Impurity scattering in unconventional density waves

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We have investigated the effect of nonmagnetic impurities on the quasi-one-dimensional unconventional density wave ground state. The thermodynamics were found to be close to those of a *d*-wave superconductor in the Born limit. Four different optical conductivity curves were found depending on the direction of the applied electric field and on the wave-vector dependence of the gap.

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I. INTRODUCTION

Recently a number of papers have been published investigating the different properties of unconventional density waves (UDW) under various conditions. The common feature of these systems is the zero average of the gap on the Fermi surface, resulting in the absence of any periodic modulation of the charge or spin density. Clearly this property makes UDW a very likely candidate for those systems in which clear thermodynamic signals of a phase transition are seen without any order parameter, which could be detected by conventional methods (i.e., x-ray or NMR methods).[1] From this the notion ''hidden order'' follows naturally.

Unconventional density wave formation is found to be possible in a large variety of systems. In the quasi-one-dimensional case, which is the natural occurrence of density waves,[2] we have investigated the basic properties of unconventional spin- and charge-density waves[3] (USDW, UCDW) and the related threshold electric field with[4] and without magnetic field.[5] UCDW turned out to be relevant in the explanation of the response of the low-temperature phase of quasi-one-dimensional α-$(BEDT\text{-}TTF)_2KHg(SCN)_4$ salts [BEDT-TTF denotes bis(ethylenedithio)tetrathiafulvalene]. In two-dimensional systems, the different unconventional phases were elaborated by Ozaki.[6] Among them, the *d*-density wave scenario, which is a special case of UCDW (orbital antiferromagnet), was proposed recently to describe the famous pseudogap phase of high-T_c superconductors.[7] Since the original proposal, several works have been published in which the properties of *d*-density waves were studied with the aim of testing the validity of the model by comparing to experimental data (see Ref. 8 and the references therein). Also the ground state of certain heavy fermion materials were suspected to be USDW (Refs. 9 and 10) which would simply explain the unsolved problem of micromagnetism. In the presence of magnetic field, the orbital antiferromagnet[11] and the spin nematic state[12] were discussed as well in two dimensions. In three-dimensional systems, the pseudogap phase of the transition-metal oxides have attracted significant attention and the staggered flux state was mentioned in the context of the possible explanations.[13]

In this paper we extend our earlier analysis[3] on pure unconventional density waves to the presence of nonmagnetic impurities. Impurities are treated in the Born scattering limit since it works very well for conventional DW. Since the Fermi surface of quasi-one-dimensional systems mainly consists of two separate sheets, two different scattering processes should be taken into account: forward and backward scattering during which an electron remains on the same or moves to the other Fermi sheet, respectively. The thermodynamics are found to be similar to those of a *d*-wave superconductor in the Born limit. Among the transport properties the quasiparticle part of the optical conductivity is evaluated. In the chain direction the phason couples strongly to the electromagnetic field, giving rise to massive collective modes in this direction. On the other hand, for electric fields applied perpendicular to the conducting chain, the conductivity shows only Fermi-liquid renormalization, and our description is valid under these circumstances.

II. FORMALISM

To start with, we consider the Hamiltonian of interacting electrons,

$$H=\sum_{\mathbf{k},\sigma}\xi(\mathbf{k})a^{\dagger}_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma}+\frac{1}{2V}\sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}}\tilde{V}(\mathbf{k},\mathbf{k}',\mathbf{q})a^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}a_{\mathbf{k},\sigma}a^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'}a_{\mathbf{k}',\sigma'}, \tag{1}$$

where $a^{\dagger}_{\mathbf{k},\sigma}$ and $a_{\mathbf{k},\sigma}$ are, respectively, the creation and annihilation operators of an electron of momentum $\mathbf{k}$ and spin σ. V is the volume of the sample. Our system is based on an

orthogonal lattice, with lattice constants a,b,c toward directions x,y,z. The system is anisotropic, the quasi-one-dimensional direction is the x axis. The kinetic-energy spectrum of the Hamiltonian is

$$\xi(\mathbf{k}) = -2t_a\cos(k_x a) - 2t_b\cos(k_y b) - 2t_c\cos(k_z c) - \mu. \quad (2)$$

In the second term of Eq. (1) we consider the interaction between on-site and nearest-neighbor electrons on the lattice as in Ref. 3. Then by rewriting the interaction in terms of Fourier-transformed variables, its antisymmetrized (therefore spin-dependent) version[14] is given by

$$\frac{N}{V}\tilde{V}(\mathbf{k},\mathbf{k}',q,\sigma,\sigma') = \delta_{-\sigma,\sigma'}\Bigg(U + \sum_i \{2V_i\cos q_i\delta_i + 2J_i\cos(k_i - k_i' + q_i)\delta_i + 2\mathrm{Re}(F_i e^{i(k_i'+k_i)\delta_i}) + 2\mathrm{Re}[C_i(e^{ik_i\delta_i} + e^{ik_i'\delta_i} + e^{i(k_i'-q_i)\delta_i} + e^{i(k_i+q_i)\delta_i})]\}\Bigg) + \delta_{\sigma,\sigma'}\sum_i (V_i - J_i)[\cos q_i\delta_i - \cos(k_i - k_i' + q_i)\delta_i], \quad (3)$$

where $i = x,y,z$ and $\delta_i = a,b,c$, the different matrix elements involve the on-site (U), nearest-neighbor direct (V_i), exchange (J_i), pair-hopping (F_i), and bond-charge (C_i) terms. This interaction is able to support a variety of low-temperature phases,[6] but we are only interested in unconventional DW (whose gap depends on the perpendicular momentum).[15,3] The latter can be either UCDW or USDW depending on the strength of the exchange and pair-hopping integrals. The single-particle electron thermal Green's function using Nambu's notation is[16,17]

$$G_\sigma(\mathbf{k}, i\omega_n) = -\int_0^\beta d\tau \langle T_\tau \Psi_\sigma(\mathbf{k},\tau)\Psi_\sigma^\dagger(\mathbf{k},0)\rangle_H e^{i\omega_n\tau}, \quad (4)$$

where Green's function is chosen to be diagonal in spin indices and the momentum space is divided into $\mathbf{k}$ and $\mathbf{k}-\mathbf{Q}$ spaces (left- and right-going electrons) by introducing the spinors,

$$\Psi_\sigma(\mathbf{k},\tau) = \begin{pmatrix} a_{\mathbf{k},\sigma}(\tau) \\ a_{\mathbf{k}-\mathbf{Q},\sigma}(\tau) \end{pmatrix}, \quad (5)$$

