

Optical properties of strongly correlated systems with spin-density-wave order

O. V. Dolgov¹ and M. L. Kulić²¹Max-Planck-Institut, FKF, Heisenbergstrasse 1, 70569 Stuttgart, Germany²Institut für Physik, Theoretische Physik II, Universität Augsburg, 86135 Augsburg, Germany

(Received 1 October 2001; revised manuscript received 30 May 2002; published 8 October 2002)

The dynamical conductivity $\sigma(\omega)$, reflectivity $R(\omega)$, and tunneling density of states $N(\omega)$ of strongly correlated systems with the commensurate spin-density wave (SDW-CS) order are studied as a function of impurity scattering rate. The theory is based on the excitonic insulator model and it is generalized to include retardation (strong coupling) and impurity effects on the SDW-CS order. The results are briefly discussed in the light of optical experiments on some heavy-fermion materials with the SDW order.

DOI: 10.1103/PhysRevB.66.134510

PACS number(s): 74.25.Gz, 75.10.-b

I. INTRODUCTION

The magnetic properties of the HF materials, which belong to the class of strongly correlated systems, are due to the competition between the Kondo effect—which leads to the screening of the $4f$ ($5f$) magnetic moment below the coherence temperature T_{coh} , and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction—which is responsible for the antiferromagnetic (AF) order.¹ The itinerant SDW magnetic order is most probably realized in UPt_3 , URu_2Si_2 , UCu_5 , while in UPd_2Al_3 it seems that an AF localized magnetic order is present. In that respect resistivity measurements on URu_2Si_2 show significant changes in $\rho(T)$ below T_N (≈ 17 K) pointing to the SDW type of magnetism, while in UPd_2Al_3 there is only a small kink in $\rho(T)$ below T_N (≈ 14 K). The latter fact is more in favor of a localized magnetic order.²⁻⁴ The neutron scattering measurements⁵⁻⁷ show that the magnetic moment in UPd_2Al_3 is much larger ($\mu \sim 0.85\mu_B$) than in UPt_3 , URu_2Si_2 , where one has $\mu \sim 0.01\mu_B$. The small magnetic moment is compatible with a SDW order.

Optical measurements in these compounds gave a possibility for the study of progressive development of the optical gap in spectra of the SDW systems UPt_3 , URu_2Si_2 —see Refs. 2 and 8–10. Infrared optical measurements in UPd_2Al_3 ,^{2,10,11} have shown no effects of the magnetic ordering on electronic properties at frequencies above 30 cm^{-1} . However, recent infrared optical measurements¹² show well pronounced (pseudo)gap behavior at rather low frequency $\omega_g \approx 0.2\text{ meV}$. We stress that ω_g was too small (compared to $T_N \approx 14$ K) in order to be explained by the simple weak coupling SDW theory,¹³ which predicts $\omega_g^{\text{SDW}}/T_{\text{SDW}} \approx 3.5$. Moreover, the recent experimental results¹⁴ give evidence for an huge increase of the optical mass at $\omega < \omega_g$ and at low temperatures $T < 2$ K. The latter fact points to a very strong and retarded quasiparticle interaction with some bosoniclike excitations, most probably spin fluctuations.

These experimental results imply a necessity for a systematic theoretical study of optical properties of the SDW metal by including possible retardation effects. In order to probe the SDW state the effect of impurities is useful tool and this is also a topic of this work. In absence of a fully microscopic theory of the SDW order our analysis is based on a semi-

microscopic model, which assumes that the conduction electrons are affected by the commensurate magnetic order with some large wave vector $\mathbf{Q} = \mathbf{G}/2$, where \mathbf{G} is the reciprocal wave vector.

In Sec. II we describe the model for systems with the commensurate spin density wave (SDW-CS) order, whose dynamics is governed by strong-coupling (retardation) equations. The effect of nonmagnetic impurities are also taken into account. We emphasize that the consideration of strong-coupling effects in some respect resembles the Eliashberg theory for superconductivity and this analogy is pursued consequently throughout the paper. Since heavy fermions are strongly correlated systems the charge fluctuation processes are suppressed in backward scattering,^{15,16} thus making negligible the effect of the interband nonmagnetic impurity scattering on the SDW order. The single-particle dynamic conductivity of the SDW-CS state is calculated in Sec. III by including impurity and strong-coupling effects, while in Sec. IV the numerical calculations for $N(\omega)$, $\sigma(\omega)$, and $R(\omega)$ are presented. The discussion of the obtained results and their possible application to some HF systems is given in Sec. V.

II. MODEL OF THE SDW METAL

A. Weak-coupling limit

The microscopic theory of the SDW metals was well elaborated in the past in the framework of the weak coupling excitonic insulator (EXIN) model.¹⁷ Since in the following we shall generalize this approach to include retardation effects we give a brief introduction of the EXIN model—see more in Refs. 18 and 19.

In the following it is assumed that the electronic system consists of several Fermi surfaces (or patches) and that at least one electron and one hole band (enumerated by indices $i = 1, 2$, respectively) fulfill the nesting condition

$$\xi_{1,\mathbf{k}} = -\xi_{2,\mathbf{k}+\mathbf{Q}} \quad (1)$$

with the energy dispersion $\xi_{1,\mathbf{k}} = \epsilon_{1,\mathbf{k}} - \mu$ and with the hole spectrum is $\xi_{2,\mathbf{k}+\mathbf{Q}} = -\epsilon_{2,\mathbf{k}} + \mu$. Other bands (or patches) are assumed not to participate in the formation of the SDW state and they create the electronic reservoir with the dispersion

$\xi_{r,\mathbf{k}}$. We assume that the SDW structure is commensurate (SDW-SC) with the wave vector $\mathbf{Q}=\mathbf{G}/2$, where \mathbf{G} is the reciprocal lattice vector, where $\xi_{1,2,\mathbf{k}+2\mathbf{Q}}=\xi_{1,2,\mathbf{k}}$ and $\xi_{1,2,\mathbf{k}+\mathbf{Q}}=\xi_{1,2,\mathbf{k}-\mathbf{Q}}$, and accordingly for operators Fermi operators $f_{1,2,\mathbf{k}+2\mathbf{Q}}=f_{1,2,\mathbf{k}}$ and $f_{1,2,\mathbf{k}+\mathbf{Q}}=f_{1,2,\mathbf{k}-\mathbf{Q}}$. The theory of the incommensurate SDW order is briefly discussed below.

