Local density of states and Friedel oscillations around a nonmagnetic impurity in unconventional density waves

András Ványolos,[1,*] Balázs Dóra,[1,2] and Attila Virosztek[1,3]
[1]*Department of Physics, Budapest University of Technology and Economics, 1521 Budapest, Hungary*
[2]*Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, 01187 Dresden, Germany*
[3]*Research Institute for Solid State Physics and Optics, P.O. Box 49, 1525 Budapest, Hungary*
(Received 29 January 2007; published 10 May 2007)

We present a mean-field theoretical study on the effect of a single nonmagnetic impurity in quasi-one-dimensional unconventional density wave. The scattering potential is treated within the self-consistent T-matrix approximation. The local density of states around the impurity exhibits resonant states in the vicinity of the Fermi level, much the same way as in d density waves or unconventional superconductors. The assumption for different forward and backward scattering, characteristic to quasi-one-dimensional systems in general, leads to a resonance state that is double peaked in the pseudogap. The Friedel oscillations around the impurity are also explored, both within and beyond the density wave coherence length ξ_0. Beyond ξ_0, we find power-law behavior as opposed to the exponential decay of conventional density wave.

DOI: 10.1103/PhysRevB.75.193101 PACS number(s): 71.45.Lr, 75.30.Fv, 71.27.+a

The effect of a single impurity on the properties of high-temperature superconductors (HTSCs) has attracted considerable attention in the past few years.[1–3] This enthusiasm is mainly due to the fact that scattering from a localized perturbation produces qualitatively different electronic structures around the impurity in the d-wave superconducting (dSC) and pseudogap phases[4,5] that are directly measurable with scanning tunneling microscopy (STM). The study of impurity induced bound states, however, is not limited to HTSC physics only. In fact, this issue has been investigated since late 1960s in the context of conventional BCS superconductors[6] and conventional charge-density waves (CDWs).[7] To the best of our knowledge, however, the single impurity problem in unconventional density wave (UDW) has not been addressed so far. An unconventional density wave is a density wave with momentum dependent gap $\Delta(\mathbf{k})$, whose average vanishes over the Fermi surface.[8,9] Therefore, these systems lack spatial variation of either charge or spin. This intriguing property is known as hidden order in recent literature.[10] For more recent developments on UDW physics, the reader may consult Ref. 9.

In this theoretical study, we aim to explore the effects of a single nonmagnetic impurity in such quasi-one-dimensional UDWs. In particular, we study the localized intragap states and Friedel oscillations induced by the scatterer.

First, we present the results for the spectral function in UDW defined by

$$A(\mathbf{r},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\alpha\beta} G_{\alpha\beta}(\mathbf{r},\mathbf{r};i\omega_n \to \omega + i0), \tag{1}$$

where G is the Green's function corresponding to the total Hamiltonian $H=H_0+H_1$. Here, H_0 is the Hamiltonian of the clean UDW.[9] The momentum dependence of its gap is chosen as $\Delta(\mathbf{k})=\Delta e^{i\phi}\sin(bk_y)$, where the phase ϕ is unrestricted due to incommensurability.[8] In addition, the interaction with the impurity responsible for the renormalization of G^0 is given by

$$H_1 = \frac{1}{V}\sum_{\mathbf{k},\mathbf{q},\sigma}\begin{pmatrix} a_{\mathbf{k+q},\sigma} \\ a_{\mathbf{k+q-Q},\sigma}\end{pmatrix}^{\dagger}\begin{pmatrix} U(0) & U(\mathbf{Q}) \\ U(\mathbf{Q}) & U(0)\end{pmatrix}\begin{pmatrix} a_{\mathbf{k},\sigma} \\ a_{\mathbf{k-Q},\sigma}\end{pmatrix}. \tag{2}$$