ω_n is the Matsubara frequency, $\mathbf{Q} = (2k_F, \pi/b, \pi/c)$ is the best nesting vector. The inverse of the above Green's function is obtained as

$$G_\sigma^{-1}(\mathbf{k}, i\omega_n) = i\omega_n - \xi(\mathbf{k})\rho_3 - \Delta_\sigma(\mathbf{k})\rho_1, \quad (6)$$

where ρ_i ($i = 1,2,3$) are the Pauli matrices acting on momentum space, $\Delta_\sigma(\mathbf{k})$ satisfies the self-consistent equation,

$$\Delta_\sigma(\mathbf{k}) = \frac{1}{V}\sum_{\mathbf{k}',\sigma'} \overline{\tilde{V}(\mathbf{k}',\mathbf{k},\mathbf{Q},\sigma,\sigma')}\langle a_{\mathbf{k}',\sigma'}^\dagger a_{\mathbf{k}'+Q,\sigma}\rangle. \quad (7)$$

In order to describe USDW, we assume Δ as an odd function of the spin ($\Delta_\sigma = -\Delta_{-\sigma}$). Assuming Δ_σ to be an even function of the spin, we would have UCDW. From now on, we will drop the spin indices since they are irrelevant for most of our discussion and most of our results applies to both unconventional charge- and spin-density waves. The spin indices will be reinserted wherever necessary. With this, the gap equation reads

$$\Delta(\mathbf{l}) = \frac{1}{V}\sum_{\mathbf{k}} \overline{P(\mathbf{k},l)}\frac{\Delta(\mathbf{k})\tanh(\beta E(\mathbf{k})/2)}{2E(\mathbf{K})}, \quad (8)$$

where $E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2}$, $\Delta(\mathbf{k}) = \Delta_\sigma(\mathbf{k})$, and the kernel of the integral equation is diagonal on the basis of the leading harmonics as[3]

$$\frac{P(\mathbf{k},\mathbf{l})}{V} = \frac{P_0}{N} + \frac{P_1}{N}\cos(k_y b)\cos(l_y b) + \frac{P_2}{N}\sin(k_y b)\sin(l_y b) + \frac{P_3}{N}\cos(k_z c)\cos(l_z c) + \frac{P_4}{N}\sin(k_z c)\sin(l_z c). \quad (9)$$

The P_i coefficients are linear combinations of the interaction matrix elements. As a consequence of the general form of the kernel, the gap will be of the form

$$\Delta(\mathbf{l}) = \Delta_0 + \Delta_1\cos(l_y b) + \Delta_2\sin(l_y b) + \Delta_3\cos(l_z c) + \Delta_4\sin(l_z c). \quad (10)$$

From now on we assume that only one kind of gap among the five possible options, whose transition temperature is the highest, opens and persists all the way down to zero temperature. For example, we find that USDW is stable with respect to UCDW if $J_y \mp F_y > 0$, where the upper (lower) sign refers to a k_y dependent gap function of cosine (sine).[3] The thermodynamic and transport properties of such a system have been worked out in Ref. 3. In the following we shall discuss the effect of impurities on UDW and determine the behavior of the basic physical quantities. The interaction of the electrons with nonmagnetic impurities is described by the Hamiltonian

$$H_1 = \frac{1}{V}\sum_{\mathbf{k},\mathbf{q},\sigma,j} e^{-i\mathbf{q}\cdot\mathbf{R}_j}\Psi_\sigma^\dagger(\mathbf{k}+\mathbf{q})U(\mathbf{R}_j)\Psi_\sigma(\mathbf{k}), \quad (11)$$

$$U(\mathbf{R}_j) = \begin{pmatrix} U(0) & U(\mathbf{Q})e^{-i\mathbf{Q}\cdot\mathbf{R}_j} \\ \overline{U(\mathbf{Q})}e^{i\mathbf{Q}\cdot\mathbf{R}_j} & U(0) \end{pmatrix}, \quad (12)$$

$\mathbf{R}_j$ is the position of the jth impurity atom. The explicit wave-vector dependence of the matrix elements[18,5] is ne-

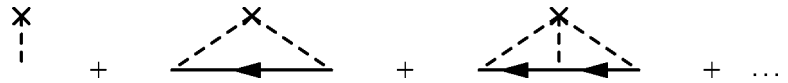

FIG. 1. Self-energy corrections due to impurity scattering. The solid line denotes the electron while the dashed line is for the electron-impurity interaction. Dashed lines coming from the same cross represent successive scattering of the electron on the same impurity.

glected since no important changes are expected from it. The usual method of treating the impurities is to average over their position in real space, and step into the wave-vector space afterwards.[17,19] Instead, we follow a rather unorthodox way: working in the Fourier space and averaging when needed. It is clear from the exponential prefactor in H_1, that only diagrams containing impurity scattering with momentum conservation at each impurity atom have finite expectation value after averaging over the position of the impurities, and translational invariance is regained.

This method can be extended into any order of impurity scattering as we will demonstrate it in the following. As to the diagrams, we will take into account only noncrossing, ladder-type diagrams.[14,17,20] To start with, we will evaluate the self-energy corrections caused by Eq. (12) at every order. This can be visualized in Fig. 1 and is given by

$$\Sigma_{\mathbf{R}}(\mathbf{k},i\omega_n)=\Sigma_{\mathbf{R}}(i\omega_n)=n_i\Bigg(U(\mathbf{R})+U(\mathbf{R})\int\frac{d^3p}{2\pi^3}G(\mathbf{p},i\omega_n)U(\mathbf{R})+U(\mathbf{R})\int\frac{d^3p}{2\pi^3}G(\mathbf{p},i\omega_n)U(\mathbf{R})$$
$$\times\int\frac{d^3p'}{2\pi^3}G(\mathbf{p}',i\omega_n)U(\mathbf{R})+\cdots\Bigg)=n_iU(\mathbf{R})+U(\mathbf{R})\int\frac{d^3p}{2\pi^3}G(\mathbf{p},i\omega_n)\Sigma_{\mathbf{R}}(i\omega_n), \tag{13}$$

where the self-energy correction turns out to be momentum independent and the $\mathbf{R}$ index in $\Sigma_{\mathbf{R}}(i\omega_n)$ means the position of an impurity over which the average will be taken in the following, n_i is the impurity concentration. Equation (13) can be solved easily, and the result is

$$\Sigma_{\mathbf{R}}(i\omega_n)=\begin{pmatrix}U_1-g & U_2e^{-i\mathbf{Q}\cdot\mathbf{R}}+f\\ \overline{U}_2e^{i\mathbf{Q}\cdot\mathbf{R}}+\overline{f} & U_1-g\end{pmatrix}\frac{n_i}{(U_1-g)^2-|f|^2-|U_2|^2-(U_2\overline{f}e^{-i\mathbf{Q}\cdot\mathbf{R}}+\overline{U}_2fe^{i\mathbf{Q}\cdot\mathbf{R}})}, \tag{14}$$

where $U_1=U(0)/[U(0)^2-|U(\mathbf{Q})|^2]$ and $U_2=U(\mathbf{Q})/[U(0)^2-|U(\mathbf{Q})|^2]$ and

$$\int\frac{d^3p}{2\pi^3}G(\mathbf{p},i\omega_n)=\begin{pmatrix}g & f\\ \overline{f} & g\end{pmatrix}. \tag{15}$$