The Hamiltonian of the two-band EXIN model has the form (σ is the spin index)

$$H = \sum_{i,\sigma,\mathbf{k}} \xi_{i,\mathbf{k}} f_{i\mathbf{k}\sigma}^\dagger f_{i\mathbf{k}\sigma} + \frac{1}{2\Omega} \sum_{ijlm\sigma,\sigma',\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ij,lm}(\mathbf{k},\mathbf{k}',\mathbf{q}) \times f_{i\mathbf{k}\sigma}^\dagger f_{j\mathbf{k}'\sigma'}^\dagger f_{l\mathbf{k}'+\mathbf{q}\sigma'} f_{m\mathbf{k}-\mathbf{q}\sigma} + H_r. \quad (2)$$

The indices $i,j=1,2$ enumerate the two nested bands of the EXIN model. For simplicity it is assumed that $V_{ij,lm}(\mathbf{k},\mathbf{k}',\mathbf{q})$ are weakly momentum dependent and for the dynamics of the model only terms $V_{12,21} \equiv V_1$, $V_{11,22} \approx V_{12,12} \equiv V_2$ are kept. The reservoir Hamiltonian H_r describes electrons of other (non-singular) bands on the Fermi surface which do not participate in the SDW state. Its importance in perturbing the SDW state is discussed below. The effects of phonons can be included easily.

In the weak coupling limit, where $V_{1,2}N(0) \ll 1$, the EXIN model admits an asymptotically exact solution in the mean-field approximation where H is replaced by the H_{MFA}

$$H_{\text{MFA}} = \sum_{i,\sigma,\mathbf{k}} \xi_{i,\mathbf{k}} f_{i,\mathbf{k}\sigma}^\dagger f_{i,\mathbf{k}\sigma} + \sum_{\sigma,\sigma',\mathbf{k},\mathbf{q}} \left[(\hat{\Delta}_{\mathbf{q}})_{\sigma,\sigma'} f_{1,\mathbf{k}+\mathbf{q}\sigma'}^\dagger f_{2,\mathbf{k}\sigma} + \text{c.c.} \right] + \sum_{\sigma,\sigma',\sigma''\mathbf{q}} (\hat{\Delta}_{\mathbf{q}})_{\sigma,\sigma'} (\hat{V}^{-1})_{\sigma'\sigma''} (\hat{\Delta}_{12,-\mathbf{q}})_{\sigma''\sigma}. \quad (3)$$

Here, $N(0)$ is the density of electronic states of the nested portions at the Fermi surface. In fact the spin-matrix $\hat{\Delta}_{\mathbf{q}}$ describes various electronic ordering phenomena $\hat{\Delta}_{\mathbf{q}} = \Delta_{\mathbf{q}}^s \sigma_0 + \hat{\Delta}_{\mathbf{q}}^t \vec{\sigma}$. Here, σ_0 , $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli spin matrices and $\Delta_{\mathbf{q}}^s$ and $\hat{\Delta}_{\mathbf{q}}^t$ are singlet and triplet (charge and spin density) order parameters, respectively. More on their physical meaning see in Refs. 18,19. Since the (triplet) SDW magnetic order is characterized by the coupling constant $V_t = V_1 + V_2$ we assume that $V_1, V_2 > 0$ and that $V_t > V_s$, i.e., the SDW order is more stable than the CDW one.

In the case of the SDW-CS order with the spin polarized along the z axis one has $\hat{\Delta}_{\mathbf{q}} = \delta_{\mathbf{q},\mathbf{Q}} \Delta \hat{\sigma}_3$ and the SDW-CS is characterized by the order parameter $\Delta_\sigma = \sigma \Delta$.^{18,19} The Hamiltonian reads (after renaming $f_{2,\mathbf{k}+\mathbf{Q},\sigma}$ by $f_{2,\mathbf{k},\sigma}$)

$$\hat{H}_{\text{SDW}} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} (f_{1\mathbf{k}\sigma}^\dagger f_{1\mathbf{k}\sigma} - f_{2\mathbf{k}\sigma}^\dagger f_{2\mathbf{k}\sigma}) + [\Delta_\sigma f_{1\mathbf{k}\sigma}^\dagger f_{2\mathbf{k}\sigma} + \text{c.c.}]. \quad (4)$$

Since the SDW physics resembles the BCS model for superconductivity we exploit this by introducing the Nambu ("spinor") operator $\Psi_{\mathbf{k}\sigma}^\dagger = (f_{1\mathbf{k}\sigma}^\dagger f_{2\mathbf{k}\sigma}^\dagger)$ and analogously the

(column) operator $\Psi_{\mathbf{k}}$. In this notation the SDW-CS Hamiltonian gets the superconductivitylike form

$$\hat{H}_{\text{SDW}} = \sum_{\mathbf{k}\sigma} \Psi_{\mathbf{k}\sigma}^\dagger [\xi_{\mathbf{k}} \hat{\tau}_3 + \Delta_\sigma \hat{\tau}_1] \Psi_{\mathbf{k}\sigma}, \quad (5)$$

where $\hat{\tau}_i$, $i=0,1,2,3$, are Pauli matrices ($\hat{\tau}_0 = \hat{1}$) operating in the electron-hole Nambu space. The Green's function $\hat{G}^0(\mathbf{k}, \omega_n)$ is given by the BCS-like solution

$$\hat{G}^0(\mathbf{k}, \omega_n) = - \frac{i \omega_n \hat{\tau}_0 + \xi_{\mathbf{k}} \hat{\tau}_3 + \Delta_\sigma \hat{\tau}_1}{\omega_n^2 + E_{\mathbf{k}}^2}, \quad (6)$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_\sigma^2}$. The SDW-CS order parameter Δ_σ fulfills the BCS like self-consistent equation

$$\Delta_\sigma = V_t \sum_{\mathbf{k}, \omega_n} G_{12, -\sigma-\sigma}^0(\mathbf{k}, \omega_n) \quad (7)$$

with $V_t = V_1 + V_2$. For small $\lambda_t = N(0)V_t$ the SDW order appears at the temperature $T_{\text{SDW}} \equiv T_c \approx 1.14 \omega_c \exp(-1/\lambda_t)$, with the cutoff energy ω_c . The gap at $T=0$ K is given by $\Delta_0/T_c = 1.75$. In solving Eq. (7) the property $\Delta_\sigma = -\Delta_{-\sigma}$ is used. Note, Eq. (7) can be generalized to describe an unconventional SDW (USDW) order parameter.^{20,21}