Here, we have neglected the small $\mathbf{q}$ dependence of the matrix elements, because in a quasi-one-dimensional DW two relevant scattering amplitudes can be distinguished: the forward $U(0)$ and the backward scattering parameter $U(\mathbf{Q})$, respectively. It is worthwhile to emphasize at this point that the allowance for different forward and backward scattering constitutes a more realistic impurity physics than the usage of a somewhat artificial pointlike scalar impurity with $U(0)=U(\mathbf{Q})\equiv U$. Nevertheless, this restricted impurity model is widely used in literature concerning the single impurity problem in conventional CDW,[7] unconventional superconductors,[3] and more recently in the context of the pseudogap phase of HTSC.[5,11]

Following Ref. 7, Dyson's equation for G can be solved easily and the T matrix responsible for the localized states reads as

$$T_{\gamma\delta}(i\omega_n) = \{t[1 - G^0(0,0;i\omega_n)t]^{-1}\}_{\gamma\delta}, \tag{3}$$

where $t_{\gamma\delta}=U(0)\delta_{\gamma\delta}+U(\mathbf{Q})\delta_{\gamma,-\delta}$. In quasi-one-dimensional UDW, besides the chain direction x, in which the model is continuous, perpendicular spatial dimensions are present, which offer the possibility for momentum dependent gap.[8,9] This is to be contrasted with the strictly one-dimensional nature of normal CDW.[7,12] As the specific $\mathbf{k}$ dependence of the gap was chosen to be $\sim\sin(bk_y)$, the relevant perpendicular direction is y, and the model remains discrete in this variable. Consequently, we take $\mathbf{r}=(x,mb,0)$, where b is the corresponding lattice constant and m is an integer indexing parallel chains.

We numerically determined and plotted $A(\mathbf{r},\omega)$ in UDW in Fig. 1 for the case $m=0$, that is, on the chain where the impurity resides. Similar results are obtained for $m\neq 0$ too. It is immediately clear that the presence of the local perturbation violates particle-hole symmetry. The fine details and fea-

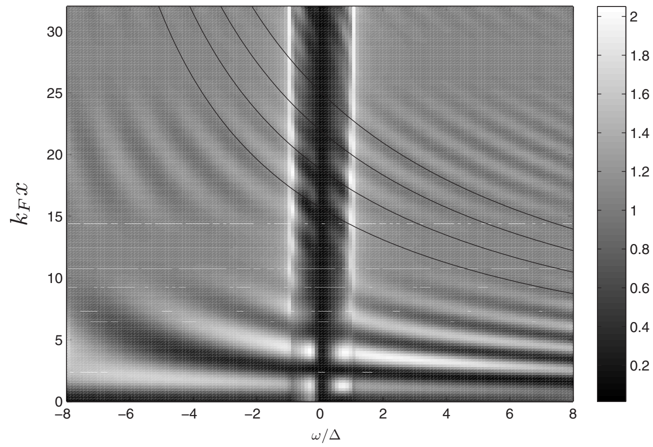

FIG. 1. The LDOS $A(\mathbf{r},\omega)/N_0$ is shown in UDW versus energy and position measured from the scatterer for $m=0$. For the numerics, $N_0U(0)=0.2$, $N_0U(\mathbf{Q})=0.7$, $v_Fk_F/\Delta=v_Fk_F/t_b=10$, and $\phi=\pi/3$ were applied. The black lines were calculated from $k_Fx=n\pi v_Fk_F/(\omega+v_Fk_F)$ with $n=5,6,7,8$ (from bottom to top) and N_0 is the normal-state DOS.

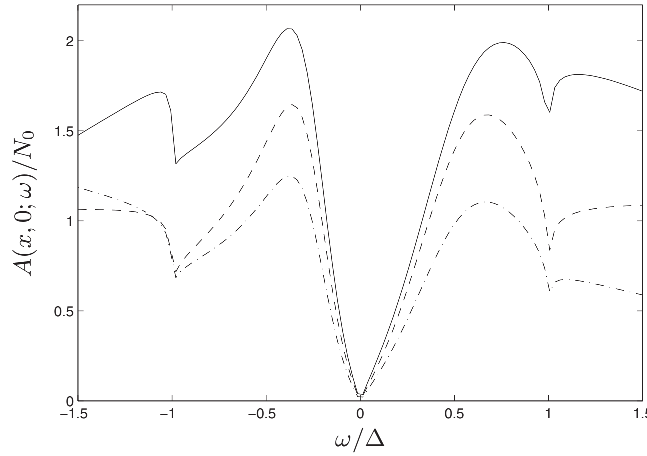

FIG. 2. The LDOS versus energy in UDW is plotted for the chain $m=0$ at fixed distances from the impurity, $k_Fx=0.9$ (dashed), 1.8 (dashed dotted), and 4 (solid). Other parameters are the same as in Fig. 1.

