the order of unity).

The function $W(\beta)$ obtained in Sec. 2 gives the distribution of β at the last point of the chain. We now need an analogous distribution function at an arbitrary point inside the chain [we designate this function by $\bar{W}(\beta)$]. We choose a certain point N at the center of the chain and construct for it two energy-minimizing solutions of Eq. (5), starting from the right and left ends of the chain. We designate the obtained functions by $\varepsilon_N^<(\varphi_N)$ and $\varepsilon_N^>(\varphi_N)$. The final minimization of the energy consists of finding the total energy $\varepsilon_N(\varphi_N) = \varepsilon_N^<(\varphi_N) + \varepsilon_N^>(\varphi_N)$.

We are interested in the region $V \ll \beta \ll \beta_0$. Therefore, taking (18) into account, we obtain

$$\varepsilon_N(\varphi_N) = -\beta_N^< \cos(\varphi_N - \gamma_N^<) - \beta_N^> \cos(\varphi_N - \gamma_N^>), \quad (35)$$

$$0 = \frac{d\varepsilon_N}{d\varphi_N} \Big|_{\varphi_N} = \beta_N^< \sin(\gamma_N - \gamma_N^<) + \beta_N^> \sin(\gamma_N - \gamma_N^>), \quad (36)$$

$$\beta_N = \beta_N^< \cos(\gamma_N - \gamma_N^<) + \beta_N^> \cos(\gamma_N - \gamma_N^>). \quad (37)$$

It is easy to verify with the aid of (35)–(37) and (21) that

$$\overline{W}(\beta) = \overline{A} \frac{\beta^2}{\beta_0^2}; \quad \overline{A} \sim 1. \quad (38)$$

In the more general case corresponding to (22) we have

$$\overline{W}(\beta) = \overline{A} \left(\frac{\beta}{\beta_0} \right)^{2n+1} \frac{1}{\beta_0}. \quad (39)$$

We obtain now the connection between $\overline{W}(\beta)$ and the state density $\rho(\omega)$. We write down the spectral expansion for the Green's function $G_{\omega=0}(x, x) = \beta_x^{-1}$ of Eq. (34) at zero frequency [see (7)]:

$$G_{\omega=0}(x, x) = \sum_n \psi_n^2(x) / E_n, \quad (40)$$

$E_n = v_F \omega_n^2 / u^2$ are the energy levels of the Schrödinger equation (34).

We are interested in states in the region of the fluctuating boundary of the spectrum, where the wave functions $\psi_n(x)$ are well localized and the spectrum is essentially discrete. Therefore the partition function in (40) is of the order of its first term:

$$\beta_x^{-1} = G_{\omega=0}(x, x) \approx \frac{\psi_1^2(x)}{E_1(x)} \approx \frac{1}{l_1(x)} \frac{1}{E_1(x)}. \quad (41)$$

Recognizing that the dimension of the bound state is $l_1 \sim (E_1 / v_F)^{-1/2}$, we obtain from (41)

$$E_1(x) \approx \beta_x^2 / v_F; \quad \omega_1(x) \approx u \beta_x / v_F. \quad (42)$$

Therefore the distribution function $\overline{W}(\beta)$ from (38) yields directly the state density $\tilde{\rho}(\omega)$ for the average length of the bound state (see e.g., Ref. 7, p. 304), $l_1 \sim v_F \beta_0^{-1} \sim R_c$:

$$\tilde{\rho}(\omega) \sim \left(\frac{\omega}{\omega_0} \right)^3 \frac{1}{\omega_0};$$

$$\omega_0 = \frac{u}{v_F} \beta_0 = \frac{u}{v_F} (c v_F V^2)^{1/2}$$

is the characteristic pinning frequency.

We ultimately obtain for the state density $\rho(\omega)$ per lattice site

$$\rho(\omega) = \frac{C}{\omega_D} \left(\frac{\omega}{\omega_0} \right)^3, \quad (43)$$

$C \sim 1$; $\omega_D \sim u p_F$ is the Debye frequency of the CDW oscillations.