Few comments are necessary. (1) The same reasoning and mathematical technique as for the two-band EXIN model are also applicable to the case of a single-band metal having planar segments at the Fermi surface with the dispersion low $\xi_{\mathbf{k}} = -\xi_{\mathbf{k}+\mathbf{Q}}$. (2) When the perfect nesting is broken it is described by the parameter δ measuring the degree of the incongruence of the Fermi surface of electrons in bands 1 and 2, i.e., $\xi_{1,\mathbf{k}} = \xi_{\mathbf{k}} - \delta$ and $\xi_{2,\mathbf{k}+\mathbf{Q}} = -\xi_{\mathbf{k}} - \delta$. In that case the Gor'kov equations are similar to those of superconductor in the Zeeman field δ . This analogy is useful in constructing the phase diagram $T_c(\delta)$ for the SDW metal. It turns out that at $T=0$ K and for $\delta < \delta^{**}$ the SDW-CS order is realized, while for $\delta^{**} < \delta < \delta^c$ the incommensurate order (SDW-IC) is more stable. The values δ^{**} , δ^c depend on the assumed microscopic model—for instance for the two-band weak-coupling EXIN model one has $\delta^{**} \approx 0.5\Delta_0$ and $\delta^c \approx 0.75\Delta_0$ —see Refs. 18 and 19, and references therein. In the following we assume that $\delta < \delta^{**}$ holds and the SDW-CS state is realized. (3) In most HF systems there are other bands on the Fermi surface (described by the reservoir Hamiltonian H_r) not participating in the formation of the SDW state. If the average density of states of these reservoir bands at the Fermi surface $N_r(0) \gg 2N(0)$ then the renormalization of the chemical potential μ by the SDW order parameter is negligible.^{18,19} We assume this case which is rather realistic for the multiband HF systems with the large fraction of the nonsingular segments at the Fermi surface. This case is also realized in the Cr metal (and in its alloys) which is a typical SDW metal. In the opposite case $N_r(0) \ll 2N(0)$ there is a significant renormalization of μ .

B. Strong-coupling generalization and impurity effects

In the following we generalize the above weak-coupling model so to comprise (a) the strong coupling retardation and (b) impurity effects.

(a) In the case when the quasiparticle interaction with some bosoniclike excitations is strong the effective interaction is frequency dependent, i.e., $V_i \rightarrow V_i(\omega_n, \mathbf{k})$. The latter gives rise to the renormalization $\omega_n \rightarrow \tilde{\omega}_{n\mathbf{k}}$, $\Delta \rightarrow \tilde{\Delta}(\omega_n, \mathbf{k}) \equiv \tilde{\Delta}_{n\mathbf{k}}$ in Eq. (6) for the Green's function—see Eqs. (10), (11). One should underline that since the SDW order is due to the Coulomb interaction and the vertex corrections to the Eliashberg equations might be important, but this is not the subject of this paper.

(b) The effect of nonmagnetic impurities on the SDW order is described by the Hamiltonian

$$\hat{H}_{\text{imp}} = \sum_{ij, \mathbf{k}, \mathbf{q}\sigma, \mathbf{R}_{\text{imp}}} \rho_{\text{imp}}(\mathbf{k}, \mathbf{R}_{\text{imp}}) u_{\text{imp}}^{ij}(\mathbf{k}) f_{i, \mathbf{q}+\mathbf{k}\sigma}^\dagger f_{j, \mathbf{q}\sigma}. \quad (8)$$

The coordinate \mathbf{R}_{imp} enumerates randomly distributed impurities. Usually and for simplicity (but without any microscopic justification) it is assumed that the intraband (“forward”) scattering (with $i=j$) is present only, while the interband (“backward”) one (with $i \neq j$) is neglected. Note that the interband scattering u^{12} renormalizes the SDW order parameter Δ already in the first order and it must be included from the very beginning what complicates the theory. However, in strongly correlated systems the nonmagnetic scattering with large momentum transfer is strongly suppressed¹⁵ and the interband scattering can be neglected, i.e., $|u_{\text{imp}}^{12}| \ll |u_{\text{imp}}^{ii}| = u_0$, $i=1,2$. In that case the leading term in \hat{H}_{imp} reads

$$\hat{H}_{\text{imp}} = \sum_{\mathbf{R}_{\text{imp}}, \mathbf{k}} \rho_{\text{imp}}(\mathbf{k}, \mathbf{R}_{\text{imp}}) u_0 \sum_{\mathbf{q}\sigma} \Psi_{\mathbf{q}+\mathbf{k}\sigma}^\dagger \hat{\tau}_0 \Psi_{\mathbf{q}\sigma}. \quad (9)$$

Since \hat{H}_{imp} is proportional to the $\hat{\tau}_0$ matrix it means that the nonmagnetic scattering breaks the SDW-CS order similarly to the effect of magnetic impurities in singlet superconductors—the effect is also proportional to $\hat{\tau}_0$. Physically it means that the scattering on random impurities prefer to make the system homogeneous by washing out the non-uniform SDW structure.

In fact there are two effects of nonmagnetic impurities on the SDW-CS state. The first one changes the chemical potential leading to a destruction of nesting effects. This effect is similar to the effect of the “Zeeman field” δ discussed in the previous subsection. It is known that by alloying Cr with some nonisoelectronic impurities (the number of electrons per unit cell is changed) the chemical potential (μ) is changed giving rise to a SDW-CS \rightarrow SDW-IC transition. However, by alloying Cr with isoelectronic impurities there is no change of μ and the only effect of such impurities is to scatter electrons.^{18,19} In the following we assume that the latter case is realized.

In the following the isotropy of the spectral functions $V_Z(\omega, \mathbf{k})$ and $V_i(\omega, \mathbf{k})$ is assumed. After the integration

over the energy and by using the fact that $\tilde{\omega}_{n\mathbf{k}\sigma} = \tilde{\omega}_{n\mathbf{k}-\sigma}$ and $\tilde{\Delta}_{m\mathbf{q}-\sigma} = -\tilde{\Delta}_{m\mathbf{q}}$ the Eliashberg equations read

$$\tilde{\omega}_n = \omega_n + \gamma_{\text{imp}} \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_n^2}} + \pi T \sum_m \lambda_Z(\omega_n - \omega_m) \frac{\tilde{\omega}_m}{\sqrt{\tilde{\omega}_m^2 + \tilde{\Delta}_m^2}}, \quad (10)$$

$$\tilde{\Delta}_n = -\gamma_{\text{imp}} \frac{\tilde{\Delta}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_n^2}} + \pi T \sum_m \lambda_t(\omega_n - \omega_m) \frac{\tilde{\Delta}_m}{\sqrt{\tilde{\omega}_m^2 + \tilde{\Delta}_m^2}}. \quad (11)$$