tures of the pattern can be nicely separated into three distinct components, each having its own microscopic origin.

(i) Perhaps the most apparent flavor of Fig. 1 are those curved stripes or waves that are becoming even denser at high energies. They are essentially nothing else but the electronic wave functions and can be obtained even in a strictly one-dimensional metal. A simple de Broglie picture can already account for the observed periodicity along the chain: $\lambda=2\pi/p$, where $p=(\omega+v_Fk_F)/v_F$ is the momentum of the electron with energy ω measured from the chemical potential in a linearized band. The very same electronic waves were found in the spectral function of one-dimensional conventional CDW.[12] Namely, in Ref. 12 the effect of open boundary on CDW was studied. Among others, it was found that the position of zeros in the STM image is determined by $k_Fx=n\pi v_Fk_F/(\omega+v_Fk_F)$, with n a natural number. This result is in complete agreement with our simple reasoning based on the de Broglie formula. Each stripe can therefore be assigned a natural number n, though these stripes do not necessarily indicate zeros in UDW. This is because the pattern in the present case depends (weakly) on the scattering amplitudes too, and an exact agreement is achieved only in the limit $U(0)=U(\mathbf{Q})\to\infty$ corresponding to the case of open boundary.

(ii) Another interesting feature of STM image is the modulated behavior along the chains with a much larger wavelength than λ. Namely, $A(\mathbf{r},\omega)$ "periodically" takes on its unperturbed value, in other words, exhibits a beat. A detailed calculation shows that on chain m whenever $J_m^2(2x/\xi)=0$, the local density of states (LDOS) is that of the unperturbed system. Here, $J_m(z)$ is the Bessel function of the first kind and $\xi=v_F/t_b$ is the characteristic length scale originating from finite interchain coupling. In density wave materials, t_b is usually of the order of the energy gap Δ, and this leads to a ξ that is comparable to the DW coherence length $\xi_0=v_F/\Delta$; in any case, it is much larger than atomic distances. This modulated behavior related to the zeros of the Bessel function is clearly missing in strictly one-dimensional models and is specific to real quasi-one-dimensional systems, may it be either a normal metal, a CDW, or even an UDW.

(iii) The most important property of the electronic structure, at least from the UDW point of view, is definitely the low-energy behavior around the Fermi level. The subgap structure of LDOS in Fig. 1 (shown enlarged in Fig. 2) is qualitatively different from that of a fully gapped DW.[7,12] Namely, in UDW considerable amount of spectral weight is accumulated in the intragap regime in the form of two virtually bound quasiparticle states. The energies of these impurity states are determined by the poles of the T matrix:

$$\Omega_\pm=\Omega'_\pm-i\Omega''_\pm=-\frac{\Delta}{N_0U_\pm}\frac{1}{\ln(4N_0|U_\pm|)}\left(1+i\frac{\pi}{2}\frac{\mathrm{sgn}(U_\pm)}{\ln(4N_0|U_\pm|)}\right), \tag{4}$$