Expanding $\Sigma_{\mathbf{R}}(i\omega_n)$ in powers of the exponential terms in the denominator of Eq. (14), the space average can be performed and the self-energy matrix is obtained as

$$\Sigma(i\omega_n)=\begin{pmatrix}\Sigma_1(i\omega_n) & \Sigma_2(i\omega_n)\\ \Sigma_3(i\omega_n) & \Sigma_1(i\omega_n)\end{pmatrix} \tag{16}$$

and its matrix elements are given by

$$\Sigma_1(i\omega_n)=n_i\frac{U(0)-g(U(0)^2-|U(\mathbf{Q})|^2)}{\sqrt{D^2-4|U(\mathbf{Q})f|^2}}, \tag{17}$$

$$\Sigma_2(i\omega_n)=n_i\frac{f}{\sqrt{D^2-4|U(\mathbf{Q})f|^2}}\Bigg(U(0)^2-|U(\mathbf{Q})|^2+\frac{2|U(\mathbf{Q})|^2}{D+\sqrt{D^2-4|U(\mathbf{Q})f|^2}}\Bigg), \tag{18}$$

$$\Sigma_3(i\omega_n)f=\Sigma_2(i\omega_n)\overline{f}, \tag{19}$$

where $D=1-2gU(0)+(g^2-|f|^2)[U(0)^2-|U(\mathbf{Q})|^2]$. In the case of $f=0$ (i.e., the average of the gap over the Fermi surface is zero), the self-energy is obtained correctly for arbitrary $U(0)$ and $U(\mathbf{Q})$, since the exponential terms disappear from the denominator of Eq. (14). Otherwise this result is valid only for a certain range of parameters due to the expansion. On the other hand, one can deduce an expression from Eq. (14) involving the different matrix elements of the self-energy, where the space average was performed rigorously,

$$\Sigma_1(i\omega_n)(1-2U(0)g+(g^2+|f|^2)[U(0)^2-|U(\mathbf{Q})|^2)]$$
$$-(\Sigma_2(i\omega_n)\overline{f}+\Sigma_3(i\omega_n)f+n_i)$$
$$\times[U(0)-g(U(0)^2-U(\mathbf{Q})^2]=0, \tag{20}$$

and this equation is satisfied with the previously obtained $\Sigma_1(i\omega_n)$, $\Sigma_2(i\omega_n)$, and $\Sigma_3(i\omega_n)$ even outside of the validity range of the expansion. Of course, this cannot be regarded as a proof but we can trust in the usefulness of this calculation outside the validity range. Moreover, in a normal metal this result gives back the known result.[14] These formulas apply also to superconductors with minor change [$U(\mathbf{R})$

$=U(0)\rho_1]$, and the self-energies in the Born and unitary limit are obtained correctly.[16,21–24] We treat our UDW system in the Born scattering limit since conventional DWs are commonly investigated in this limit.[25] The interaction gives rise to the self-energy, which is in the Born approximation (considering only the lowest-order terms),

$$\Sigma(\mathbf{k},i\omega_n)=\frac{n_i}{V}\sum_{\mathbf{q}}\frac{1}{N}\sum_{\mathbf{R}}U(\mathbf{R})G(\mathbf{k}-\mathbf{q},i\omega_n)U(\mathbf{R}), \tag{21}$$

where the summation is the only remaining operation from averaging over the impurity atoms. From this, one obtains for a DW

$$G(\mathbf{k},i\omega_n)=-\frac{i\tilde{\omega}_n+\xi(\mathbf{k})\rho_3+\tilde{\Delta}_n(\mathbf{k})\rho_1}{\tilde{\omega}_n^2+\xi(\mathbf{k})^2+\tilde{\Delta}_n(\mathbf{k})^2}, \tag{22}$$

where both the frequency and the gap are renormalized in the conventional case,

$$\omega_n=\tilde{\omega}_n-\frac{\Gamma_1+\Gamma_2}{2}\frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2+\tilde{\Delta}_n^2}}, \tag{23}$$

$$\Delta=\tilde{\Delta}_n+\frac{\Gamma_1}{2}\frac{\tilde{\Delta}_n}{\sqrt{\tilde{\omega}_n^2+\tilde{\Delta}_n^2}}. \tag{24}$$

$\Gamma_1=\pi n_i|U(0)|^2 g(0)$ is the forward-scattering parameter, $\Gamma_2=\pi n_i|U(\mathbf{Q})|^2 g(0)$ is the backward scattering parameter,[26] $g(0)$ is the density of states per spin in the metallic state. As in other similar problems,[20] it is convenient to introduce the quantity $u_n=\tilde{\omega}_n/\tilde{\Delta}_n$, which relates to physical quantities,

$$\omega_n=\Delta u_n\left(1-\alpha\frac{1}{\sqrt{u_n^2+1}}\right), \tag{25}$$

$\Gamma=\Gamma_1+\Gamma_2/2$, $\alpha=\Gamma/\Delta$ is the pair-breaking parameter. As opposed to this, in unconventional DW self-energy corrections from impurities do not renormalize the gap but the Matsubara frequency

$$\omega_n=\tilde{\omega}_n-\frac{\Gamma_1+\Gamma_2}{\pi}\frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2+\Delta^2}}K\left(\frac{\Delta}{\sqrt{\tilde{\omega}_n^2+\Delta^2}}\right),$$

$$\tilde{\Delta}_n(\mathbf{k})=\Delta(\mathbf{k})=\Delta\sin(bk_y)\ \text{ or }\ \Delta\cos(bk_y). \tag{26}$$

This is written in a more useful dimensionless form

$$\omega_n=\Delta u_n\left[1-\frac{2}{\pi}\frac{\alpha}{\sqrt{u_n^2+1}}K\left(\frac{1}{\sqrt{u_n^2+1}}\right)\right], \tag{27}$$

where $\Gamma=(\Gamma_1+\Gamma_2)/2$, $\alpha=\Gamma/\Delta$, $u_n=\tilde{\omega}_n/\Delta$ and Γ_1 and Γ_2 are the same quantities as in a conventional DW, $K(z)$ is the complete elliptic integral of the first kind. Here the combination of the scattering rates is different from the conventional DW's case due to the lack of renormalization of the order parameter. We choose the Born scattering limit because this limit works very well for conventional DW. We believe that by neglecting the explicit wave-vector dependence of the impurity matrix elements, we made a useful approximation as far as the character of the physics is concerned and we are able to capture the characteristic changes caused by impurities. However, in order to describe very fine, characteristic phenomena to DW such as the threshold electric field,[27–30] we cannot use simple *s*-wave scatterers as it is shown in Refs. 4 and 5.