Here $\gamma_{\text{imp}} [= 2\pi n_i N(0) V_0^2]$ is the impurity scattering rate. Note, that γ_{imp} enters equations for $\tilde{\omega}_{n\mathbf{k}}$ and $\tilde{\Delta}_{n\mathbf{k}}$ with different signs, which is due to the τ_0 matrix in Eq. (9). This leads to the detrimental (breaking) effect of nonmagnetic impurities on the SDW-CS state. The coupling functions $\lambda_l(\omega_n - \omega_m) = \lambda_{Z,t}(\omega_n - \omega_m)$ depend on the spectral functions $\alpha_l^2 F_l(\omega)$

$$\lambda_l(\omega_n - \omega_m) = \int_0^\infty d\omega \alpha_l^2 F_l(\omega) \frac{2\omega}{\omega^2 + (\omega_n - \omega_m)^2}. \quad (12)$$

III. DYNAMIC CONDUCTIVITY OF THE SDW-CS METAL

In HF systems with SDW order and complex multiband Fermi surface there are contributions to the dynamic conductivity $\sigma_{jj}(\omega)$ ($j=x,y,z$) due to SDW and reservoir electrons. We calculate first $\sigma_{jj}^{\text{SDW}}(\omega)$ which is due to electrons participating in the SDW-CS state. It is given by

$$\sigma_{jj}^{\text{SDW}}(\omega) = \frac{i\Pi_{jj}^{\text{SDW}}(\mathbf{q} \rightarrow 0, i\omega_n \Rightarrow \omega + i0^+)}{\omega}, \quad (13)$$

where $\Pi^{\text{SDW}}(i\omega_n)$ is the current-current correlation function

$$\Pi_{jj}^{\text{SDW}}(\mathbf{q}, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \langle T \hat{J}_j(\mathbf{q}, \tau) \hat{J}_j(-\mathbf{q}, 0) \rangle. \quad (14)$$

Since we study the optical properties in the London limit ($\mathbf{q} \rightarrow \mathbf{0}$) the current operator $\hat{J}_j(\mathbf{q}, \tau)$ of the SDW-CS metal reads

$$\hat{J}_j(\mathbf{q}, \tau) = \frac{e}{m} \sum_{\sigma, \mathbf{p}} v_j \left(\mathbf{p} + \frac{\mathbf{q}}{2} \right) \Psi_{\mathbf{p}\sigma}^\dagger \hat{\tau}_3 \Psi_{\mathbf{p}+\mathbf{q}\sigma}, \quad (15)$$

where in obtaining $\hat{J}_j(\mathbf{q}, \tau)$ the nesting property $\mathbf{v}_F(\mathbf{k}_F) = -\mathbf{v}_F(\mathbf{k}_F + \mathbf{Q})$ of the Fermi velocity is used. Note, that $\hat{J}_j(\mathbf{q}, \tau)$ contains the $\hat{\tau}_3$ matrix, while in the superconducting (SC) state it contains $\hat{\tau}_0$. This makes profound differences in transport properties of these two systems.

By neglecting the vertex correction in $\Pi(\mathbf{q}, i\omega_n)$ (index j is omitted) one obtains

$$\Pi^{\text{SDW}}(\mathbf{q}=\mathbf{0}, i\omega_n) \approx \frac{\omega_{pl}^2}{4\pi} T \sum_{m\sigma} \Pi_{\sigma}^{\text{SDW}}(\omega_n, \omega_m), \quad (16)$$

where

$$\Pi_{\sigma}^{\text{SDW}}(\omega_n, \omega_m) = \int d\xi_{\mathbf{k}} S_P \{ \hat{\tau}_3 \hat{G}_{\sigma\sigma}(\mathbf{k}, \omega_n + \omega_m) \hat{\tau}_3 \hat{G}_{\sigma\sigma}(\mathbf{k}, \omega_m) \}. \quad (17)$$

Here, $\omega_{j,pl} = (8\pi e^2 N(0) \langle v_j^2 \rangle)^{1/2}$ is the bare plasma frequency and \mathbf{v} is the Fermi velocity.

After the integration over the energy variable one obtains

$$\sigma^{\text{SDW}}(\omega) = \frac{\omega_{j,pl}^2}{16\pi i \omega} \int d\omega' \left\{ \frac{\tanh\left(\frac{\omega_-}{2T}\right)}{D^R} \left[1 - \frac{\tilde{\omega}_-^R \tilde{\omega}_+^R - \tilde{\Delta}_-^R \tilde{\Delta}_+^R}{\sqrt{(\tilde{\omega}_-^R)^2 - (\tilde{\Delta}_-^R)^2} \sqrt{(\tilde{\omega}_+^R)^2 - (\tilde{\Delta}_+^R)^2}} \right] \right. \\ \left. - \frac{\tanh\left(\frac{\omega_+}{2T}\right)}{D^A} \left[1 - \frac{\tilde{\omega}_-^A \tilde{\omega}_+^A - \tilde{\Delta}_-^A \tilde{\Delta}_+^A}{\sqrt{(\tilde{\omega}_-^A)^2 - (\tilde{\Delta}_-^A)^2} \sqrt{(\tilde{\omega}_+^A)^2 - (\tilde{\Delta}_+^A)^2}} \right] \right. \\ \left. - \frac{\tanh\left(\frac{\omega_+}{2T}\right) - \tanh\left(\frac{\omega_-}{2T}\right)}{D^a} \left[1 - \frac{\tilde{\omega}_-^A \tilde{\omega}_+^R - \tilde{\Delta}_-^A \tilde{\Delta}_+^R}{\sqrt{(\tilde{\omega}_-^A)^2 - (\tilde{\Delta}_-^A)^2} \sqrt{(\tilde{\omega}_+^R)^2 - (\tilde{\Delta}_+^R)^2}} \right] \right\}, \quad (19)$$