where $U_\pm=U(0)\pm U(\mathbf{Q})$, and we have assumed the impurity scattering to be close enough to the unitary limit so that the result can be computed to logarithmic accuracy with $\ln(4N_0|U_\pm|)\gg 1$. It is only in this limit that the two bound states are well defined with $\Omega''_\pm\ll|\Omega'_\pm|$. The finite lifetime results from the finite density of states in the subgap coming from nodal quasiparticles $[A^0(\omega)\sim|\omega|$ for small $\omega]$. In contrast to this, in conventional DW with constant gap the binding energies of the corresponding impurity states are purely real, leading to infinitely sharp resonances and well-defined undamped states.[7] Equation (4) and the presence of impurity induced quasiparticle states in the UDW gap are in precise agreement with that found in dSC (Ref. 4 and 13) and in d density wave (dDW).[5,11] However, in dDW only one such impurity state has been found, which is due to the limitation of the strictly pointlike impurity potential applied there. Indeed, for such a potential $U_-=0$ and the pole structure of the T matrix exhibits a single resonance only. Note also that in dSC a double peaked resonance is found: one state on both positive (electron) and negative (hole) biases. This structure, however, arises from the particle-hole mixing, an essential feature of pairing in SC, and has nothing to do with different forward and backward scattering.

Now, we turn our attention to the analysis of density oscillations caused by the impurity in the Born limit. The investigation of this issue is motivated by the findings of Ref. 7, valid in one-dimensional CDW. It was found that at zero temperature below the coherence length $\xi_0=v_F/\Delta$, the charge density around the impurity is just the sum of the contributions corresponding to the CDW and the Friedel oscillations. Beyond ξ_0, however, exponential decay was found, as the necessary electron-hole pairs with energy smaller than 2Δ are not available. Here, Friedel oscillations essentially cannot build up. Our aim is to perform an analog but finite temperature calculation in UDW, and find the total density

$$n(\mathbf{r})=\sum_{\alpha\beta}G_{\alpha\beta}(\mathbf{r},\mathbf{r};\tau=-0). \tag{5}$$

Since in UDW no periodic modulation of charge is present, we expect robust Friedel oscillations showing up below ξ_0. On the other hand, as UDW is gapless, we expect the oscillations beyond the coherence length to exhibit power-law behavior as opposed to exponential decay.

To get started, we first present the results for a quasi-one-dimensional metal. For $|x|\gg k_F^{-1}$, one obtains

$$n(x,m)=n_0-n_0N_0U(\mathbf{Q})\pi \times(-1)^mJ_m^2\left(\frac{2x}{\xi}\right)P\left(\frac{2\pi|x|}{\xi_1}\right)\frac{\cos(2k_Fx)}{2k_F|x|}, \tag{6}$$

where $n_0=k_F/(\pi bc)$ is the homogeneous density, $\xi_1=v_F/T$ is the thermal length scale, and $P(z)=z\sinh^{-1}(z)$. Apparently, in a normal metal only backscattering contributes to Friedel oscillations. The oscillations are modulated by a smooth envelope $P(z)$, that in the zero-temperature limit correctly simplifies to $P(z\to 0)=1$. On the other hand, at small but finite temperature the long-range behavior is replaced by an exponential decay according to $P(z\gg 1)\approx 2ze^{-z}$. This qualitative change arises from the smearing of the Fermi surface at finite T. As to the effect of impurity on the parallel chains, it has been taken into account by the Bessel function. In the extreme limit of decoupled one-dimensional chains, where $t_b\to 0$, one readily finds $J_m(2x/\xi)\to\delta_{m0}$, indicating the fact that screening takes place on the chain only where the impurity resides and all the others are completely unaffected. At finite interchain coupling, the square of the Bessel function serves as a modulating function: due to its quasiperiodic zeros, it results in a beat in the induced charge density with wavelength $\lambda\approx\pi\xi/2$, that is certainly much larger than that of the Friedel oscillation, π/k_F.