III. THERMODYNAMICS OF IMPURE UDW

Since the thermodynamic properties of a pure UDW are identical to those of a *d*-wave superconductor[3,31] and the impurity effects on a conventional DW are similar to those in *s*-wave superconductors, we expect behaviors very similar to those in a *d*-wave superconductor treated in the Born limit. However, the main difference is that we distinguish two different scattering processes (forward and backward scattering) while in the superconducting world there is only one. Consequently the different combinations of the Γ's are far from being trivial. The gap equation is obtained as

$$1=\rho(0)TP_i\sum_n\left[E\left(\frac{1}{\sqrt{1+u_n^2}}\right)\sqrt{1+u_n^2}-K\left(\frac{1}{\sqrt{1+u_n^2}}\right)\frac{u_n^2}{\sqrt{1+u_n^2}}\right], \tag{28}$$

where $E(z)$ is the complete elliptic integral of the second kind $\rho(0)=g(0)abc$. The change in the transition temperature is given by the Abrikosov-Gor'kov formula

$$-\ln\left(\frac{T_c}{T_{c_0}}\right)=\psi\left(\frac{1}{2}+\rho\right)-\psi\left(\frac{1}{2}\right), \tag{29}$$

where T_c and T_{c_0} are the transition temperatures of the impure and clean system, respectively, $\rho=\Gamma/2\pi T_c$, $\psi(z)$ is the digamma function. Note that this formula is also valid for any kind of unconventional superconductor in the presence of impurities considered either in the Born or in resonant scattering limit.[32] The critical impurity scattering rate is given by

$$\Gamma_c=\frac{\pi T_{c_0}}{2\gamma}=\frac{\sqrt{e}\Delta_{00}}{4}. \tag{30}$$

The gap maximum is the same as the one of a *d*-wave SC in the Born limit,[33]

$$\ln\frac{\Delta_{00}}{\Delta(0,\Gamma)}=\frac{8}{\pi^2}\frac{\Gamma}{\Delta}\int_{C_0}^{\infty}(K-E)\left(E-K\frac{x^2}{1+x^2}\right)dx+2\left\langle\sin^2 y\,\mathrm{arcsinh}\frac{C_0}{\sin y}\right\rangle, \tag{31}$$

where $\langle\cdots\rangle$ means $1/2\pi\int_0^{2\pi}dy\ldots$, the argument of K and E reads as $1/\sqrt{x^2+1}$. C_0 is the value of u_n at zero frequency,

$$\sqrt{1+C_0^2}=\frac{2}{\pi}\alpha K\left(\frac{1}{\sqrt{1+C_0^2}}\right), \tag{32}$$

vanishing as the impurity scattering parameter disappears as $C_0=4\exp(-\pi/2\alpha)$, while for large α, $C_0=\alpha$ as in Ref. 34. Close to T_c, Δ vanishes in a square-root manner as does usually in mean-field treatments,

$$\Delta^2=8(2\pi T_c)^2\frac{1-\rho\psi'(\frac{1}{2}+\rho)}{-\frac{3\psi''(\frac{1}{2}+\rho)}{2}-\rho\frac{\psi'''(\frac{1}{2}+\rho)}{3}}\left(1-\frac{T}{T_c}\right). \tag{33}$$

Close to absolute zero, the following formula is obtained:

$$\Delta(T)=\Delta(0)-\frac{\pi^2}{3}\frac{C_0}{\Gamma}\left(\frac{K}{E}-1\right)\left\{1-\frac{4}{\pi}\left[\frac{2\alpha}{\pi}\int_{C_0}^{\infty}(K-E)\times\left(E-K\frac{x^2}{1+x^2}\right)dx+C_0\sqrt{1+C_0^2}\left(E-K\frac{C_0^2}{1+C_0^2}\right)\right]\right\}^{-1}T^2, \tag{34}$$

where the T^3 decrease of the pure case turned into a faster T^2 one, the argument of K and E under the integral is the same as in Eq. (31), otherwise it reads as $1/\sqrt{1+C_0^2}$.

From this, one can assume that the effect of the impurity scattering in the limit of low temperatures is to reduce the power-law exponent by 1. As a result we expect the exponent of temperature to be the same as that in a conventional DW in the gapless region.[16,25] The analogy looks obvious since in neither of these two systems there is a lower bound of the excitation energy. The correspondence works only at low temperatures $T\ll T_c$ when the only energy scale is the temperature. Now we derive expressions for the grand canonical potential and for the specific heat. In doing this, we use the well-known relation involving an integral over the coupling constant of the interaction[14]

$$\Omega-\Omega_0=\int_0^1\frac{d\lambda}{\lambda}\langle\lambda H_{int}\rangle, \tag{35}$$

where H_{int} is the interaction causing the phase transition. This formula gives us the thermodynamic potential difference between the normal and the DW phase. Since we work on a grand canonical ensemble, the appropriate thermodynamic potential at $T=0$ is obtained as

$$\Omega(0)=-N\rho(0)\left[\frac{\Delta^2}{4}-\frac{2}{\pi}\Delta^2C_0\sqrt{C_0^2+1}+\frac{\Gamma^2}{3}+\frac{2\Delta^3C_0^3}{3\Gamma}-\frac{4\Gamma\Delta}{\pi^2}\int_{C_0}^{\infty}(K-E)\left(E-K\frac{x^2}{1+x^2}\right)dx\right]. \tag{36}$$

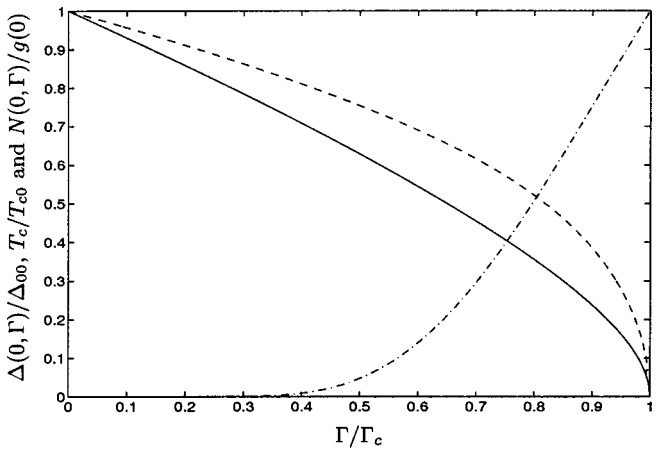

FIG. 2. $\Delta(0,\Gamma)/\Delta_{00}$ (dashed line), T_c/T_{c0} (solid line) and $N(0,\Gamma)/g(0)$ (dashed-dotted line) are shown as a function of Γ/Γ_c for an unconventional density wave.

At small Γ, the leading correction is the last integral, enhancing the potential as in the normal SDW case. The low temperature specific heat reads

$$C(T)=\frac{2\pi^2}{3}g(0)\frac{\Delta C_0}{\Gamma}T. \tag{37}$$

This expression also reaches the normal state value with increasing Γ. The specific heat jump is

$$\Delta C(T)=\frac{16\pi^2g(0)T_c}{-\frac{3\psi''(\frac{1}{2}+\rho)}{2}-\rho\frac{\psi'''(\frac{1}{2}+\rho)}{3}}[1-\rho\psi'(\tfrac{1}{2}+\rho)]^2. \tag{38}$$

In Fig. 2 we show $\Delta(0,\Gamma)$ and T_c as a function of the scattering rate.