where $D^{R,A} = \sqrt{(\tilde{\omega}_+^{R,A})^2 - (\tilde{\Delta}_+^{R,A})^2} + \sqrt{(\tilde{\omega}_-^{R,A})^2 - (\tilde{\Delta}_-^{R,A})^2}$ and $D^a = \sqrt{(\tilde{\omega}_+^R)^2 - (\tilde{\Delta}_+^R)^2} - \sqrt{(\tilde{\omega}_-^A)^2 - (\tilde{\Delta}_-^A)^2}$. Here, $\omega_{\pm} = \omega' \pm \omega/2$, and the index $R(A)$ correspond to the retarded (advanced) branches of the complex function $F^{R(A)} = \text{Re}F \pm i \text{Im}F$. These expressions are similar to the ones for the optical conductivity of strong-coupling superconductors (see Ref. 23) but with different sign in the term $\tilde{\Delta}_-^{R,A} \tilde{\Delta}_+^{R,A}$ in the coherence factors, i.e., in front of the terms $\tilde{\Delta}_-^{R,A} \tilde{\Delta}_+^{R,A}$. This fact was used sometimes to describe experimental data in systems with C(S)DW by using the famous Mattis-Bardeen expression for the optical conductivity with the coherence factor of the first kind.^{24,25} The latter formula works properly in two limiting cases: (a) in the nonlocal Pippard limit and (b) in the very dirty limit ($l \ll \xi_0$). However, none of these limits is valid for the SDW-CS state in the HF systems since these are in the normal-skin (local) limit, and as mentioned before normal impurities are pair breaking and destroy SDW itself, i.e., it must be fulfilled $l > \xi_0$ with ξ_0 the SDW coherence length.

Since in most of the HF systems with the SDW magnetic order the optical measurements show the (generalized)

$$\Pi^{\text{SDW}}(\omega_n, \omega_m) = \frac{\tilde{\omega}_m(\tilde{\omega}_m + \tilde{\omega}_{m+n}) + \tilde{\Delta}_m(\tilde{\Delta}_m + \tilde{\Delta}_{m+n})}{R_m P_{mn}} \\ - \frac{\tilde{\omega}_{m+n}(\tilde{\omega}_{m+n} + \tilde{\omega}_m) + \tilde{\Delta}_{m+n}(\tilde{\Delta}_{m+n} + \tilde{\Delta}_m)}{R_m P_{mn}} \quad (18)$$

with $R_m = \sqrt{\tilde{\omega}_m^2 + \tilde{\Delta}_m^2}$ and $P_{mn} = \tilde{\omega}_m^2 - \tilde{\omega}_{m+n}^2 + \tilde{\Delta}_m^2 - \tilde{\Delta}_{m+n}^2$. By comparing this expression with the corresponding one for superconductors²² one sees that Π_{jj}^{SDW} contains the coherence factors $\tilde{\Delta}_m(\tilde{\Delta}_m + \tilde{\Delta}_{m+n})$ and $\tilde{\Delta}_{m+n}(\tilde{\Delta}_{m+n} + \tilde{\Delta}_m)$ while in the SC state one has $\tilde{\Delta}_m(\tilde{\Delta}_m - \tilde{\Delta}_{m+n})$ and $\tilde{\Delta}_{m+n}(\tilde{\Delta}_{m+n} - \tilde{\Delta}_m)$. This profound difference is reflected in different behavior of the optical conductivities $\sigma^{\text{SDW}}(\omega)$ and $\sigma^{\text{SC}}(\omega)$.

It gives

Drude-like behavior at low frequencies $\omega \ll 2\Delta_{\text{SDW}}^0$, the latter contribution (σ^D) is due to other (reservoir) electrons at the Fermi surface which are described by the Hamiltonian H_r . One expects that the total conductivity is a sum of both components $\sigma \approx \sigma^{D,r} + \sigma^{\text{SDW}}$. This problem will be discussed in the Sec. V.

IV. NUMERICAL RESULTS FOR THE SDW-CS STATE

In the following $N(\omega)$ and $\sigma^{\text{SDW}}(\omega)$ are calculated for various scattering rates γ_{imp} . The spectral function $\alpha_i^2 F_i(\omega)$ is taken in the form of a broadened Einstein-like bosonic spectrum centered at the frequency Ω and with the coupling constant $\lambda \equiv \lambda_i(\omega=0) = 5$.

(i) *Tunneling density of states $N(\omega)$* . The calculated $N(\omega)$ in the clean limit ($\gamma_{\text{imp}}=0$) is shown in Fig. 1. As expected it has strong BCS-like singularity due to the gap opening in the quasiparticle spectrum. Since the nonmagnetic impurities are SDW-breaking this leads to a strong suppression of $N(\omega)$, by smoothing it and shifting its maximum to lower energies. For $\gamma_{\text{imp}} \sim \Delta_0$ it shows the gapless behavior—a

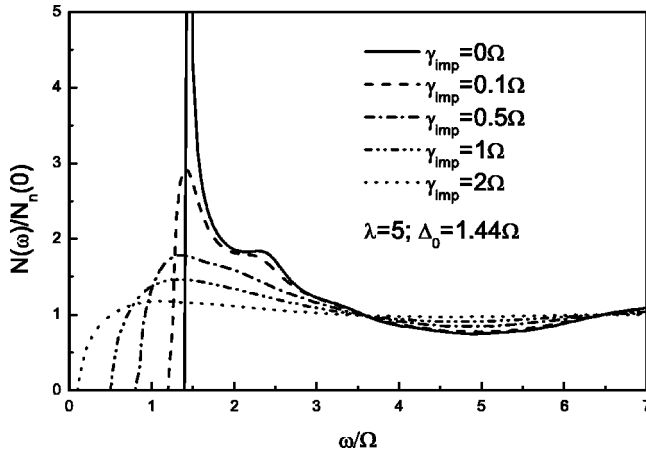


FIG. 1. Tunneling density of states $N(\omega)$ for the broadened Einstein spectrum with $\lambda_t=5$ for various impurity scattering rates γ_{imp} .

property analogous to the case of superconductors with magnetic impurities. It turns out that due to large $\lambda (=5)$ there is clear dip in $N(\omega)$ for $\omega > \Delta_0$ [with $N(\omega)/N_n(0) < 1$] followed by a broad peak at larger ω . We emphasize that the dip structure, followed by the peak at higher frequencies, appears always in the strong-coupling Eliashberg theory of superconductors for sufficiently large coupling constant λ and it is weakly dependent on the shape of the bosonic spectral function.²⁶ Similar behavior of the tunneling density of states $N(\omega)$ has been seen also in the tunneling conductivity of UPd₂Al₃ but in the superconducting state,²⁷ which together with the above theoretical and numerical results points to a strong scattering of quasiparticles on some bosoniclike excitations. Since the above equations for the Green functions and $N(\omega)$ hold also for singlet superconductors with the same spectral function, $\alpha_t^2 F_t(\omega)$ at $T < T_c < T_N$, the results shown in Fig. 1 confirm earlier conclusions^{27,28} that superconductivity in UPd₂Al₃ is in the very strong-coupling regime ($\lambda \gg 1$). Regarding the theoretical results for $N(\omega)$, which are shown in Fig. 1, it would be interesting to search experimentally for possible strong-coupling effects—the dip structure and second peak, in SDW metals at temperatures $T_c < T < T_N$.