The corresponding formula for the impurity induced charge response in a quasi-one-dimensional conventional CDW reads as

$$n(x,m)=n_0-(-1)^mn_1\cos(2k_Fx+\phi)-n_0N_0 \times U(\mathbf{Q})\pi(-1)^mJ_m^2\left(\frac{2x}{\xi}\right)F\left(\frac{2|x|}{\xi_0}\right)\frac{\cos(2k_Fx)}{2k_F\xi_0}, \tag{7}$$

where

$$F(z)=2K_1(z)-2e^{i\phi}\cos(\phi) \times\left(\frac{\pi}{2}-zK_0(z)-\frac{\pi}{2}z[L_1(z)K_0(z)+L_0(z)K_1(z)]\right). \tag{8}$$

Here, $n_1=\Delta/|g|$ with g being the density wave coupling constant. Furthermore, $K_n(z)$ and $L_n(z)$ are the modified Bessel function of the second kind and the Struve function. The first two terms in Eq. (7) are the usual CDW charge modulation. In a pure CDW without impurity, ϕ is unrestricted due to incommensurability. However, introducing the perturbing potential, the phase gets pinned to $\phi(U(\mathbf{Q})>0)=0$ or $\phi(U(\mathbf{Q})<0)=\pi$.[7] In either case, $F(z)$ remains the same, and within the CDW coherence length it simplifies to $F(z\ll 1)\approx 2z^{-1}$. Therefore, in this region the Friedel oscillations are precisely those of a metal. At distances much larger than ξ_0, $F(z\gg 1)\approx\sqrt{2\pi}z^{-3/2}e^{-z}$, and exponential decay is obtained in agreement with Ref. 7. Strictly speaking, Eq. (7) is valid only at absolute zero temperature. However, its validity still holds for low temperatures where $\beta\Delta(T)=\xi_1/\xi_0\gg 1$. Indeed, the exponential cutoff ($\sim\exp[-2\pi|x|/\xi_1]$) introduced by finite T clearly has no observable effect as long as $\xi_1\gg\xi_0$. Finite interchain coupling t_b results in a quasi-one-dimensional CDW structure. Its effect coincides exactly with that found for normal metal because of the same factors of Bessel functions appearing in Eqs. (6) and (7).

Now, we finally turn our attention to UDW. We have just seen during the calculation of the CDW response that within ξ_0 the metallic result applies. This is because at such distances only high-energy electron-hole pair excitations contribute to density oscillations, and far from the Fermi energy a fully gapped CDW behaves the same as a normal metal. This latter statement is equally true for an UDW as well. Therefore, we conclude that in UDW ground state within the coherence length, the density oscillations are the same as that of a normal metal given by the zero-temperature limit of Eq. (6). Note here that in UDW due to the vanishing average of the gap over the Fermi surface, the anomalous contribution to the total density due to the condensate is missing, $n_1=0$. On the other hand, at large distances nodal excitations dominate the static charge response. To make the picture whole, for $|x|\gg\xi_0$ asymptotic expansion to leading order yields

$$n(x,m)-n_0=n_0N_0U(\mathbf{Q})(-1)^m\left[\sin^2\left(\frac{2x}{\xi}-\frac{\pi}{2}m\right)\times\frac{\cos(2k_Fx+2\phi)}{2k_F\xi_0}\frac{2m^2}{z(2z^2+m^2)^2}-\cos^2\left(\frac{2x}{\xi}-\frac{\pi}{2}m\right)\frac{\cos(2k_Fx)}{2k_F\xi_0}\frac{4z}{(2z^2+m^2)^2}\right], \tag{9}$$

where $z=|x|/\xi_0$. It certifies our expectations about the power-law decay ($\sim r^{-3}$) at large distances. At finite T, charge response is affected only at distances $|x|\gg\xi_1$, where the factor $\exp[-2\pi|x|/\xi_1]$ becomes dominant. However, as long as $\beta\Delta(T)=\xi_1/\xi_0\gg 1$, the power-law behavior can, in principle, be observed in the range $\xi_0\ll|x|\ll\xi_1$. In Fig. 3, the density oscillations along the chain $m=0$ are compared in a CDW and an UDW. Beyond the coherence length, the CDW response is hardly observable while it is considerably larger in UDW. Furthermore, the aforementioned beat due to finite interchain coupling can be clearly seen in the latter case too. This complex behavior signals the presence of the nodal density wave and seems to be more accessible in experiments than the detection of an exponential decay of CDW. In the latter case, clear CDW background is present too, that is certainly measurable by other means. In UDW candidates, however, measuring Friedel oscillations (for example, in STM measurements) might serve as a useful tool in identifying the low-temperature phase and to reveal hidden order.

