Conductivity of one-dimensional incommensurate system

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Near an incommensurate–commensurate phase transition, all impurities that interact with a one-dimensional incommensurate system must be regarded as strong. This makes it possible to obtain the low-frequency conductivity $\sigma(\omega)$. If $\omega_2<\omega<\omega_1$, where $\omega_2\ll\omega_1$ and $\omega_1\to 0$ as the phase transition is approached, then $\sigma(\omega)\propto\omega^{-1+\eta}$, $\eta\propto l_s/\bar{l}$, where l_s is the soliton width and $\bar{l}$ is the average between the impurities. On the other hand, if $\omega<\omega_2$ the conductivity is proportional to $\exp(-\pi c/\bar{l}\omega)$.

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1. INTRODUCTION

The conductivity of one-dimensional systems, such as of a charge-density wave, has been the subject of a large number of studies.[1-5] It is known[1] that in the absence of impurities or of friction, a one-dimensional charge-density wave that is incommensurate with the lattice can be displayed without changing its energy. This means that the dc conductivity due to the charge-density wave in infinite. It was shown[2,3] that in the absence of a periodic potential the influence of the impurities makes the conductivity tend to zero like $\exp(-\text{const}/\omega)$ as the frequency $\omega\to 0$. The conductivity $\sigma(\omega)$ at finite temperature was obtained earlier[4] for a charge-density wave, both commensurate and incommensurate with the lattice, in the absence of impurities. The joint action of the periodic substrate potential and of friction was considered in Ref. 6. Feigelman[5] obtained the conductivity of a charge-density wave interacting with weak impurities. In the present paper, the low-frequency conductivity at zero temperature is obtained near the point of an incommensurate–commensurate phase transition.

By an appropriate choice of the measurement units of the time t and of the coordinate x, the Hamiltonian of a charge-density wave interacting with a periodic potential can be reduced to the form[4,7,8]

$$\mathcal{H}=\int\left[\frac{1}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2+\frac{1}{2}\left(\frac{\partial\varphi}{\partial x}-\delta\right)^2+V(\varphi)\right]dx, \tag{1}$$

where φ is the phase of the charge-density wave, $V(\varphi)$ is a periodic potential with period b, and δ is the difference between the initial periods of the charge-density wave and of the potential $V(\varphi)$. Exactly the same Hamiltonian describes the behavior of a commensurate system of atoms interconnected by springs and located on an aperiodic substrate having a period b. In this case δ is equal to the difference between the equilibrium length of the spring and the substrate period. The ground state of a system having a Hamiltonian (1) depends essentially on the value of the parameter δ. If δ is less than a certain critical value δ_c,

$$\delta_c=\frac{1}{b}\int_0^b[2(V(\varphi)-V_{min})]^{1/2}d\varphi, \tag{2}$$

it is more advantageous for the system to be in a commensurate state in which φ does not depend on x and assumes a value such that $V(\varphi)$ is a minimum. This means that at $\delta<\delta_c$ all the atoms are located at the minima of the substrate potential.

On the other hand, if $\delta>\delta_c$, the favored situation is the production of solitons, which are sections having a width $\sim l_s$ that does not depend on δ, on which $d\varphi/dx$ is relative large. The distance between the solitons

$$\mathcal{L}\sim l_s\ln[\delta_c/(\delta-\delta_c)]$$

is large near the commensurate–incommensurate phase transition (C–I transition), which takes place at $\delta=\delta_c$. In the commensurate phase, all the atoms are located at the minima of the substrate potential. It is therefore impossible to displace them without changing the energy, and the conductivity is $\sigma(\omega=0)=0$. In the incommensurate phase, the soliton structure can be displaced without changing its energy. Therefore the conductivity at zero frequency is limited only by the impurities.

We shall assume that the impurities are pinned to the lattice, i.e., are located, say, at minima of the substrate potential. We shall also assume that their action is such that they make these minima even deeper. Thus, it is more advantageous for the atoms to be located where the impurities are located. This interaction with the impurities can be described, for example, by the Hamiltonian

$$\mathcal{H}_i=-V_i\int dx\sum_m\delta(x-x_m)\cos\frac{2\pi}{b}\varphi(x), \tag{3}$$

where m is the number of the impurity.