(ii) *Dynamitic conductivity $\sigma^{\text{SDW}}(\omega)$ and reflectivity $R(\omega)$.* Due to the peculiar coherence effects in the SDW-CS state the dynamitic conductivity $\sigma^{\text{SDW}}(\omega)$ differs significantly from the corresponding one in s -wave superconductors—see Eq. (19). The numerical calculations of $\sigma_1(\omega) \equiv \text{Re} \sigma^{\text{SDW}}(\omega)$ are shown in Fig. 2. In the clean limit ($\gamma_{\text{imp}}=0$) and at very low temperatures ($T \ll \Delta_0$) $\sigma_1(\omega)$ is singular at $\omega=2\Delta_0$. For finite $\gamma_{\text{imp}} (< \Delta_0)$ $\sigma_1(\omega)$ is broadened and its maximum is shifted to lower ω , as it is seen in Fig. 2. It is also apparent from Fig. 2 that for $\gamma_{\text{imp}}=0.1\Delta_0$ the suppression, broadening and shift (to lower frequency) of σ_1 are very pronounced, already for the large mean-free path, $l \sim 20 \xi_{\text{SDW}}$, i.e., isoelectronic nonmagnetic impurities affect the SDW-CS condensate appreciably. This property is robust and practically independent on the shape of the spectral function. We stress that this pronounced impurity dependence of $\sigma^{\text{SDW}}(\omega)$ may serve as an important

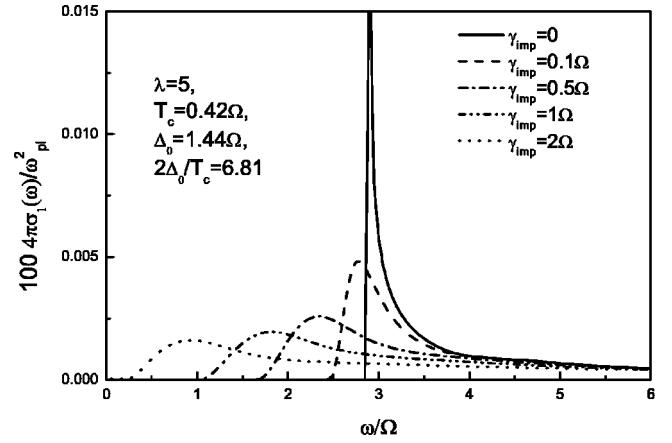


FIG. 2. Real part of the dynamic conductivity $\sigma^{\text{SDW}}(\omega)$ for various impurity scattering rate γ_{imp} .

check of the SDW-CS state in HF systems.

The reflectivity along the j axis $R(\omega) = \{[\sqrt{\varepsilon(\omega)} - 1]/[\sqrt{\varepsilon(\omega)} + 1]\}^2$ is defined by the dielectric function $\varepsilon(\omega) = \varepsilon_\infty + 4\pi i \sigma^{\text{SDW}}(\omega)/\omega$. The numerical results for $R(\omega)$ are shown in Fig. 3 for $\sigma_1(\omega)$ from Fig. 2, and for the assumed $\varepsilon_\infty=9$. A rather rich structure in $R(\omega)$ is seen, which is partly due to the strong-coupling limit ($\lambda=5$) of the theory. In the clean case there is a peak at $\omega=2\Delta_0$ followed by the minimum around $\omega/\Omega \approx 5$ which is just the position of the dip in the density of states shown in Fig. 1, while the maximum of the shoulder at $\omega/\Omega \approx 7.5$ corresponds to the second maximum in $N(\omega)$.

Usually, experimental results for $\sigma(\omega)$ are modeled by the generalized Drude formula with ω -dependent scattering rate $\Gamma_{\text{eff}}(\omega)$ and the optical mass $m^*(\omega)$

$$\sigma^{\text{SDW}}(\omega) = \frac{\omega_{pl}^2}{4\pi} \frac{1}{\Gamma_{\text{eff}}(\omega) - i\omega m_{\text{SDW}}^*/m_\infty}. \quad (20)$$

As the result we obtain that in the SDW-CS state m_{SDW}^* is negative (not shown), while $\Gamma_{\text{eff}}(\omega)$ —shown in Fig.

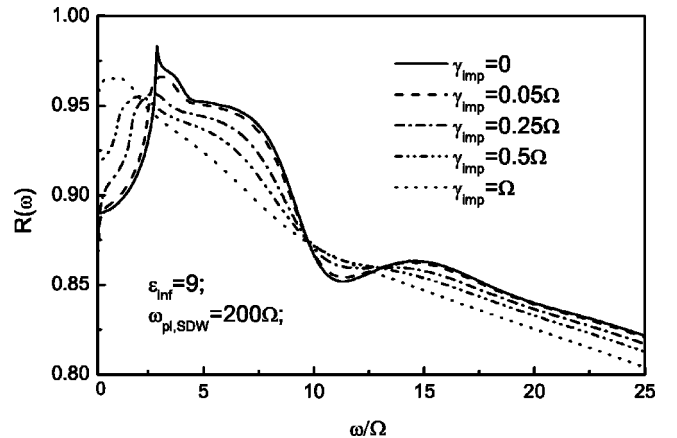


FIG. 3. Reflectivity in the SDW state $R^{\text{SDW}}(\omega)$ for $\sigma^{\text{SDW}}(\omega)$ in Fig. 2 and for various impurity scattering rates γ_{imp} .

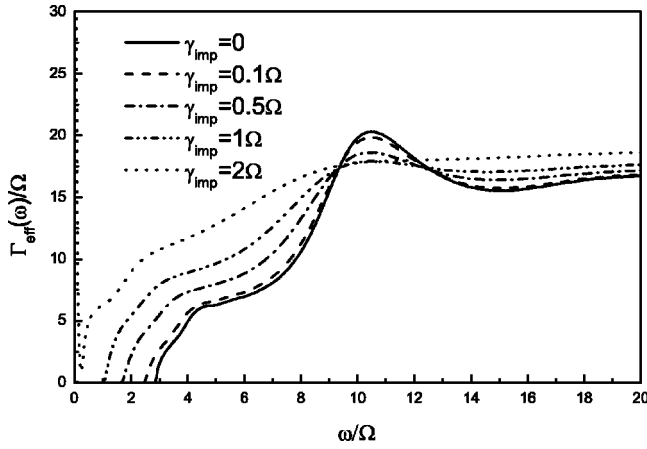


FIG. 4. Optical relaxation rate $\Gamma_{\text{eff}}^{\text{SDW}}(\omega)$ [see Eq. (20)] for various impurity scattering rates γ_{imp} .