We have studied the effect of a single nonmagnetic impurity in quasi-one-dimensional unconventional density wave. We found double peaked quasiparticle resonance in the pseudogap that follows from the generalization to different scattering amplitudes. The energies and lifetimes are found to be the same as those of dDW or dSC. Both the static charge response and STM images along neighboring chains reflect the quasi-one-dimensional nature of UDW: a unique beat property in real space was obtained, which is related to finite interchain coupling. Robust Friedel oscillations of a normal metal show up below the coherence length. On the other hand, contrary to the exponential decay of fully gapped CDW, beyond the coherence length power-law behavior was anticipated and found. This algebraic behavior at large distances signals the presence of nodal density wave and could be accessible in STM experiments.

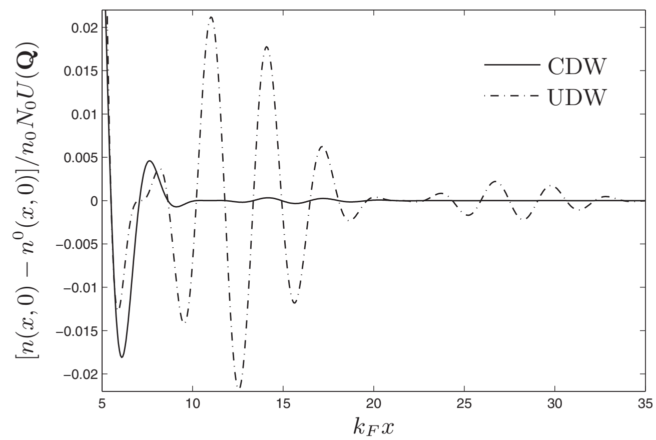

FIG. 3. The impurity induced electronic density is shown for a conventional CDW (solid) and an UDW (dashed-dotted) on the $m=0$ chain. It is calculated from Eqs. (7) and (9). For plotting, $k_F\xi_0=k_F\xi=10$ was applied and $n^0(x,0)$ denotes the unperturbed density without impurity. The CDW response freezes out exponentially at large distances. The UDW contribution, on the other hand, is much larger, which leads to the fact that the beat property is well observable too, in the present case with $k_F\lambda\approx\pi k_F\xi/2\approx 15$.

This work was supported by the Hungarian National Research Fund under Grants No. OTKA NDF45172, No. NI70594, No. T046269, and No. TS049881.

*Electronic address: vanyolos@kapica.phy.bme.hu

[1] S. H. Pan, E. W. Hudson, K. M. Lang, H. Eisaki, S. Uchida, and J. C. Davis, Nature (London) **403**, 746 (2000).
[2] E. W. Hudson, S. H. Pan, A. K. Gupta, K. W. Ng, and J. C. Davis, Science **285**, 88 (1999).
[3] A. V. Balatsky, I. Vekhter, and J. X. Zhu, Rev. Mod. Phys. **78**, 373 (2006).
[4] A. V. Balatsky, M. I. Salkola, and A. Rosengren, Phys. Rev. B **51**, 15547 (1995).
[5] H. V. Kruis, I. Martin, and A. V. Balatsky, Phys. Rev. B **64**, 054501 (2001).
[6] H. Shiba, Prog. Theor. Phys. **40**, 435 (1968).
[7] I. Tüttő and A. Zawadowski, Phys. Rev. B **32**, 2449 (1985).
[8] B. Dóra and A. Virosztek, Eur. Phys. J. B **22**, 167 (2001).
[9] B. Dóra, K. Maki, and A. Virosztek, Mod. Phys. Lett. B **18**, 327 (2004).
[10] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001).
[11] D. K. Morr, Phys. Rev. Lett. **89**, 106401 (2002).
[12] B. Dóra, Europhys. Lett. **70**, 362 (2005).
[13] M. I. Salkola, A. V. Balatsky, and D. J. Scalapino, Phys. Rev. Lett. **77**, 1841 (1996).