IV. DENSITY OF STATES IN UDW

By use of Green's function, the density of states per spin is given by

$$N(\omega)=-\frac{1}{2\pi V}\sum_{\mathbf{k}}\mathrm{Im\,Tr}(G^R(\mathbf{k},\omega))=g(0)\frac{1}{\alpha}\mathrm{Im}(u), \tag{39}$$

where $u=iu_n(i\omega_n=\omega+i\delta)$. After some algebra, the low-energy behavior reads

$$N(\omega)=g(0)\frac{C_0\Delta}{\Gamma}\left[1+\frac{\pi^2}{8E^2}\left(\frac{K}{E}+\frac{1}{C_0^2}-1\right)\left(\frac{\omega}{\Gamma}\right)^2\right]. \tag{40}$$

The residual density of states (i.e., the DOS at the Fermi energy) is finite at any finite Γ, disappears exponentially as Γ goes to zero, but takes the normal-state value as Γ approaches to infinity. Since $N(0)$ is almost zero for $\Gamma<0.5\Gamma_c$, we do not expect relevant changes in the static quantities (such as the specific heat, the spin susceptibility at $T\to0$) at low impurity concentrations. The notion ''gapless''

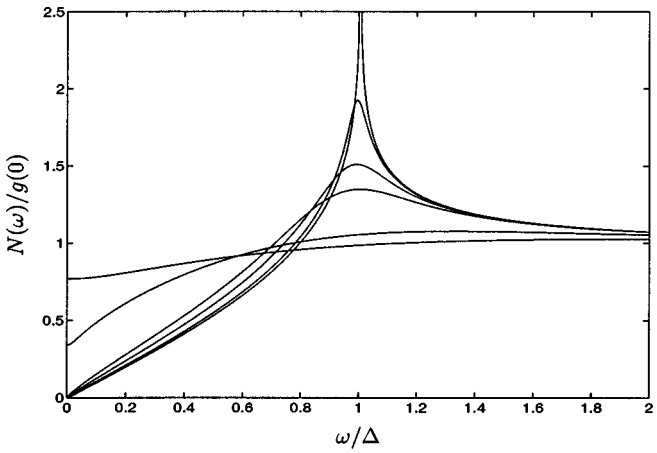

FIG. 3. Density of states plotted as a function of the reduced energy for different scattering amplitudes: $\alpha=0$, 0.01, 0.05, 0.1, 0.5, and 1 with peak position at $\omega=\Delta$ from top to bottom.

makes no sense in this case since even in pure UDW the gap vanishes at the Fermi energy leading to the possibility of arbitrary small energy excitations. At the value of the order parameter, the divergent peak of the pure system is broadened and $N(\omega)$ is always finite as a result of the impurities, shown in Fig. 3. Compared to the DOS of the conventional DW,[25] the states below the gap maximum are filled in, and the peak at Δ disappears more rapidly as α increases than in the case of momentum independent gap. At high energies it reaches the normal state value as

$$N(\omega)=g(0)\left(1+\frac{\Delta^2}{4}\frac{\omega^2-\Gamma^2}{(\omega^2+\Gamma^2)^2}\right). \tag{41}$$

In Fig. 2, we show the Γ dependence of the residual density of states.

V. DENSITY CORRELATOR

We turn our attention to the behavior of the static, long-wavelength density correlation function[25] using the thermal Green's function

$$\chi_0(T)=-\frac{1}{\beta}\sum_{\mathbf{p},\mathbf{k},\sigma,n}\mathrm{Tr}\overline{(G(\mathbf{p},\mathbf{k},i\omega_n)G(\mathbf{k},\mathbf{p},i\omega_n))} \tag{42}$$

where the overbar means averaging over the position of the impurity atoms. This requires calculating the averaged Green's function and the vertex corrections. In the following we focus on the vertex corrections, $\Lambda(\mathbf{p},i\omega_n)$. With this, our equation becomes simpler,

$$\chi_0(T)=-\frac{1}{\beta}\sum_{\mathbf{p},\sigma,n}\mathrm{Tr}[G(\mathbf{p},i\omega_n)\Lambda(\mathbf{p},i\omega_n)G(\mathbf{p},i\omega_n)]. \tag{43}$$

In the standard ladder approximation the vertex corrections are determined by the integral equation

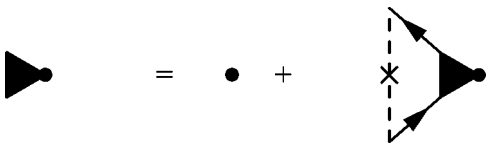

FIG. 4. The vertex correction in the Born limit is shown. The dot is the vertex function, the open triangle represents the vertex correction due to impurity scattering.

$$\Lambda(\mathbf{p},i\omega_n)=1+\frac{n_i}{V}\sum_{\mathbf{q}}\frac{1}{N}\sum_{\mathbf{R}}U(\mathbf{R})G(\mathbf{q},i\omega_n)\times\Lambda(\mathbf{q},i\omega_n)G(\mathbf{q},i\omega_n)U(\mathbf{R}), \tag{44}$$

which is shown in diagrammatic language in Fig. 4. Assuming $\Lambda(\mathbf{p},i\omega_n)=\Lambda(i\omega_n)$, and making the following ansatz:

$$\Lambda(i\omega_n)=\begin{pmatrix}\Lambda_1(i\omega_n) & \Lambda_2(i\omega_n)\\ \Lambda_2(i\omega_n) & \Lambda_1(i\omega_n)\end{pmatrix}, \tag{45}$$

the vertex corrections can be obtained as

$$\Lambda_1=\left(1-\frac{2}{\pi}\alpha\frac{K-E}{\sqrt{1+u_n^2}}\right)^{-1}, \tag{46}$$

$$\Lambda_2=0, \tag{47}$$

where the argument of K and E reads as $1/\sqrt{1+u_n^2}$. Substituting this into Eq. (43), the susceptibility reads

$$\chi_0(T)=2g(0)\left(1-\frac{2}{\Delta\beta}\sum_n\frac{\frac{K-E}{\sqrt{u_n^2+1}}}{1-\alpha\frac{K-E}{\sqrt{u_n^2+1}}}\right). \tag{48}$$

