High-frequency conductivity of charge-density-wave condensates at low temperatures

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Making use of Zamolodchikov's S matrix for the sine-Gordon system in $(1+1)$ dimensions, we calculate the frequency-dependent electric conductivity of the charge-density-wave (CDW) condensate at $T=0$ K. It is assumed that the phase of the CDW wave function obeys a sine-Gordon equation. The conductivity has a square-root threshold structure at $\omega=2m$ associated with soliton-antisoliton pair production, where m is the soliton energy. Furthermore below $|\omega|=2m$, the conductivity has a series of resonance peaks due to the creation of the soliton-antisoliton bound states at $\omega_n=2m\sin[\pi(2n+1)/2\lambda]$, with n the integer and λ the dimensionless coupling constant ($\lambda >> 1$) of the system.

I. INTRODUCTION

The low-temperature conductivities of the quasi-one-dimensional charge-density-wave condensates like tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ), $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$ (KCP), and $NbSe_3$ are of current interest. In the low-temperature region (say the temperature below 10 K), the quasiparticle density becomes negligible and it is believed that the electric conductivity should be dominated by ϕ solitons[1] [which are the kinks in the phase ϕ of the charge-density-wave (CDW) condensate].

According to Lee, Rice, and Anderson,[2,3] the dynamics of the CDW condensate is described by the Lagrangian density

$$\mathcal{L}=N_0\left[\phi_t^2-c_0^2\phi_x^2-2\left(\frac{\omega_0}{N}\right)^2(1-\cos N\phi)\right]-\frac{e}{\pi}\epsilon\,, \quad (1)$$

where

$$N_0=\frac{1}{4\pi v}\left[1+\eta^{-1}\left(\frac{2\Delta}{\omega_Q}\right)^2\right],$$

$$c_0=v\left[1+\eta^{-1}\left(\frac{2\Delta}{\omega_Q}\right)^2\right]^{-1/2},\quad \eta=\frac{1}{\pi v}g^2\,, \quad (2)$$

where v, Δ, and ω_Q are the Fermi velocity, the quasiparticle energy gap, and the phonon energy with $Q=2p_F$, and η is the dimensionless electron-phonon coupling constant. Furthermore, ω_0 is the pinning frequency and N is an integer. In the following we assume that $s<c_0<v$, where s is the phonon velocity.[3] Finally, the last term in Eq. (1) describes the coupling of ϕ to the external electric field ϵ.

As shown by Rice *et al.*,[1] the nonlinear solution (ϕ soliton) of Eq. (1) carries the electric charge and gives rise to the low-temperature dc conductivity of activated form with E_ϕ the soliton energy as the activation energy. This may account for the observed dc conductivity of TTF-TCNQ (Ref. 4) and KCP,[5] if the pinning frequency ω_0 is of the order of 10 K.

At even lower temperatures, where no thermally activated solitons are available, one of us (K.M.)[6] has shown that the conductivity is dominated by soliton-antisoliton pair production due to the electric field, which is strongly nonlinear in ϵ. However, the above calculation is limited to the frequency region $|\omega| << 2E_\phi$, where the pair production takes place via quantum-mechanical tunneling processes.

The object of the present paper is to study the electric conductivity of the model given in Eq. (1) in the whole frequency region (at $T=0$ K); from zero frequency to slightly above the pair creation threshold ($\omega\simeq 2E_\phi$). Recently Kaup and Newell[7] have shown within the classical field theory that the above sine-Gordon system absorbs the electromagnetic wave with $\omega\lesssim 2E_\phi$ via dipole excitation of breathers (i.e., the soliton and antisoliton bound pairs). However, in the low-temperature region which we are interested in, the full quantum-mechanical treatment of the Lagrangian (1) is required. For example, in the quantum limit the breathers are allowed to have only discrete energies[8] unlike the classical case.

About two years ago the S matrix as well as the electromagnetic vertex for soliton-antisoliton production of the sine-Gordon system was discovered by Zamolodchikov.[9,10] His results allow us to construct the exact frequency-dependent conductivity of the sine-Gordon system at $T=0$ K.