4—has also a rich structure due to the strong-coupling effects resembling those in the superconducting state.²⁹

V. DISCUSSION

In real HF systems with SDW order electrons participating in the SDW state and those from the reservoir contribute to $\sigma_{ij}(\omega)$. The reservoir part gives rise to the (generalized) Drude conductivity $\sigma^D(\omega)$ at frequencies $\omega < 2\Delta_0$. For a quantitative analysis the bosonic spectral function is needed, as well as the plasma frequency, etc. In absence of these relevant informations we assume for simplicity that these two effects are additive and that the contribution of the reservoir is described by the simple Drude part with constant scattering rate and optical mass, i.e., $\sigma(\omega) = \sigma^{\text{SDW}}(\omega) + \sigma^D(\omega) = \sigma^{\text{SDW}}(\omega) + \omega_{pl,D}^2/4\pi(-i\omega + \gamma_D)$. It is again fit by the generalized Drude formula

$$\sigma(\omega) = \frac{\omega_{pl,D}^2 + \omega_{pl,SDW}^2}{4\pi} \frac{1}{-i\omega m^*(\omega)/m_\infty + \Gamma_{\text{eff}}(\omega)}. \quad (21)$$

The real part of the conductivity $\sigma(\omega)$ is numerically calculated by assuming for simplicity $\gamma_D = 2\gamma_{\text{imp}}$, $\omega_{pl,D}^2 = \omega_{pl,SDW}^2$ and it is shown in Fig. 5, while $m^*(\omega)/m_\infty$ and $\Gamma_{\text{eff}}(\omega)$ are shown in Fig. 6. The rich structure in $m^*(\omega)/m_\infty$ and $\Gamma_{\text{eff}}(\omega)$ is partially due the properties of $N(\omega)$ and $\sigma(\omega)$ and to the assumed parametrization in Eq. (21). In that respect it is worth of mentioning that there is an increase of the optical mass $m^*(\omega)$ by factor 2 with respect to m_∞ which is in fact not due to any inelastic quasiparticle scattering, but it is due only to the fitting method of $\sigma(\omega)$ by Eqs. (20) and (21). This interesting result tells us how dangerous is to interpret the optical mass as the quasiparticle mass. Such a misinterpretation of the optical mass was made very frequently in interpreting optic measurements in HTS materials.

We stress, that in order to compare to experimental results in real SDW heavy fermion materials the realistic values for $\omega_{pl,D}^2$, $\omega_{pl,SDW}^2$, m_∞ , etc., are needed, as well as optic measurements in the low-frequency region $\omega < \omega_g$. The most appropriate candidate for the application of the above theory

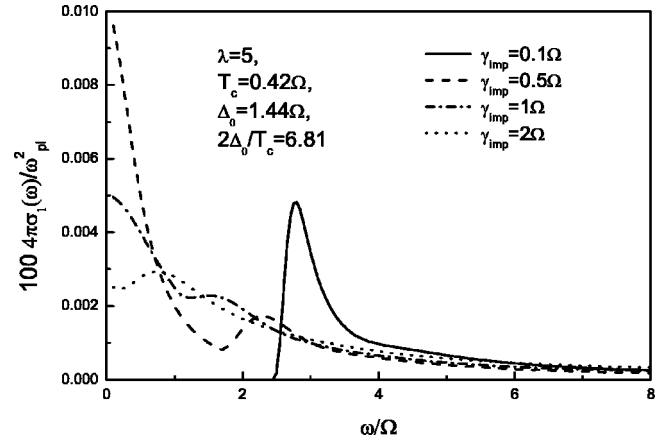


FIG. 5. Real part of the total conductivity $\sigma_1^D(\omega) + \sigma_1^{\text{SDW}}(\omega)$ for $\sigma_1^{\text{SDW}}(\omega)$ in Fig. 2 and for various impurity scattering rates γ_{imp} .

seems to be URu₂Si₂, which can be considered as a typical example of the HF systems with the SDW-SC order. For such a purpose it would be necessary to study the optical spectra of this material in which a controllable amount of the isoelectronic impurities are introduced.

In conclusion, we have studied the retardation (strong-coupling) and impurity effects on the dynamic conductivity $\sigma(\omega)$ and tunneling density of states $N(\omega)$ in strongly correlated metals (such as heavy fermions) with commensurate SDW order. It is shown that nonmagnetic impurities, with strongly suppressed interband (backward) impurity scattering in strongly correlated systems, affect $N(\omega)$, $\sigma(\omega)$, and $R(\omega)$ significantly. Such impurities broaden and shift the maxima of $N(\omega)$ to lower frequencies and are SDW breaking. The latter effect might be an important test for the itinerant character of the SDW order in the HF systems. It is shown that in systems with a multiband Fermi surface, containing SDW and reservoir electrons and if $\sigma(\omega)$ is additive then the optic mass is increased at low frequencies only because of additivity of $\sigma(\omega)$ without any additional inelastic scattering mechanism. This result demonstrates clearly that

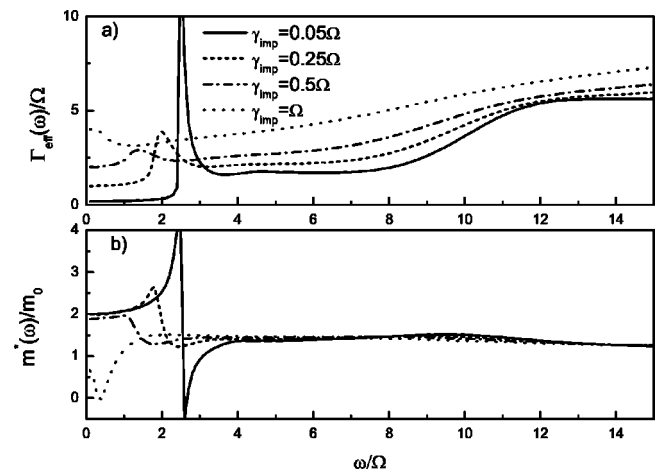


FIG. 6. Optical relaxation rate $\Gamma_{\text{eff}}(\omega)$ and the effective mass $m^*(\omega)$ extracted from $\sigma(\omega)$ in Fig. 5 for various impurity scattering rates γ_{imp} .

the interpretation of the quasiparticle mass to be proportional (or even equal) to the optical mass may lead to wrong conclusions regarding the inelastic quasiparticle scattering mechanisms. The proposed theory can be with minor changes extended to systems with unconventional spin density wave order, as well as to charge-density wave order.