At zero temperature it equals the total density of states at the Fermi surface,

$$\chi_0(0)=2g(0)\frac{C_0\Delta}{\Gamma}. \tag{49}$$

In the low-temperature limit we obtain

$$\chi_0(T)=2g(0)\frac{C_0}{\Gamma}\left[\Delta(T)+\frac{\pi^4}{24E^2}\left(\frac{K}{E}-1+\frac{1}{C_0^2}\right)\left(\frac{T}{\Gamma}\right)^2\right], \tag{50}$$

where the argument of K and E is the same as in Eq. (34). Close to T_c, an expression similar to the normal SDW describes the susceptibility,

$$\chi_0(T) = 2g(0)\left(1+\frac{2\psi''(\frac{1}{2}+\rho)(1-\rho\psi'(\frac{1}{2}+\rho))}{-\frac{3\psi''(\frac{1}{2}+\rho)}{2}-\rho\frac{\psi'''(\frac{1}{2}+\rho)}{3}}\left(1-\frac{T}{T_c}\right)\right). \tag{51}$$

We refrain from the evaluation of the **Q**th Fourier component of the density correlation function because in UDW this is not the quantity that signals the phase transition, random-phase approximation corrections will not lead to divergence, since the dominant unconventional channel does not couple to charge or spin density.[3] In conventional CDW or SDW, the **Q**th Fourier component of the charge density or the spin density turned out to be the order parameter of the phase transition, respectively. As opposed to this, in the unconventional scenario, the following phases and related order parameters are found:

Phase	Gap	Order parameter: the **Q**th Fourier component of the
UCDW	$\Delta\cos(bk_y)$	Electric current density
UCDW	$\Delta\sin(bk_y)$	Kinetic-energy density
USDW	$\Delta\cos(bk_y)$	Spin current density
USDW	$\Delta\sin(bk_y)$	Spin kinetic-energy density

These phases are already known as orbital antiferromagnet,[11] bond-order wave,[6] spin nematic state[12] and axial spin bond-order wave,[6] respectively, in the context of the two-dimensional Hubbard model. Electron-hole condensate with momentum dependent gap was also mentioned in the context of excitonic insulator.[35,36] Generally these order parameters can be called as the effective charge or spin density.[3] The autocorrelation function of the above quantities will be divergent at T_c in the corresponding phase, because these quantities are relevant to the phase transitions.

VI. OPTICAL CONDUCTIVITY

The optical conductivity contains relevant informations about the possible excitation of a system. Since in real materials impurities are always present, the evaluation of the optical conductivity in impure systems is of prime importance. As it is known, the electrical conductivity of a conventional DW is divided into a pair-breaking (interband) and a normal (intraband) contribution.[37] Hence a Lorentzian-like normal contribution appears at all the frequencies, while the pair-breaking term is zero as long as $\omega<2\Delta$. This separation can be done in the unconventional case, although here both processes contribute to all frequencies due to the finite density of states at the Fermi energy. Introducing two notations,

$$I_n(\omega)=\int_0^\infty\left(\tanh\frac{\beta(x+\omega)}{2}-\tanh\frac{\beta x}{2}\right)\mathrm{Re}\{F[u(\omega+x),u(x)] - F[u(\omega+x),\overline{u(x)}]\}dx, \tag{52}$$

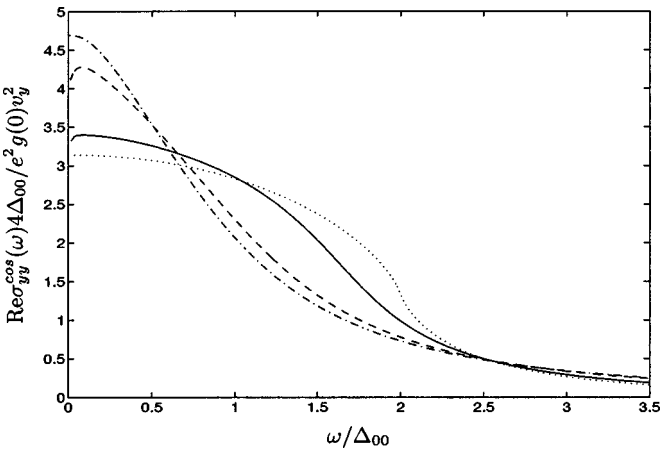

FIG. 5. Real part of the electric conductivity in the y direction for $\Delta(\mathbf{k})=\Delta\cos(bk_y)$ is plotted as a function of the reduced energy for different scattering amplitudes: $\alpha=0$ (dotted line), 0.1 (solid line), 0.5 (dashed line), and 1 (dashed-dotted line), $\Gamma_1=2\Gamma_2$.

$$I_{pb}(\omega)=\int_0^\omega\tanh\frac{\beta(\omega-x)}{2}\mathrm{Re}[F(u(\omega-x),-\overline{u(x)}) - F(u(\omega-x),-u(x))]dx, \tag{53}$$

the conductivity is given by

$$\mathrm{Re}\,\sigma_{aa}=-e^2g(0)v_a^2\frac{4}{\Delta\pi}\frac{I_n(\omega)+I_{pb}(\omega)}{\omega}, \tag{54}$$

where $v_x=v_F$, $v_y=\sqrt{2}bt_b$, and $v_z=\sqrt{2}ct_c$. The different $F(u,u')$ functions and the dc conductivities are discussed in the following

(i) $\Delta(\mathbf{k})=\Delta\cos(k_yb)$, $a=y$.

$$F(u,u')=\frac{1}{u'^2-u^2}\left[\sqrt{1-u'^2}\left\{E'\left(-uu'-\frac{2}{3}+\frac{u'^2}{3}\right)+K'\left(uu'-\frac{u'^2}{3}\right)\right\}+\sqrt{1-u^2}\left\{E\left(uu'+\frac{2}{3}-\frac{u^2}{3}\right)+K\left(-uu'+\frac{u^2}{3}\right)\right\}\right]. \tag{55}$$

In the definition of the different $F(u,u')$ functions the argument of E and K is $1/\sqrt{1-u^2}$, while for E' and K' $1/\sqrt{1-u'^2}$ has to be used. This is the simplest case, the vertex corrections vanish due to the mismatch of wave-vector dependence of the velocity and the gap. As the scattering strength enhances, it becomes the dominant energy scale and the curves take more and more the form of a Lorentzian as can readily be checked in Fig. 5. The dc conductivity is calculated at $T=0$,

$$\sigma_{yy}^{dc,cos}=e^2g(0)v_y^2\frac{4}{\Delta\pi}\left(E\sqrt{1+C_0^2}-\frac{\pi C_0^2}{2\alpha}\right). \tag{56}$$

In the dc conductivities, the argument of E and K is the same as in Eq. (34).