It is known that the interaction between solitons is proportional to $\exp(-\mathcal{L}/l_s)$, where $\mathcal{L}$ is the distance between them.[9] In this case there is a simple connection between l_s and the second derivative of the potential $V(\varphi)$ at its minimum point:

$$l_s=\left(\frac{d^2V(\varphi)}{d\varphi^2}\Big|_{\varphi=0}\right)^{-1/2}. \tag{4}$$

We shall assume that $V(\varphi)$ has a minimum at the point $\varphi=0$. Near the C-I transition, when the distance between the solitons $\mathcal{L}$ increases to infinity, the interaction between them becomes arbitrarily weak. At the same time, the energy of the interaction with the impurities is independent of the proximity to the C-I transition point. Consequently, near the C-I transition all the impurities should be regarded as strong, i.e., such that they fix uniquely $\varphi(x)$ at their location. To find the

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ground state and the conductivity of an incommensurate system it suffices therefore to consider a section of length l between two neighboring impurities, and then average over the length of this section with weight $\sim\exp(-l/\bar{l})$, where $\bar{l}$ is the average distance between the impurities.

2. GROUND STATE

We obtain the ground state on a section of length l between impurities. The energy of this section is

$$\mathcal{H}=\int_0^l\left[\frac{1}{2}\left(\frac{\partial\varphi}{\partial x}-\delta\right)^2+V(\varphi)\right]dx. \tag{5}$$

From the condition that the energy be a minimum we obtain the balance equation for $\varphi(x)$:

$$\frac{d^2\varphi}{dx^2}=\frac{dV(\varphi)}{d\varphi}, \tag{6}$$

which has a simple first integral

$$\frac{1}{2}\left(\frac{d\varphi}{dx}\right)^2=\mathcal{E}+V(\varphi), \tag{7}$$

where $\mathcal{E}$ is the integration constant. Near the C-I transition the value of $\mathcal{E}$ is close to $-V_{\min}$.

The $\varphi(x)$ dependence that follows from (7) and constitutes a sequence of solitons separated by a distance

$$\mathcal{L}=\int_0^b\frac{d\varphi}{[2(\mathcal{E}+V(\varphi))]^{1/2}} \tag{8}$$

is shown in Fig. 1. The parameter $\mathcal{E}$ is determined from the boundary conditions. The boundary conditions satisfied by $\varphi(x)$ are

$$\varphi(x=0)=0,\quad \varphi(x=l)=Nb. \tag{9}$$

These conditions follow from the fact that the phase φ is fixed at the impurities, and the impurities are located at minima of the substrate potential.

Near the C-I transition it is possible, using (7)–(9) as well as the proximity of $\mathcal{E}$ to $-V_{\min}$, to represent $\mathcal{H}$ in the form

$$\mathcal{H}=Nb\left[-(\delta-\delta_c)+\alpha\frac{b}{l_s}\exp\left(-\frac{l}{l_sN}\right)\right], \tag{10}$$

where α is a certain numerical constant that depends on the concrete form of the potential $V(\varphi)$. The first term in the square brackets of (10) is the self-energy of one soliton, which is negative at $\delta>\delta_c$. The second term describes exponentially weak repulsion of the solitons. At a given length l, it is necessary to find a value of N such that $\mathcal{H}(N)$ is a minimum. The distance between the solitons $\mathcal{L}$ is in this case

$$\mathcal{L}=l/N. \tag{11}$$

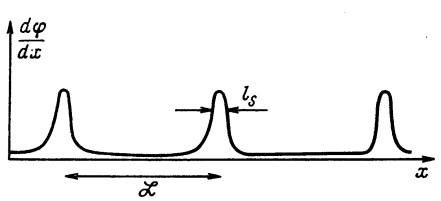

FIG. 1.