For this purpose we shall first transform the

Lagrangian density (1) into the standard form.[11]

$$\mathcal{L}'=\frac{1}{2}\partial_\mu\phi\partial^\mu\phi-(\alpha/\beta^2)[1-\cos(\beta\phi)] , \tag{3}$$

where

$$\mathcal{L}\,dx=\mathcal{L}'dx' ,\quad x'=x/c_0 ,$$

$$\phi'=\frac{1}{2}(N_0c_0)^{1/2}\phi ,\quad \alpha=\omega_0^2 ,$$

$$\beta=(8\pi)^{1/2}N\left[1+\eta^{-1}\left(\frac{2\Delta}{\omega_Q}\right)^2\right]^{-1/4} \tag{4}$$

$$=(8\pi)^{1/2}N(c_0/v)^{1/2} .$$

In Eq. (3) we have rewritten x' and ϕ' as x and ϕ. From Eq. (4) we have

$$0<\beta^2<<8\pi , \tag{5}$$

which implies that the energy spectrum of the soliton-antisoliton bound states is given by[8]

$$E_n=2m\sin(n\pi/2\lambda) , \tag{6}$$

where $m=E_\phi(\equiv 8\omega_0\beta^{-2})$ is the soliton energy

$$\lambda=8\pi\beta^{-2}-1$$

and n is an integer. In the present model $\lambda>>1$ we expect a large number of the soliton-antisoliton bound-state levels. We shall see later that the electric field couples only with those states with odd n. Therefore, at low temperatures these bound states contribute to a series of δ-function-like absorption spectrum in the electric conductivity.

II. FORMULATION

The electric conductivity is given by the imaginary part of the photon self-energy $\Pi(q^2)$ (the Kubo formula)

$$\sigma(\omega)=\frac{1}{\omega}\,\mathrm{Im}\,\Pi(q^2)\big|_{q^2=\omega^2} , \tag{7}$$

which is defined in terms of the polarization tensor in the $1+1$ dimensions as

$$\Pi^{\mu\nu}(q)=ie^2\int d^2x\,e^{iqx}\langle 0|T[j^\mu(x)j^\nu(0)]|0\rangle$$
$$=-(g^{\mu\nu}-q^\mu q^\nu q^{-2})\,\Pi(q^2) , \tag{8}$$

where the current operator $j^\mu(x)$ is defined by

$$j^\mu(x)=\pi^{-1}\epsilon^{\mu\nu}\partial_\nu\phi(x) \tag{9}$$

and $\epsilon^{\mu\nu}$ is the antisymmetric tensor. (Hereafter we adopt standard notations of the relativistic field theory in the $1+1$ dimensions and set $c_0\equiv 1$.)

Inserting intermediate states, one has

$$\mathrm{Im}\,\Pi(q^2)=\frac{e^2}{2}\int\int dp_1\,dp_2\left[\frac{m^2}{E_1E_2}\right]\sigma^2(p_1+p_2-q)\,\langle 0|j^\mu(0)|p_1\bar{p}_2\rangle\,\langle p_1\bar{p}_2|j_\mu(0)|0\rangle , \tag{10}$$

where

$$m=E_\phi ,\quad E_1=(m^2+\vec{p}_1^{\,2})^{1/2} ,$$

etc. Here $|p_1\bar{p}_2\rangle$ denotes the state with a soliton (fermion) with relativistic two momentum p_1 and an antisoliton (antifermion) with p_2. Making use of the equivalence between the sine-Gordon system (3) and the massive Thirring model,[11]

$$L=i\bar{\psi}\gamma_\mu\partial^\mu\psi-\frac{1}{2}g\,\bar{\psi}\gamma^\mu\psi\,\bar{\psi}\gamma_\mu\psi , \tag{11}$$

with

$$g=\pi(4\pi/\beta^2-1) ,$$

the current matrix elements may be parameterized in terms of two-dimensional spinors as

$$\langle 0|j^\mu(0)|p_1\bar{p}_2\rangle\equiv u(p_1)\gamma^\mu v(p_2)G(q^2) , \tag{12}$$

such that

$$\mathrm{Im}\,\Pi(q^2)=e^2\frac{m^2}{2Ep}|G(q^2)|^2 , \tag{13}$$

where $u(p_1)$ and $v(p_1)$ are two-component spinor-wave functions for particle with momentum p_1, and antiparticle with momentum p_2, respectively, and

$$E=\frac{1}{2}s ,\quad p=\frac{1}{2}(s-4m^2)^{1/2} ,\quad s=q^2 ,$$

are individual energy and momentum of the produced pair, the latter resulting in the characteristic square-root singularity at the threshold.