(ii) $\Delta(\mathbf{k})=\Delta\sin(k_yb)$, $a=y$.

$$F(u,u')=\frac{1}{u'^2-u^2}\Bigg[\sqrt{1-u^2}E\left(-uu'+\frac{4}{3}+\frac{u^2}{3}\right)-\sqrt{1-u'^2}E'\left(-uu'+\frac{4}{3}+\frac{u'^2}{3}\right)-\frac{u'^2}{\sqrt{1-u'^2}}K'\left(-uu'+\frac{2}{3}+\frac{u'^2}{3}\right)$$
$$+\frac{u^2}{\sqrt{1-u^2}}K\left(-uu'+\frac{2}{3}+\frac{u^2}{3}\right)\Bigg]+\frac{\Gamma_1}{\Delta\pi}\frac{1}{(u+u')^2}\frac{\left(E'\sqrt{1-u'^2}-E\sqrt{1-u^2}+\frac{u'^2}{\sqrt{1-u'^2}}K'-\frac{u^2}{\sqrt{1-u^2}}K\right)^2}{1+\frac{\Gamma_1}{\Delta\pi}\frac{1}{u+u'}\left(\frac{u'}{\sqrt{1-u'^2}}K'+\frac{u}{\sqrt{1-u^2}}K\right)}, \quad (57)$$

the third row of the equation comes from the vertex corrections. As Γ increases, the peak at 2Δ is broadened and moves closer to zero frequency. The dc conductivity is obtained at $T=0$,

$$\sigma_{yy}^{dc,sin}=4e^2g(0)v_y^2\frac{C_0^2(K-E)}{\Delta\pi\sqrt{C_0^2+1}+\Gamma_1(K-E)}, \quad (58)$$

where the second term in the denominator is clearly the effect of the vertex corrections. The conductivity is shown in Fig. 6.

(iii) $\Delta(\mathbf{k})=\Delta\sin(k_yb)$ or $\Delta\cos(k_yb)$, $a=z$.

$$F(u,u')=\frac{1}{2(u'^2-u^2)}\left(2\sqrt{1-u^2}E-2\sqrt{1-u'^2}E'+K'\frac{u'(u-u')}{\sqrt{1-u'^2}}+K\frac{u(u-u')}{\sqrt{1-u^2}}\right), \quad (59)$$

the vertex corrections vanish because the velocity depends on different perpendicular wave-vector component (k_z) than the gap (k_y). As Γ increases, the peak at 2Δ is broadened and moves closer to zero frequency. The dc conductivity is obtained at $T=0$ as

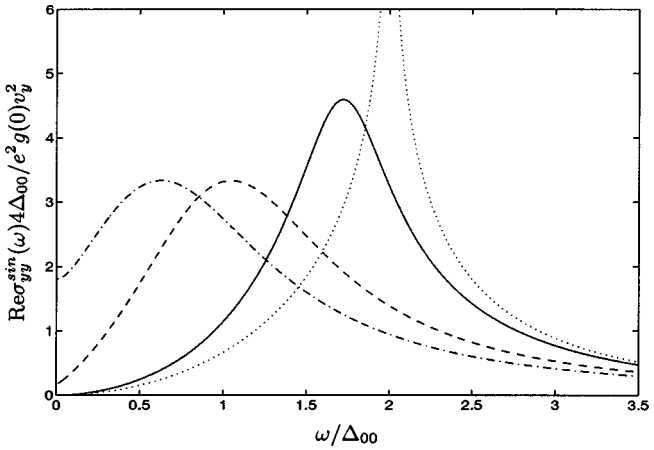

FIG. 6. Real part of the electric conductivity in the y direction for $\Delta(\mathbf{k})=\Delta\sin(bk_y)$ is plotted as a function of the reduced energy for different scattering amplitudes: $\alpha=0$ (dotted line), 0.1 (solid line), 0.5 (dashed line), and 1 (dashed-dotted line), $\Gamma_1=2\Gamma_2$.

$$\sigma_{zz}^{dc}=2e^2g(0)v_z^2\frac{E}{\Delta\pi\sqrt{C_0^2+1}}. \quad (60)$$

The optical conductivity is usually the same in the x and z direction apart from constant factors, since the velocity in these directions does not interfere with the gap. But in the presence of impurities this general relation does not hold any more due to the presence of different vertex corrections. A very similar breakdown of equality is found in the relation between the static spin susceptibility and the condensate density ($\rho_s=1-\chi_0/\chi_n$), which are not related to each other if impurity scattering is considered.[19,24] The conductivity is shown in Fig. 7.

For the sake of completeness we present the result for the quasiparticle part of the conductivity in the chain direction keeping in mind that collective modes also appear in this direction.

(iv) $\Delta(\mathbf{k})=\Delta\sin(k_yb)$ or $\Delta\cos(k_yb)$, $a=x$.

$$F(u,u')=\frac{\pi\Delta}{2(\Gamma_1-\Gamma_2)}\left\{\left[1-\frac{\Gamma_1-\Gamma_2}{\Delta\pi}\left(-K\frac{u(u'-u)}{\sqrt{1-u^2}}-K'\frac{u'(u'-u)}{1-u'^2}+2E\sqrt{1-u^2}-2E'\sqrt{1-u'^2}\right)\right]^{-1}-1\right\}. \quad (61)$$

This formula gives the quasiparticle part of the optical conductivity in the chain direction, although collective modes also show up here significantly modifying the conductivity. The consideration of impurity scattering and collective modes (even in the simplest random-phase approximation) together is a very difficult task to deal with[38,39] and is beyond the scope of the present investigation. The dc conductivity is obtained at $T=0$,

$$\sigma_{xx}^{dc}=2e^2g(0)v_x^2\frac{E}{\Delta\pi\sqrt{C_0^2+1}-(\Gamma_1-\Gamma_2)E}. \quad (62)$$

The conductivity seems to transfer more and more spectral weight to the zero-frequency peak with growing impurity scattering rate, transforming the curve into a Lorentzian-like one (Fig. 8).

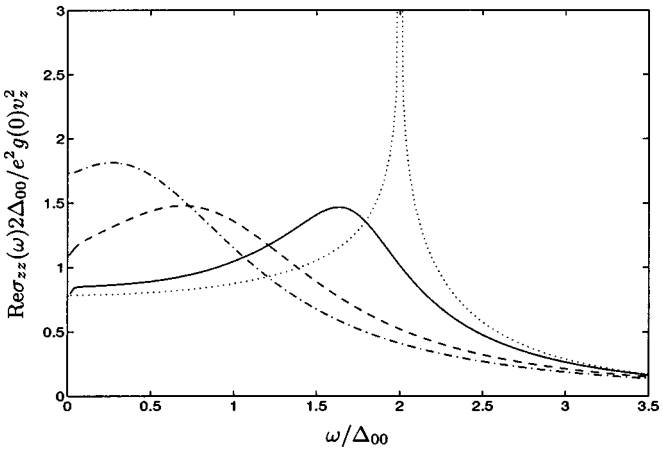

FIG. 7. Real part of the electric conductivity in the z direction is plotted as a function of the reduced energy for different scattering amplitudes: $\alpha=0$ (dotted line), 0.1 (solid line), 0.5 (dashed line), and 1 (dashed-dotted line), $\Gamma_1=2\Gamma_2$.