If $l<l_s\ln[\alpha b/l_s(\delta-\delta_c)]$, then there is not even one soliton between the impurities. The length over which the formation of precisely N solitons is profitable satisfies at $N\ll\ln[\alpha b/l_s(\delta-\delta_c)$ the condition

$$l_sN\ln[\alpha bN/l_s(\delta-\delta_c)]<l<l_s(N+1)\ln[\alpha b(N+1)/l_s(\delta-\delta_c)]. \tag{12}$$

On the other hand, if $N\gg\ln[\alpha b/l_s(\delta-\delta_c)]$, then the limits of the variation of l at a given N are determined from the equation

$$\left(1+\frac{l}{l_sN}\right)\frac{\alpha b}{l_s(\delta-\delta_c)}\left(1-\frac{1}{2}\frac{l}{l_s}\frac{1}{N(N-1)}\right)<\exp\left(\frac{l}{l_sN}\right)$$
$$<\left(1+\frac{l}{l_sN}\right)\frac{\alpha b}{l_s(\delta-\delta_c)}\left(1+\frac{1}{2}\frac{l}{l_s}\frac{1}{N(N+1)}\right). \tag{13}$$

3. LOW-FREQUENCY CONDUCTIVITY

In the absence of a periodic potential $V(\varphi)$, the low-frequency conductivity was obtained by Gor'kov.[2] I shall follow hereafter his paper for the most part. The equation of motion of $\varphi(x,t)$ in the presence of a homogeneous time-dependent external force F follows from the Hamiltonian (1):

$$\frac{\partial^2\varphi}{\partial t^2}-\frac{\partial^2\varphi}{\partial x^2}+\frac{dV(\varphi)}{d\varphi}=F(t). \tag{14}$$

The conductivity is proportional to the average velocity $\langle\partial\varphi(\omega)/\partial t\rangle$ that the particles acquire under the influence of the force $F(\omega)$. Since only an effect linear in $F(t)$ is taken into account in the calculation of the conductivity, φ can be represented in the form

$$\varphi=\varphi_0(x)+\psi(x,\ t), \tag{15}$$

where $\varphi_0(x)$ is given by the solution of Eq. (7) and describes N solitons located on a segment of length l, while $\psi(x,t)$ is small. Since we are seeking the conductivity at low frequencies that do not exceed (as will be shown later)

$$\frac{2}{l_s}\left(\frac{\delta-\delta_c}{\delta_c}\right)^{1/2},$$

it follows that the impurities must be regarded strong as before. Therefore ψ satisfies the following boundary conditions

$$\psi(x=0)=\psi(x=l)=0. \tag{16}$$

The equation satisfied by ψ follows directly from (14):

$$-\frac{d^2\psi}{dx^2}-\omega^2\psi+\frac{d^2V(\varphi_0)}{d\varphi_0^2}\psi=F(\omega). \tag{17}$$

The particle velocity $\partial\psi(\omega)/\partial t$ is obtained from the equation

$$\frac{\partial\psi}{\partial t}(\omega,x,l)=-i\omega\int_0^l G(x,x')F(\omega)dx', \tag{18}$$

where $G(x,x')$ is the Green's function of the operator in the left-hand side of (17):

$$G(x,x')=-\sum_k\frac{\psi_k(x)\psi_k^*(x')}{\omega^2-\omega^2(k)+i\omega 0}, \tag{19}$$

where ψ_k are the eigenfunctions of the operator in the left-hand side of (17), $\omega^2(k)$ are the corresponding eigenvalues, and k numbers the eigenfunctions.

I shall calculate only the real part of the conductivity, which after averaging over x turns out to be proportional to

$$\sigma(\omega)\sim\pi\frac{\omega}{l}\sum_{k}\left|\int_{0}^{l}\psi_{k}(x)\,dx\right|^{2}\delta(\omega^{2}-\omega^{2}(k)). \tag{20}$$

The function ψ_k satisfy a linear differential equation similar to the Schrödinger equation

$$\frac{d^{2}\psi_{k}}{dx}+\psi_{k}\left(\omega^{2}(k)-\frac{d^{2}V(\varphi_{0})}{d\varphi_{0}^{2}}\right)=0. \tag{21}$$

In this equation, the potential energy $d^2V(\varphi_0)d\varphi_0^2$ depends essentially on x only in regions of length l_s near the soliton centers. Therefore ψ_k and $\omega^2(k)$ can be sought by the strong-coupling method. Then $\psi_k(x)$, which satisfies the boundary condition $\psi_k(x=0)=0$, is given by

$$\psi_{k}(x)=A\sum_{n=-\infty}^{+\infty}\tau\left(x-n\mathscr{L}-\frac{\mathscr{L}}{2}\right)\times\left[\exp\left[iq\left(n\mathscr{L}+\frac{\mathscr{L}}{2}\right)\right]-\exp\left[-iq\left(n\mathscr{L}+\frac{\mathscr{L}}{2}\right)\right]\right]. \tag{22}$$