For the sine-Gordon Lagrangian (3) (or the massive Thirring model) the form factor $G(q^2)$ has been determined[10] as

$$G(q^2)\equiv G(\theta)=\frac{\cosh[\frac{1}{2}(i\pi-\theta)]}{\cosh[\frac{1}{2}\lambda(i\pi-\theta)]}e^{iT(i\pi-\theta)} , \tag{14}$$

with

$$T(z)=\int_0^\infty\frac{dy}{y}\,\frac{\sin^2\left(\frac{zy}{2\pi}\right)\sinh\left[\frac{1}{2}\left(1-\frac{1}{\lambda}\right)y\right]}{\sinh y\,\sinh\left(\frac{y}{2\lambda}\right)\cosh\frac{1}{2}y} . \tag{15}$$

Here $\frac{1}{2}\theta$ is the rapidity of the particles in the center of mass frame

$$\sinh\frac{\theta}{2}=\frac{p}{m}\,,\quad \cosh\frac{\theta}{2}=\frac{E}{m}\,,$$
$$q^2=s=2m(1+\cosh\theta) \tag{16}$$

As we have noted already the parameter $\lambda(>0)$ is expressed in terms of β or g as

$$\lambda=1+\frac{2g}{\pi}=\frac{8\pi}{\beta^2}-1\;. \tag{17}$$

In particular, in the case of the charge-density-wave condensate, we have $\lambda>>1$. From the $\cosh[\frac{1}{2}(i\pi+\theta)]$ denominator, the form factor $G(\theta)$ has poles at

$$\theta_n=i\pi\left(1-\frac{n}{\lambda}\right),\quad n=1,3,5,\ldots,[\lambda]\;, \tag{18}$$

corresponding to bound states with masses

$$M_n=2m\sin(2n\pi/\lambda)\;. \tag{19}$$

Comparing with the mass spectrum of the bound states (6), one notes that the electromagnetic field couples to bound states with odd n, the state with $c=-1$, only, where c is the charge conjugation operator. These bound states give rise to a series of resonance poles in the complex electric conductivity.

The above form factor is derived from the S matrix for fermion (soliton) and antifermion (antisoliton) scattering in the $c=-1$ state[9,10]

$$S_{f\bar f}^{(-)}(\theta)\equiv e^{2i\delta_{f\bar f}^{(-)}(\theta)}=-\frac{\cosh[\frac{1}{2}\lambda(i\pi+\theta)]}{\cosh[\frac{1}{2}\lambda(i\pi-\theta)]}S_{ff}(\theta)\;, \tag{20}$$

where $S_{ff}(\theta)$ is the two-fermion scattering amplitude[9]

$$S_{ff}(\theta)=\prod_{l=1}^{\infty}\frac{\Gamma[\lambda(2l-\hat\theta)]\,\Gamma[1+\lambda(2l-2-\hat\theta)]\,\Gamma[\lambda(2l-1+\hat\theta)]\,\Gamma[1+\lambda(2l-1+\hat\theta)]}{\Gamma[\lambda(2l+\hat\theta)]\,\Gamma[1+\lambda(2l-2+\hat\theta)]\,\Gamma[\lambda(2l-1-\hat\theta)]\,\Gamma[1+\lambda(2l-1-\hat\theta)]}\;,$$

with

$$\hat\theta=-i\theta/\pi \tag{21}$$

and follows uniquely by postulating (a) the absence of a left-hand cut in the s plane, i.e.,

$$G(i\pi+\theta)=G(i\pi-\theta)\,,\quad \theta>0\;, \tag{22}$$

(b) the discontinuity over the right-hand cut according to Watson's theorem

$$\frac{G(\theta)}{G(-\theta)}=e^{2i\delta_{f\bar f}^{(-)}(\theta)}\,,\quad \theta>0\;, \tag{23}$$