ACKNOWLEDGMENTS

The authors thank B. Gorshunov for discussions. M.L.K. acknowledges the support of the Deutsche Forschungsgemeinschaft (DFG) through the SFB 484 project at University of Augsburg.

-
- ¹G.R. Stewart, *Rev. Mod. Phys.* **56**, 755 (1984); P. Fulde, J. Keller, G. Zwicknagl, in *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1988), Vol. 41, p. 1.
- ²L. Degiorgi, S. Thieme, H.R. Ott, M. Dressel, G. Grüner, Y. Dalichaouch, M.B. Maple, C. Geibel, and F. Steglich, *Z. Phys. B: Condens. Matter* **102**, 367 (1997).
- ³C. Geibel, C. Schank, S. Thies, H. Kitazawa, C.D. Bredl, A. Böhm, M. Rau, A. Grauel, R. Caspary, R. Helfrich, U. Ahlheim, G. Weber, and F. Steglich, *Z. Phys. B: Condens. Matter* **84**, 1 (1991).
- ⁴T.T.M. Palstra, A.A. Menovsky, and J.A. Mydosh, *Phys. Rev. B* **33**, 6527 (1986).
- ⁵N. Sato, N. Aso, G.H. Lander, B. Roessli, T. Komatsubara, and Y. Endoh, *J. Phys. Soc. Jpn.* **66**, 1884 (1998); N. Metoki, Y. Haga, Y. Koike, and Y. Onuki, *Phys. Rev. Lett.* **80**, 5417 (1998).
- ⁶A. Krimmel, P. Fischer, B. Roessli, H. Malleta, C. Geibel, C. Schank, A. Grauel, A. Loidl, and F. Steglich, *Z. Phys. B: Condens. Matter* **86**, 161 (1992); A. Krimmel, A. Loidl, R. Eccleston, C. Geibel, and F. Steglich, *J. Phys.: Condens. Matter* **8**, 1677 (1996).
- ⁷L. Paolasini, J.A. Paixao, and G.H. Lander, *J. Phys.: Condens. Matter* **5**, 8905 (1993).
- ⁸S. Donovan, A. Schwartz, and G. Grüner, *Phys. Rev. Lett.* **79**, 1401 (1997).
- ⁹D.A. Bonn, J.D. Garrett, and T. Timusk, *Phys. Rev. Lett.* **61**, 1305 (1988).
- ¹⁰L. Degiorgi, H.R. Ott, M. Dressel, G. Grüner, and Z. Fisk, *Europhys. Lett.* **26**, 221 (1994).
- ¹¹M. Dressel, L. Degiorgi, G. Grüner, P. Wachter, N. Sato, T. Komatsubara, and Y. Uemura, *Physica B* **199&200**, 173 (1994); L. Degiorgi, M. Dressel, G. Grüner, P. Wachter, N. Sato, and T. Komatsubara, *Europhys. Lett.* **25**, 311 (1994).
- ¹²M. Dressel, B. Gorshunov, N. Kasper, B. Nebendahl, M. Huth, and H. Adrian, *J. Phys.: Condens. Matter* **12**, L633 (2000); M. Dressel, N. Kasper, B. Gorshunov, K. Petukhov, D. N. Peligard, M. Huth, and H. Adrian (unpublished).
- ¹³G. Grüner, *Density Waves in Solids* (Addison-Wesley, Reading, 1994).
- ¹⁴M. Dressel, N. Kasper, K. Petukhov, B. Gorshunov, G. Grüner, M. Huth, and H. Adrian, cond-mat/0201167 (unpublished).
- ¹⁵M.L. Kulić and R. Zeyher, *Phys. Rev. B* **49**, 4395 (1994); *Physica C* **199-200**, 358 (1994); R. Zeyher and M.L. Kulić, *Phys. Rev. B* **53**, 2850 (1996).
- ¹⁶M.L. Kulić, *Phys. Rep.* **338**, 1 (2000).
- ¹⁷L.V. Keldysh and Yu.V. Kopaev, *Sov. Phys. Solid State* **6**, 2219 (1965).
- ¹⁸E. Fawcett, *Rev. Mod. Phys.* **60**, 209 (1988); **66**, 25 (1994).
- ¹⁹V. V. Tugushev, in *Electronic Phase Transitions*, edited by W. Hanke and Yu. V. Kopaev (Elsevier, British Vancouver, 1992), p. 237; N.I. Kulikov and V.V. Tugushev, *Sov. Phys. Usp.* **27**, 954 (1984).
- ²⁰B. Dora and A. Virosztek, *Eur. Phys. J. B* **22**, 167 (2001).
- ²¹Xiao Yang and C. Nayak, cond-mat/0108407 (unpublished).
- ²²N.E. Bickers, D.J. Scalapino, R.T. Collins, and Z. Schlesinger, *Phys. Rev. B* **42**, 67 (1990).
- ²³S.B. Nam, *Phys. Rev.* **156**, 1234 (1967); W. Lee, D. Rainer, and W. Zimmermann, *Physica C* **159**, 535 (1989); O.V. Dolgov, A.A. Golubov, and S.V. Shulga, *Phys. Lett. A* **147**, 317 (1990); F. Marsiglio, R. Akis, and J.P. Carbotte, *Phys. Rev. B* **45**, 9865 (1992).
- ²⁴L. Degiorgi, M. Dressel, A. Schwartz, B. Alavi, and G. Grüner, *Phys. Rev. Lett.* **76**, 3838 (1996); M. Dressel, *Physica C* **317-318**, 89 (1999).
- ²⁵A.P. Kampf, *Phys. Rep.* **249**, 220 (1994).
- ²⁶D.J. Scalapino, J.R. Schrieffer, and J.W. Wilkins, *Phys. Rev.* **148**, 263 (1966); G. Varelogiannis, *Z. Phys. B: Condens. Matter* **104**, 411 (1997).
- ²⁷M. Jourdan, M. Huth, and H. Adrian, *Nature (London)* **398**, 47 (1999).
- ²⁸N.K. Sato, N. Aso, K. Miyake, R. Shilna, P. Thalmeier, G. Varelogiannis, C. Geibel, F. Steglich, P. Fulde, and T. Komatsubara, *Nature (London)* **410**, 340 (2001).
- ²⁹R. Combescot, O.V. Dolgov, D. Rainer, and S.V. Shulga, *Phys. Rev. B* **53**, 2739 (1996).