To calculate the conductivity $\sigma(\omega)$ connected with the CDW, it must be noted that (see Refs. 2 and 9)

$$\sigma(\omega) \sim \int \langle \omega \operatorname{Im} G_+(x, x) \rangle dx,$$

i.e., it differs from $\rho(\omega)$ by integration with respect to x , which introduces a factor on the order of the dimension $l(\omega)$ of the state with energy ω . Recognizing that $l(\omega) \sim v_F^{1/2} E^{-1/2}(\omega) \sim u \omega^{-1}$, we obtain

$$\sigma(\omega) \sim \text{const} \frac{\omega^2}{\omega_0^3}. \quad (44)$$

[We have left out of (44) all the constant factors that

do not depend on the impurities.]

In the case of a potential $V(\varphi)$ of general form we obtain with the aid of (39)

$$\rho(\omega) = \frac{C}{\omega_D} \left(\frac{\omega}{\omega_0} \right)^{2n+1}, \quad (45)$$

$$\sigma(\omega) \sim \frac{1}{\omega_0} \left(\frac{\omega}{\omega_0} \right)^{2n}. \quad (46)$$

We emphasize once more that the results (43)–(46) pertain to the intermediate frequency region $Vu/v_F \ll \omega \ll \omega_0$. In the region $\omega \ll Vu/v_F$ the states are formed on account of low-probability fluctuations on the "Poisson tail," therefore

$$\rho(\omega), \sigma(\omega) \sim \exp(-\text{const}/\omega).$$

5. DISCUSSION OF RESULTS

We have developed here a method that permits a quantitative approach to the investigation of the ground state of one-dimensional classical ordered system which substantial disorder (by substantial disorder is meant one that alters qualitatively the properties of the ground state). In addition to the considered problem of the charge-density wave, the results are directly applicable to a one-dimensional planar magnet with random anisotropy (see Appendix A) and in general to any one-dimensional system with a random field that interacts with a zero-gap mode of the phonon type.

The original results of the paper are represented by formulas (45) and (46) for the state density and for the CDW conductivity at low frequencies. The exponent η depends on the form of the interaction potential $V(\varphi + Qx)$ of the impurity with the CDW phase. For a potential containing a single harmonic, $\eta = 1$, and in the presence of a small second-harmonic component [See (23a)] the exponent is given by (23). In the considered case of weak impurities the interaction potential $V(\varphi + Qx)$ is directly proportional to the modulation $\delta\rho(\varphi + Qx)$ of the charge density of the CDW, therefore the coefficient a in (23) is directly the ratio of the amplitudes of the second and first Bragg peaks connected with the CDW superstructure. Thus, a direct connection (23) is predicted between the form of the structure factor of the CDW and the behavior of $\rho(\omega)$ and $\sigma(\omega)$ at low frequencies.

It should be noted that the function $\sigma(\omega) \sim \omega^2$ was obtained earlier by Fukuyama and Lee.² This result was obtained with the aid of an impurity diagram technique, with all the diagrams with crossing dashed lines discarded (the effective-medium approximation). In our problem this approximation is utterly unjustified, since the discarded diagrams are of the same order as the retained ones. Therefore the agreement between the result obtained by this method and our result [formula (44)] without the use of perturbation theory is quite surprising and worthy of a separate investigation. We note, incidentally, that this agreement holds only for the case of a potential with a single harmonic, ($V(\varphi) = V \cos\varphi$); for an arbitrary potential the answer contains the nontrivial exponent, whereas the method of Fukuyama and Lee² would yield the earlier result $\eta = 1$.