and (c) the absence of any physical sheet singularity other than the bound-state poles displayed in the form factor of Eq. (14). For our purpose it is useful to rewrite the infinite tail of the product (21) as an integral representation

$$S_{ff}(\theta)=\frac{\Gamma[\lambda(2-\hat\theta)]\,\Gamma(1-\lambda\hat\theta)\,\Gamma[\lambda(1+\hat\theta)]\,\Gamma[1+\lambda(1+\hat\theta)]}{\Gamma[\lambda(2+\hat\theta)]\,\Gamma(1+\lambda\hat\theta)\,\Gamma[\lambda(1-\hat\theta)]\,\Gamma[1+\lambda(1-\hat\theta)]}e^{J(\theta)}\;, \tag{24}$$

where

$$J(\theta)=\int_0^\infty\frac{dy}{y}\,\frac{e^{-2y}\sinh\left(\frac{\theta}{i\pi}y\right)\sinh\left[\frac{y}{2}\left(1-\frac{1}{\lambda}\right)\right]}{\sinh(y/2\lambda)\cosh\frac{1}{2}y}\;. \tag{25}$$

Here use is made of the formula

$$\ln\frac{\Gamma(a-z)}{\Gamma(a+z)}=\int_0^\infty\frac{dy}{y}\left[-2\lambda z e^{-y/\lambda}+e^{y/\lambda(1/2-a)}\sinh(zy)/\sinh\left(\frac{y}{2\lambda}\right)\right]\;. \tag{26}$$

The integral (25) converges for

$$\mathrm{Im}\,\theta < \pi(2+1/\lambda) \tag{27}$$

due to the fact that we have explicitly kept the first $l=1$ factor (20): its t-channel poles at $\theta_n^* = i\pi(n/\lambda)$ would destroy the convergence for $\mathrm{Im}\,\theta \geq 1/\lambda$ if it were included into the integral representation.

III. LIMITING BEHAVIORS

It is now useful to discuss two regions separately.

A. Threshold region $q^2 \gtrsim 4m^2$

Close to threshold the conductivity for the free-fermion case is dominated by the p^{-1} divergence in Eq. (13). The form factor $G(q^2)$ introduces the following modification: If λ is not an odd integer, Eq. (14) shows

$$G(q^2) = -i\sinh(\tfrac{1}{2}\theta)\sec(\tfrac{1}{2}\pi\lambda)e^{T_{th}} . \tag{28}$$

The $\sinh\frac{1}{2}\theta(\equiv p/m)$ factor destroys the threshold peak such that

$$\mathrm{Im}\,\Pi(q^2) = \frac{e^2 p}{2E}\left[\sec\left(\frac{\pi\lambda}{2}\right)\right]^2 e^{2T_{th}} ,$$

with

$$2T_{th} \equiv 2T(i\pi) = -\int_0^\infty \frac{dy}{y}\left\{\tanh^2\frac{y}{2}\coth\frac{y}{2\lambda} - \tanh\frac{y}{2}\right\} . \tag{29}$$

Equation (29) is numerically evaluated as a function of λ and shown in Fig. 1. The exponential $e^{2T_{th}}$

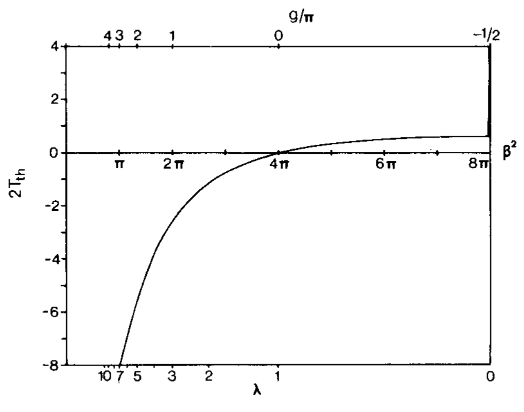

FIG. 1. $T_{th}(\lambda)$, which appears in the threshold expression of the electric conductivity, as a function of λ.