The dc conductivities are shown in Fig. 9 at $T=0$ as a function of the impurity scattering parameter. In the perpendicular direction, the dc conductivities take the same value at the critical scattering parameter, while the dc conductivity in the chain direction is exactly 3/2 times larger as follows from Eqs. (63) and (64) in the $\omega=0$ limit, if $\Gamma_1=2\Gamma_2$. In spite of the similar thermodynamics of d-wave SC (Refs. 33 and 34) and UDW, the transport properties of these two systems are completely different due to the distinct coherence factors coming from the different condensates. In a SC, there is always a Dirac delta peak at zero frequency, and the stronger the impurity scattering, the larger the spectral weight of this peak transferred to the finite frequency part of the conductivity. In UDW, the Dirac delta contribution disappears as soon as any finite impurity concentration is present, and the areas under the different curves are equal, but their form approaches that in the normal metal as Γ enhances.

The normal-state electric conductivities are given by the usual Lorentzians,

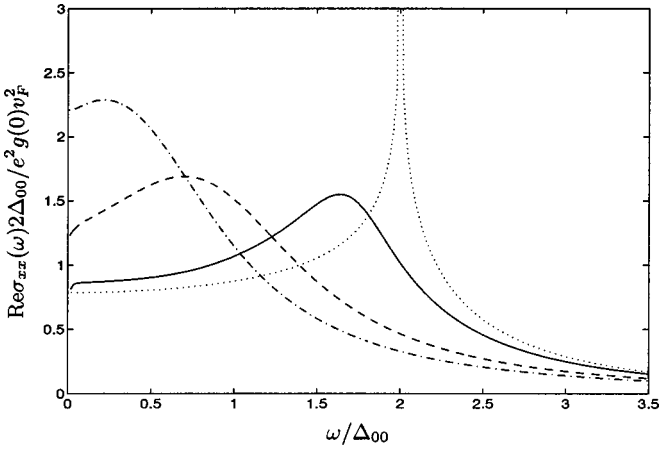

FIG. 8. Real part of the electric conductivity in the chain direction is plotted as a function of the reduced energy for different scattering amplitudes: $\alpha=0$ (dotted line), 0.1 (solid line), 0.5 (dashed line), and 1 (dashed-dotted line), $\Gamma_1=2\Gamma_2$.

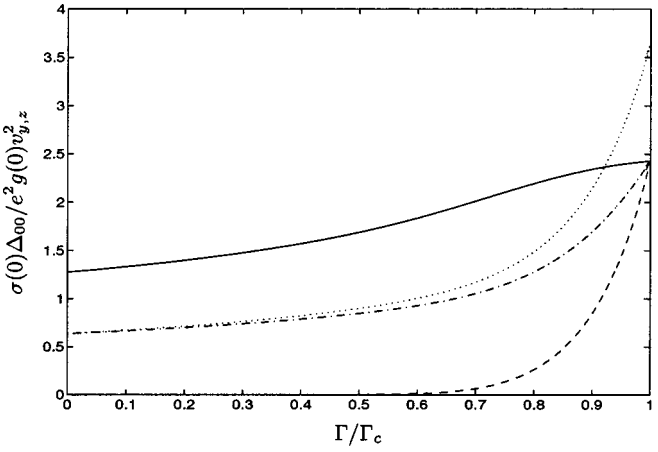

FIG. 9. The dc conductivity plotted at $T=0$ as a function of the reduced scattering rate for $\Gamma_1=2\Gamma_2=4\Gamma/3$ for a cosinusoidal (sinusoidal) gap in the y direction, solid (dashed line), in the z direction, dashed-dotted line; and in the x direction, dotted line.

$$\mathrm{Re}\,\sigma_{xx}(\omega)=e^2g(0)2v_F^2\frac{2\Gamma_2}{\omega^2+(2\Gamma_2)^2}, \tag{63}$$

$$\mathrm{Re}\,\sigma_{yy,zz}(\omega)=e^2g(0)2v_{y,z}^2\frac{\Gamma_1+\Gamma_2}{\omega^2+(\Gamma_1+\Gamma_2)^2}. \tag{64}$$

In the chain direction only backscattering can cause current damping as it is known from transport theory, which is manifested in the absence of the forward-scattering parameter in $\mathrm{Re}\sigma_{xx}(\omega)$.

VII. CONCLUSION

We have studied the effect of nonmagnetic impurities in unconventional density waves. In this respect there is no difference between USDW and UCDW due to the spin independence of the interaction with impurities. In s-wave superconductors nonmagnetic impurities have no influence on the thermodynamics of the system, while impure d-wave superconductors suffer important changes. This is known as Anderson's theorem, but equivalent conclusion has been reached independently by Abrikosov and Gor'kov. It says that if a static perturbation does not break the time-reversal symmetry and does not cause a long-range spatial variation of the order parameter, the thermodynamic properties of the superconductor remain unchanged in the presence of perturbation. As opposed to this, any kind of DW is destroyed in the presence of impurities, although the identity of the thermodynamics of s-wave superconductor to conventional DW and d-wave superconductor to unconventional DW is well established without impurities. Impurities have a pair-breaking effect on the condensate, resulting in a universal formula between the transition temperature and the scattering parameter, named after Abrikosov and Gor'kov. It seems to be valid for superconductors with all kinds of symmetries and now for density waves as well, independent of whether the Born or the resonant scattering limit is taken. Since conventional DW were studied in the Born limit, we found ap-

propriate to use the same approximation for the unconventional scenario. We have examined the system with the standard noncrossing approximation, and calculated the self-energy corrections for infinite order in the scattering potential, but only the lowest nontrivial correction was retained for the Born limit. The thermodynamics of UDW were found to be very similar to that in *d*-wave superconductors with nonmagnetic impurities, but the existence of two different types of scattering processes (forward and backward) was called for in the microscopic theory. In unconventional DW, at any finite scattering strength the valley of the density of states at the Fermi energy is filled in, leading to normal electronlike behaviors very close to absolute zero, but the reduced density of states compared to the normal state bears the effect of the condensate. The order parameter does not get renormalized due to impurities because we assumed *s*-wave scattering for simplicity. The specific heat increases linearly with temperature due to the finite density of states at the Fermi energy. Interestingly, impure UDW was found to be very similar to the gapless region of conventional DW very close to the critical scattering rate as far as the temperature exponents are concerned close to absolute zero because of the absence of any finite lower barrier of the excitation energy.

But at the transport properties all the similarities ended. The optical conductivity in the chain direction is dominated by the phason contribution, and incorporating the effect of impurities in the theory is beyond the scope of this study. Instead we concentrated on the perpendicular direction. In the optical conductivity, self-energy and vertex corrections were taken into account in the ladder-type noncrossing approximation. Depending on the symmetry of the order parameter and the chosen direction, four qualitatively different curves are deduced, although σ_{xx} is certainly dressed by collective modes due to coupling to the phason propagator. In the perpendicular directions, the possibility of low-frequency excitations rapidly increases, transferring increasing amount of spectral weight to $\omega=0$. The dc conductivities at $T=0$ sharply differ from each other, hence they can help to provide one with decisive conclusion when comparing these results to experimental data.

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