As noted in the derivation of the distribution function W the solution used by us for the balance equation is one of the local energy minima (not necessarily the absolute one). This calls for a certain refinement of the region of applicability of our results. The expressions obtained by us for $\rho(\omega)$ and $\sigma(\omega)$ constitute the contributions made to these quantities by the phonon modes localized in the random potential produced because the system selects any one of the local energy minima. In addition to the phonons, the system should contain excitations of the soliton type, which transfer the distribution of the phases from one local minimum to another. Since the characteristic times for such excitations should be quite large (especially at low temperatures), it is meaningful to formulate the problem in such a way that the solitons need not be taken into account at all. To obtain the characteristics of the system it would then be necessary to average over the possible metastable states in which the system can turn out to be. Actually, however, there is no special need for this, since our results depend not on the concretely chosen phase distribution that realizes the local minimum, but only on the equation that this distribution satisfies. Since the result is obtained by us unambiguously, it should be the same for any of these local minima, so that there is no need to average over them.

When total equilibrium thermodynamics is considered, account must be taken of the soliton contribution, and this limits the region of applicability of our results. Consider, for example the heat capacity of the system at low temperatures $T \ll \omega_0$. The contribution of the phonon states with density $\rho(\omega)$ from (43) is

$$C_{ph} \sim \frac{T^4}{\omega_D \omega_0^3}. \quad (47)$$

We estimate now the density of the soliton state: the characteristic scale of the function $\varepsilon(\varphi)$ is of the order β_0 , so that the probability of finding to minima of $\varepsilon(\varphi)$ that differ by ω in energy is of the order $\omega \beta_0^{-1}$. This probability is normalized to a length of the order of $R_c \sim v_F \beta_0^{-1}$.

The presence of solitons leads thus to a state density that is finite at $\omega = 0$ and has a value per lattice site

$$\rho_{\text{solit}}(0) \sim 1/\varepsilon_F; \quad \varepsilon_F = v_F p_F.$$

We note that our solitons are similar in many respects to the two-level excitations considered in Ref. 11.

The corresponding contribution to the heat capacity is

$$C_{\text{solit}} \sim T/\varepsilon_F,$$

the heat capacity therefore takes the form (47) at the temperatures

$$\omega_0 (u/v_F)^{1/2} \ll T \ll \omega_0. \quad (48)$$

As seen from (48), the existence of a region where our analysis is valid for full-equilibrium thermodynamics is the result of the classical character of the CDW, as expressed by the condition $u \ll v_F$ (Ref. 1).

It should also be noted that at $T \neq 0$ there should exist a finite conductivity $\sigma(0)$ at zero frequency and a singular dielectric susceptibility $\chi(k) \sim (R_p k)^{-2}$ at small

momenta [the last effect was considered by Brazovskii for the case of strong pinning, but the existence of finite $\rho_{\text{solit}}(0)$ was not taken into account]. These phenomena are due entirely to excitations of the soliton type.

In conclusion, the author thanks L. P. Gor'kov and V. L. Pokrovskii for numerous discussions of the work.

APPENDIX A

The energy of a chain of classical planar spins with random anisotropy of second order is of the form

$$H = -J \sum_n S_n S_{n+1} - D \sum_n (S_n \xi_n)^2, \quad (A.1)$$

where $S_n = (S \cos \theta_n, S \sin \theta_n)$; $\xi_n = (\cos \alpha_n, \sin \alpha_n)$; α_n is a random phase uniformly distributed over a circle. Changing over to the variable $\varphi_n = 2\theta_n$, we obtain

$$H = \frac{JS^2}{8} \sum_n (\varphi_n - \varphi_{n+1})^2 - \frac{DS^2}{2} \sum_n \cos(\varphi_n - 2\alpha_n). \quad (A.2)$$

Comparing with (2), we see that the considered problems are identical, apart from the substitutions $cv_F \rightarrow 1/4 JS^2$, $V \rightarrow 1/2 DS^2$; the weak-pinning condition $cv_F \gg V$ corresponds to weak anisotropy $D \ll J$. A ferromagnet with a Heisenberg (three-component) spin can also be treated by the proposed method; the difference lies in the fact that it becomes necessary to consider a function $\varepsilon(\theta, \varphi)$ that depends on two angles rather than one.