Here A is a normalization constant, q is the wave vector, and $\tau(x)$ is a function defined by the equations

$$\tau(x)=[2(V(\varphi_{1})-V_{min})]^{-1/2}, \tag{23}$$

$$x=\int_{0}^{\varphi_{1}}\frac{d\varphi}{[2(V(\varphi)-V_{min})]^{1/2}}. \tag{24}$$

If q satisfies the condition

$$q=\pi k/l, \tag{25}$$

where k is an integer, then $\psi_k(x)$ of (22) satisfies also the second boundary condition $\psi_k(x=l)=0$. The integral of ψ_k, which enter in $\sigma(\omega)$, is equal to

$$\int_{0}^{l}\psi_{k}dx=2Ab/i\sin\left(\frac{\pi}{2}\frac{k}{N}\right), \tag{26}$$

if k is an odd integer. On the other hand if k is even, this integral is zero. The normalization constant A turns out to be

$$A=(2Nb\delta_{c})^{-1/2} \tag{27}$$

at $k\neq N$ and

$$A=(4Nb\delta_{c})^{-1/2} \tag{28}$$

at $k=N$.

The frequency of the natural oscillation with wave vector q is given by

$$\omega^{2}(k,\mathscr{L})=\omega_{0}^{2}(\mathscr{L})\sin^{2}\frac{q\mathscr{L}}{2}=\omega_{0}^{2}(\mathscr{L})\sin^{2}\left(\frac{\pi}{2}\frac{k}{N}\right), \tag{29}$$

where $\omega_0^2(\mathscr{L})$ is equal to

$$\omega_{0}^{2}(\mathscr{L})=\frac{4\alpha}{l_{s}^{2}}\frac{b}{l_{s}\delta_{c}}\exp\left(-\frac{\mathscr{L}}{l_{s}}\right). \tag{30}$$

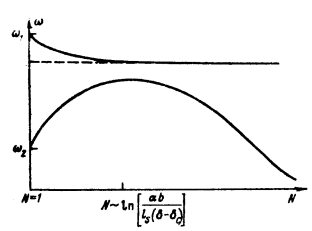

FIG. 2.

Substituting (26)–(29) in (20), and averaging over the distance l between the impurities, we obtain

$$\sigma(\omega)\sim\left(\frac{\pi\omega b}{l\delta_{c}}\right)\sum_{N=1}^{\infty}\frac{1}{N}\int_{l_{min}(N)}^{l_{max}(N)}\exp\left(-\frac{l}{\bar{l}}\right)\frac{dl}{l}\times\left\{\sum_{\substack{k=2m+1<N\\ m\geq 0}}\frac{2}{\sin^{2}(\pi/2\cdot k/N)}\delta(\omega^{2}-\omega_{0}^{2}(\mathscr{L})\sin^{2}\left(\frac{\pi}{2}\frac{k}{N}\right))+\sum_{\substack{N=2m+1\\ m\geq 0}}^{\infty}\delta(\omega^{2}-\omega_{0}^{2}(\mathscr{L}))\right\}. \tag{31}$$

Here m is an integer, $l_{min}(N)$ and $l_{max}(N)$ are determined from the condition (12) at $N\ll\ln[\alpha b/l_s(\delta-\delta_c)]$ and from the condition (13) at $N\gg\ln[\alpha b/l_s(\delta-\delta_c)]$.

The contribution made to the conductivity $\sigma(\omega)$ from segments with N solitons will differ from zero only if natural oscillations with frequency $\omega(k)=\omega$ exist on these segments. From the restrictions (12) it follows that at $N\ll\ln[\alpha b/l_s(\delta-\delta_c)]$ the natural frequencies of system consisting of N solitons lie in the range

$$\frac{4}{l_{s}^{2}}\left(\frac{\delta-\delta_{c}}{\delta_{c}}\right)\left[\frac{l_{s}}{\alpha b}(\delta-\delta_{c})\right]^{1/N}(N+1)^{-(1+1/N)}\sin^{2}\frac{\pi}{2N}<\omega^{2}<\frac{4}{l_{s}^{2}}\left(\frac{\delta-\delta_{c}}{\delta_{c}}\right)\frac{1}{N}. \tag{32}$$

The character of the dependences of $\omega_{max}^2(N)$ and $\omega_{min}^2(N)$ is shown for all in Fig. 2.