goes through unity for $\lambda=1$ (free-fermion case). It decreases as $e^{-1.7\lambda}$ for large $\lambda \gg 1$, since strong attraction presents an obstacle to the production of free pairs. Correspondingly, for the repulsive case [i.e., $\lambda\epsilon(1,0)$], although this is very unlikely in our model, there is an enhancement by $e^{0.6} \simeq 1.82$ at $\lambda=0$. If one goes beyond $\lambda=0$ (this is already the unphysical region in our model) there is a discontinuous jump to infinity indicating instability of the vacuum with respect to pair production. At the same point $\lambda=0, \beta^2=8\pi$ has been shown before,[11] in the context of the sine-Gordon theory, to have a bottomless energy. The resulting phase transition was investigated by Luther,[12] who argued that there would be a rearrangement of the vacuum with the new $\lambda_{\text{new}} > 0$.

If λ happens to hit odd integers > 1, the original $(s-4m^2)^{-1/2}$ threshold behavior becomes again visible, since

$$G(q^2) = (-1)^{\lambda-1/2}\frac{2}{\lambda}e^{T_{th}} . \tag{30}$$

The reason for this is the arrival of a bound-state pole $\lambda=n$ at the threshold point. Its approach $\lambda \to n$ is signaled by the $(\frac{1}{2}\sec\pi\lambda)^2$ factor in Eq. (29).

Summing up the conductivity near the threshold is given by

$$\sigma(\omega) = \sigma_0(\lambda)\frac{[\omega^2-(2m)^2]^{1/2}}{\omega} , \tag{31}$$

with

$$\sigma_0(\lambda) = \frac{e^2}{2}\left[\sec\left(\frac{\pi\lambda}{2}\right)\right]^2 e^{2T_{th}(\lambda)} \tag{32}$$

for $\lambda \neq n$.

B. Resonance peaks below the threshold

Let us consider now the resonance peaks in the conductivity caused by the bound-state poles. Inserting the bound states $|B_n(q)\rangle$ into Eq. (10), we find their contribution

$$\mathrm{Im}\,\Pi(q^2) = \frac{e^2}{2}\sum_{n:\text{odd}} g_n^2\left\{4\pi\frac{m^2}{m_n^2}\right\}\delta(q^2-m_n^2) , \tag{33}$$

with g_n being the dimensionless direct photon-"vector" meson (i.e., the $c=-1$ soliton-antisoliton bound-state) coupling defined by[13]

$$\langle 0|j^\mu|B_n(q)\rangle \equiv 2mg_n\epsilon^\mu(q) . \tag{34}$$

There is only one polarization vector $\epsilon^\mu(q) = (\hat{q}^1,\hat{q}^0)$ for a massive vector meson in $1+1$ dimensions. The coupling can be determined by making use of the factorization property of invariant amplitudes at poles. By the reduction formalism, $G(q)^2$ and $S_{f\bar{f}}$ must behave close to the pole $q^2=m_n^2$ according to

$$(q^2-m_n^2+i\epsilon)^{-1}\langle 0|j^\mu|B_n(q)\rangle\langle B_n(q)|j_\mu|p_1\bar{p}_2\rangle \tag{35}$$

and

$$(q^2-m_n^2+i\epsilon)^{-1}i\left(\frac{m^2}{2Ep}\right)\langle p_1\bar{p}_2|j^\mu|B_n(q)\rangle \times\langle B_n(q)|j_\mu|p_1\bar{p}_2\rangle\ , \tag{36}$$

respectively. The kinematic factor $i(m^2/2Ep)$ in the second expression appear, since the invariant scattering amplitude A is defined in terms of S via

$$S\equiv\hat{1}-i(2\pi)^2\delta^2(p_F-p_I)A\ , \tag{37}$$

where p_F and p_I are two momenta of the final state and the initial state. For the $c=-1$ states with our normalization, $\hat{1}$ stands for the δ functions

$$\hat{1}\to\frac{1}{2}\left[(2\pi)^2\frac{E_1E_2}{m^2}\delta(p_1'-p_1)\times\delta(p_2'-p_2)+(p_1'\leftrightarrow p_2')\right]. \tag{38}$$

But $(2\pi)^2\delta^2(p_F-p_I)$ can be rewritten as $m^2/2Ep$ times the above expression such that

$$S=\left[1-i\left(\frac{m^2}{2Ep}\right)A\right]\hat{1}\ . \tag{39}$$

Therefore one has

$$g_n^2=\frac{1}{4m^2}\frac{(\text{Res}\,G)^2}{(im/2Ep)\text{Res}\,S}\bigg|_{q^2=m_n^2}\ . \tag{40}$$