APPENDIX B

We seek $\varepsilon(\varphi)$ corresponding to the potential (23a) in the form

$$\varepsilon_N(\varphi) = -z_N \cos(\varphi - \gamma_N) - ay_N \cos 2(\varphi - \gamma_N) \quad (B.1)$$

and obtain the asymptotic form of $W(z)$ at $z \ll \beta_0$. The equations for γ_N , z_N , and y_N are obtained in analogy with (10) and (19):

$$\gamma_{N+1} - \gamma_N = -\frac{V}{z_N + 4ay_N} [\sin(\gamma_N + Qx_{N+1}) + 2a \sin 2(\gamma_N + Qx_{N+1})], \quad (B.2)$$

$$z_{N+1} = z_N \cos(\gamma_{N+1} - \gamma_N) + V \cos(\gamma_{N+1} + Qx_{N+1}), \quad (B.3)$$

$$y_{N+1} = y_N \cos 2(\gamma_{N+1} - \gamma_N) + V \cos 2(\gamma_{N+1} + Qx_{N+1}). \quad (B.4)$$

The corresponding equation for the distribution function $\mathcal{P}(z, y)$ is

$$\frac{1}{4} \frac{\partial^2 \mathcal{P}}{\partial z^2} + \frac{1}{2} \frac{\partial^2 \mathcal{P}}{\partial z \partial y} + \frac{1}{4} \frac{\partial^2 \mathcal{P}}{\partial y^2} - \frac{\partial}{\partial z} \left[\left(\frac{1}{2(z+4ay)} - \frac{1+4a^2}{4(z+4ay)^2} z \right) \mathcal{P} \right] - \frac{\partial}{\partial y} \left[\left(\frac{2a}{z+4ay} - \frac{1+4a^2}{(z+4ay)^2} y \right) \mathcal{P} \right] = 0. \quad (B.5)$$

Integrating (B.5) with respect to y we get

$$\frac{1}{4} \frac{d^2 W}{dz^2} - \frac{d}{dz} \left(\frac{1-4a^2}{4z} W - \frac{4a^2}{z^2} W_2 \right) = 0; \quad (B.6)$$

here

$$W(z) = \int \mathcal{P}(z, y) dy, \quad W_2(z) = \int \mathcal{P}(z, y) y^2 dy;$$

in the derivation of (B.6) we used the condition $a \ll 1$.

It will be shown that $W_2(z) = Az^2 W(z)$; therefore Eq. (B.6) has the solution

$$W(z) = \text{const} \cdot z^\eta; \quad \eta = 1 - 4a^2 - 16a^2A. \quad (\text{B. 7})$$

For a final determination of η we must find A in the zeroth order in a . Multiplying (B. 5) by y and y^2 and integration, we obtain equations for

$$W_1(z) = \int \mathcal{P}(z, y) y \, dy \quad \text{and} \quad W_2(z).$$

We have

$$\frac{1}{4} \frac{d^2 W_1}{dz^2} - \frac{1}{4} \frac{d}{dz} \left(\frac{W_1}{z} \right) - \frac{W_1}{z^2} = \frac{1}{2} \frac{dW}{dz}, \quad (\text{B. 8})$$

$$\frac{1}{4} \frac{d^2 W_2}{dz^2} - \frac{1}{4} \frac{d}{dz} \left(\frac{W_2}{z} \right) - 2 \frac{W_2}{z^2} = \frac{dW_1}{dz} - \frac{1}{2} W. \quad (\text{B. 9})$$

Substituting $W(z) = z$ in (B. 8) and (B. 9) we obtain

$$W_1(z) = -z^2/3; \quad W_2(z) = z^4/3.$$

Thus, $A = 11/6$ and we get for η :

$$\eta = 1 - 100/3a^2. \quad (\text{B. 10})$$

We have $\beta = \partial^2 \mathcal{E} / \partial \varphi^2 |_{\varphi=\gamma} = z + 4ay$. Since $\bar{y}(z) = z^{-1} W_1(z) \sim z$, $a \ll 1$, the distribution function $W(\beta)$ takes the form (B. 7) with the same value of η .

¹P. A. Lee, T. M. Rice, and P. W. Anderson, *Sol. State Comm.* **17**, 1089 (1975).

