

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 ($\lambda \gg 1$) 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 quasi-particle density becomes negligible and it is believed that the electric conductivity should be dominated by ϕ solitons¹ [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 quasi-particle 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 $|\omega| \ll 2E_\phi$, 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 ($\omega \approx 2E_\phi$). Recently Kaup and Newell⁷ have shown within the classical field theory that the above sine-Gordon system absorbs the electromagnetic wave with $\omega \leq 2E_\phi$ 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 energies⁸ 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

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

where

$$\begin{aligned} \mathcal{L} dx &= \mathcal{L}' dx' , \quad x' = x/c_0 , \\ \phi' &= \frac{1}{2} (N_0 c_0)^{1/2} \phi , \quad \alpha = \omega_0^2 , \\ \beta &= (8\pi)^{1/2} N \left[1 + \eta^{-1} \left(\frac{2\Delta}{\omega_Q} \right)^2 \right]^{-1/4} \\ &= (8\pi)^{1/2} N (c_0/v)^{1/2} . \end{aligned} \quad (4)$$

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

$$0 < \beta^2 \ll 8\pi , \quad (5)$$

which implies that the energy spectrum of the soliton-antisoliton bound states is given by⁸

$$E_n = 2m \sin(n\pi/2\lambda) , \quad (6)$$

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 $\lambda \gg 1$ 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)

$$\sigma(\omega) = \frac{1}{\omega} \text{Im} \Pi(q^2) \Big|_{q^2 = \omega^2} , \quad (7)$$

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

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

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

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

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

$$\text{Im} \Pi(q^2) = \frac{e^2}{2} \int \int dp_1 dp_2 \left(\frac{m^2}{E_1 E_2} \right) \sigma^2(p_1 + p_2 - q) \langle 0 | j^\mu(0) | p_1 \bar{p}_2 \rangle \langle p_1 \bar{p}_2 | j_\mu(0) | 0 \rangle , \quad (10)$$

where

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

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

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

with

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

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

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

such that

$$\text{Im} \Pi(q^2) = e^2 \frac{m^2}{2E p} |G(q^2)|^2 , \quad (13)$$

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 determined¹⁰ as

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

with

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

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

$$\sinh \frac{\theta}{2} = \frac{p}{m}, \quad \cosh \frac{\theta}{2} = \frac{E}{m}, \quad (16)$$

$$q^2 = s = 2m(1 + \cosh \theta).$$

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

$$\lambda = 1 + \frac{2g}{\pi} = \frac{8\pi}{\beta^2} - 1. \quad (17)$$

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

has poles at

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

corresponding to bound states with masses

$$M_n = 2m \sin(2n\pi/\lambda). \quad (19)$$

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}

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

where $S_{ff}(\theta)$ is the two-fermion scattering amplitude⁹

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

with

$$\hat{\theta} = -i\theta/\pi \quad (21)$$

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

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

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

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

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

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

where

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

Here use is made of the formula

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

The integral (25) converges for

$$\text{Im } \theta < \pi(2 + 1/\lambda) \quad (27)$$

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 $\text{Im } \theta \geq 1/\lambda$ if it were included into the integral representation.

III. LIMITING BEHAVIORS

It is now useful to discuss two regions separately.

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

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

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

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

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

with

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

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

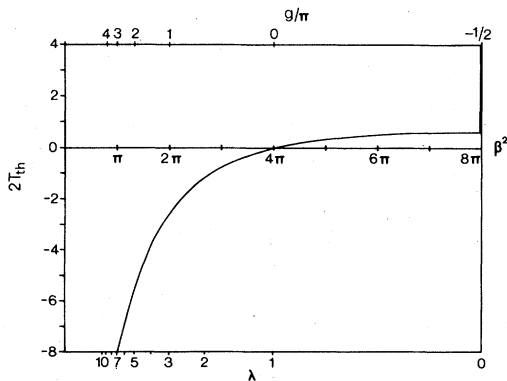


FIG. 1. $T_{th}(\lambda)$, which appears in the threshold expression of the electric conductivity, as a function of λ .

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., $\lambda \in (1, 0)$], although this is very unlikely in our model, there is an enhancement by $e^{0.6} \approx 1.82$ 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 $\lambda_{new} > 0$.

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

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

The reason for this is the arrival of a bound-state pole $\lambda=n$ at the threshold point. Its approach $\lambda \rightarrow n$ 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

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

with

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

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

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

with g_n being the dimensionless direct photon-"vector" meson (i.e., the $c=-1$ soliton-antisoliton bound-state) coupling defined by¹³

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

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

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

and

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

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

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

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

$$\hat{1} \rightarrow \frac{1}{2} \left[(2\pi)^2 \frac{E_1 E_2}{m^2} \delta(p_1' - p_1) \right. \\ \left. \times \delta(p_2' - p_2) + (p_1' \leftrightarrow p_2') \right]. \quad (38)$$

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

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

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

Thus

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

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 occurrence 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., $\lambda - n_{\max} \ll 1$), 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

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

Equations (45) and (46) indicate that the coupling

Therefore one has

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

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

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

such that

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

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 $\lambda \gg n$, the integral (15) gives

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

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

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

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

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 quasi-linear CDW systems.

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