Now $G(q^2)$ and S have the same poles $(2/\lambda)(1/\theta-\theta_n)$ from

$$\left[\text{sech}\left(\frac{\lambda}{2}(i\pi-\theta)\right)\right]^{-1}.$$

Therefore we can directly take the θ residues multiplied by

$$\frac{\partial q^2}{\partial\theta}=4m^2\cosh\frac{\theta}{2}\sinh\frac{\theta}{2}=4Ep\ , \tag{41}$$

such that

$$g_n^2=-\frac{1}{\lambda}\frac{|\cos(\pi n/2\lambda)|^2}{\sin\pi\lambda}\left(\frac{e^{2T(i\pi-\theta)}}{e^{2i\delta_{ff}(\theta)}}\right)_{\theta=\theta_n} \tag{42}$$

The above expression gives the intensity of individual resonance, associated with the creation of the soliton-antisoliton bound states.

Some limiting cases g_n^2 can be calculated analytically. For $\lambda>>n$, the integral (15) gives

$$2T(i\pi-\theta_n)\sim-\frac{n^2}{2\lambda},\quad e^{2T}=\exp\left(-\frac{n^2}{2\lambda}\right). \tag{43}$$

The $S_{ff}(\theta)$ matrix, on the other hand, yields

$$e^{2i\delta_{ff}(\theta_n)}=-\frac{\pi}{\sin\pi\lambda}\frac{\Gamma(\lambda+n)\,\Gamma(2\lambda-n)\,\Gamma(1+2\lambda-n)\,e^{J(\theta_n)}}{\Gamma(\lambda-n)\,\Gamma(3\lambda-n)\,\Gamma(1+\lambda-n)\,\Gamma(n)\,\Gamma(1+n)}\to-\frac{\pi}{\sin\pi\lambda}\frac{\lambda^{2n}}{n!(n-1)!}\ . \tag{44}$$

Thus

$$g_n^2=\frac{1}{\pi}n!(n-1)!\lambda^{-(2n+1)}e^{-n^2/2\lambda}\ \text{for}\ \lambda>>n\ . \tag{45}$$

Note that the factor $\sin\pi\lambda$ cancels, thereby guaranteeing positive definiteness of g_n^2 [which is equivalent to positive norms of the states $|B_n(q)\rangle$!]. Its origin lies in the occurence of t-channel poles at $\theta_n^*=i\pi n/\lambda$ in $e^{2i\delta_{ff}(\theta)}$, one of which coincides with the s-channel pole as well as sign flip.

When the last bound state lies very close to the threshold (i.e., $\lambda-n_{\max}<<1$), one has another limiting behavior

$$e^{2i\delta_{ff}}\sim\frac{\pi}{\sin\pi\lambda}(\lambda-n)_{\max},\quad e^{2T}\simeq e^{2T_{th}}$$

and

$$g_n^2\simeq\frac{\pi}{4\lambda^3}(\lambda-n_{\max})e^{2T_{th}(\lambda)}\ . \tag{46}$$

Equations (45) and (46) indicate that the coupling constant g_n^2 initially decreases rapidly with increasing n, but begins to saturate near the threshold.

Finally the conductivity below the threshold $(|\omega|<2E_\phi)$ is given

$$\sigma(\omega)=2\pi e^2\frac{E_\phi^2}{\omega^3}\sum_{n:\text{odd}}g_n^2\delta(\omega^2-E_n^2)\ . \tag{47}$$

IV. CONCLUDING REMARKS

Limiting ourselves to $T=0$ K, we constructed the complex electric conductivity of the one-dimensional sine-Gordon system (1). Making use of Zamolodchikov's S matrix, we have shown that the electromagnetic wave can excite soliton-antisoliton bound states with the odd quantum number. The dipole coupling constants are explicitly determined. Furthermore, we have analyzed the threshold structure of the conductivity near $\omega\simeq 2m$. It is hoped that these results will be tested in some of the quasilinear CDW systems.

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