- ²H. Fukuyama and P. A. Lee, *Phys. Rev.* **B17**, 535 (1977).
³W. J. Gunning, A. J. Heeger, J. F. Schegolev, S. P. Zolotukhin, *Sol. State Comm.* **25**, 981 (1978). J.-J. Andre, A. Beeber, and F. Gauntier, *Ann. de Phys.* **1**, 145 (1976). K. C. Carneiro, G. Shirane, S. A. Werner, and S. Kaiser, *Phys. Rev.* **B13**, 4258 (1976).
⁴D. C. Mattis, *Phys. Lett.* **A56**, 421 (1976). G. Toulouse, *Comm. Phys.* **2**, 115 (1977). J. Villain, *J. Phys.* **C10**, 1717 (1977).
⁵D. J. Scalapino, M. Sears, and R. A. Ferrel, *Phys. Rev.* **B6**, 3409 (1972).
⁶H. Schmidt, *Phys. Rev.* **105**, 425 (1957).
⁷S. A. Gradeskul and L. A. Pastur, *Fiz. Nizk. Temp.* **1**, 277 (1975) [*Sov. J. Low Temp. Phys.* **1**, 135 (1975)].
⁸Y. Ymry and S.-k Ma, *Phys. Rev. Lett.* **35**, 1399 (1975).
⁹L. P. Gor'kov, *Pis'ma Zh. Eksp. Teor. Fiz.* **25**, 384 (1977) [*JETP Lett.* **25**, 358 (1977)].
¹⁰K. B. Efetov, *Zh. Eksp. Teor. Fiz.* **75**, 1885 (1978) [*Sov. Phys. JETP* **48**, 949 (1978)].
¹¹P. W. Anderson, B. I. Halperin, and C. M. Varma, *Phil. Mag.* **25**, 1 (1972).
¹²S. A. Brazovskii, *Zh. Eksp. Teor. Fiz.* **76**, 1000 (1979) [*Sov. Phys. JETP* **49**, 557 (1979)].
¹³R. Harris, M. Plischke, and M. J. Zuckermann, *Phys. Rev. Lett.* **31**, 160 (1973).

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Effect of a strong magnetic field on the spin-reorientation transition in DyCo_{5,3}

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Magnetization and magnetostriction measurements have been made on the intermetallic compound DyCo_{5,3} in strong pulsed magnetic fields (up to 250 kOe), at temperatures close to the spin-reorientation transition that is observed in this compound and that is of the easy-plane, easy-cone, easy-axis type. The experimental data are compared with theoretical relations obtained by consideration of a model of a two-sublattice ferrimagnet, each sublattice of which has its own magnetocrystalline anisotropy; the uniaxial anisotropy constants of the sublattices have different signs and are comparable in magnitude with the intersublattice exchange interaction. It is shown that such a model describes the magnetic properties of DyCo_{5,3} in strong fields; values of the anisotropy constants of the sublattices are obtained from the experimental data. It is significant that in the analysis of magnetization curves it was necessary to allow for a noncollinear magnetic structure that occurs in strong fields, and also for a dependence of the value of the magnetic moment of the Dy sublattice on direction.

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INTRODUCTION

The compound DyCo_{5,3}, like other rare-earth compounds RCo₅, has a hexagonal crystallographic structure of the CaCu₅ type (space group *P6/mmm*). This structure may be regarded as consisting of alternating layers of cobalt atoms, placed perpendicular to the hexagonal axis; the atoms of the rare-earth metal (REM) occupy hexagonal positions in every second layer.^{1,2} A decisive role in the formation of the magnetism in RCo₅ is played by the Co-Co exchange interaction,

which causes the high Curie temperatures³ (about 1000 K) of these compounds. The R-Co interaction is about an order of magnitude weaker; the exchange interaction within the R sublattice can as a rule be neglected. Thus the REM atoms constitute a paramagnetic system located in an effective field produced by the Co sublattice. The compounds RCo₅ with light REM have ferromagnetic ordering; those with heavy, ferrimagnetic.

A distinctive feature of many RCo₅ compounds is the fact that at low temperatures their uniaxial magnetic