It follows from (32) and Fig. 2 that the highest possible oscillation frequency, namely

$$\omega_{1}=\frac{2}{l_{s}}\left(\frac{\delta-\delta_{c}}{\delta_{c}}\right)^{1/2}, \tag{33}$$

is possessed by a system containing only one soliton. The contribution of this system to $\sigma(\omega)$ vanishes only at $\omega<\omega_2$, where ω_2 is given by

$$\omega_{2}=\frac{\omega_{1}}{4}\left(\frac{l_{s}}{\alpha b}(\delta-\delta_{c})\right)^{1/2}\propto(\delta-\delta_{c}). \tag{34}$$

If $\omega<\omega_2$, contributions to the conductivity $\sigma(\omega)$ are made only by states with very large N. The conductivity is then proportional to

$$\sigma(\omega<\omega_{2})\sim\exp(-\pi c/l\omega), \tag{35}$$

where c is the speed of sound in the soliton system and varies near the C-I transition approximately like $(\delta-\delta_c)^{1/2}$. Inasmuch as $\omega<\omega_2\sim(\delta-\delta_c)$ in (35), the argument of the exponential is $\gtrsim(\delta-\delta_c)^{-1/2}$ and is large.

An equation of the type (35) was obtained by Gor'kov.[2] In his paper, however, in view of the absence of a periodic potential $V(\varphi)$, the speed of sound c was independent of the proximity to the transition point.

We show now that at $\omega_2<\omega<\omega_1$ the state with a single soliton makes the largest contribution to $\sigma(\omega)$. In fact,

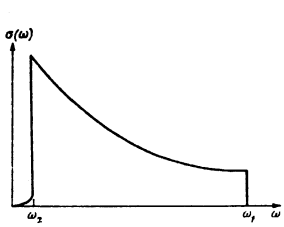

FIG. 3.

when the number of solitons is increased by unity, it is necessary to increase the length l by approximate $l_s \ln[\alpha b/l_s(\delta-\delta_c)]$. Therefore at $l_s \ln[b/l_s(\delta-\delta_c)] \gg \bar{l}$ the contribution to the conductivity from the states with more than one soliton is exponentially small compared with the contribution from states with one soliton. And since $\bar{l}$ does not depend on the proximity to the C-I transition, it is always possible to satisfy in a sufficiently close proximity to this transition, when $\delta - \delta_c \to 0$, the condition

$$l_s \ln[\alpha b/l_s(\delta-\delta_c)] \gg \bar{l}. \tag{36}$$

We obtain now the contribution made to the conductivity by states with $N=1$. Integration with respect to l in (31) is elementary and yields

$$\sigma(\omega) \sim \frac{\pi b}{l\delta_c}\left(\frac{l_s}{l}\right)\frac{1}{\omega}\exp\left(-\frac{l}{\bar{l}}\right), \tag{37}$$

where l is connected with ω by the condition

$$l = l_s \ln[(4\alpha/l_s^2)(b/l_s\delta_c)\omega^{-2}]. \tag{38}$$

It follows from (37) and (38) that

$$\sigma(\omega) \sim 1/\omega^{1-\eta}, \tag{39}$$

where $\eta = 2l_s/\bar{l}$. Thus, if the soliton width l_s is much less than average distance $\bar{l}$ between the impurities, $\sigma(\omega)$ increases with decreasing ω from ω_1 to ω_2. If, however, $l_s \gg \bar{l}$, then $\sigma(\omega)$ decreases when ω decreases from ω_1 to ω_2. At $\omega > \omega_1$ the conductivity $\sigma(\omega)$ is zero. At $\omega < \omega_2$ the conductivity is exponentially small and is given by (35). The variation of the conductifity $\sigma(\omega)$ with frequency at $l_s \ll \bar{l}$ is shown in Fig. 3.

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