Mid-gap states in particle-hole pairing systems

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Abstract

Motivated by a recent proposal for the pseudogap phase in underdoped cuprate superconductors, we examine the normal-metal–*d*-density-wave (DDW) junctions. It is shown that the electronic structure of the DDW state in semi-infinite plane can be investigated within a more general 1D particle-hole pairing system, and furthermore the existence of the mid-gap state is determined by the number of zeros of the corresponding bulk Green's function.

Key words: *d*-density wave; mid-gap states; zero-bias conductance peak; Keldysh-Green's function

It is observed in experiments that there are signatures of a "partial" gap well above the superconducting temperature T_c in underdoped cuprate superconductors. This anomalous regime in the phase diagram of the cuprate superconductors is termed the pseudogap phase[1]. Experiments also find that the pseudogap is consistent with a *d*-wave structure. Recently Chakravarty et al. proposed that the pseudogap phase of the underdoped cuprate is possibly the *d*-density-wave (DDW) state.[2] It is therefore of interest to examine the possible signatures for such states in experiments.

The *d*-wave-like structure of DDW prompts the question as to the existence of zero-bias conductance peak (ZBCP), well-known in the metal-*d*-wave superconductor (ND) junction[3], in tunneling measurements. It has been realized that the ZBCP in ND junctions originates from the mid-gap states that arise at certain interface orientations. It is usually analyzed in the mean-field level applying the Bogoliubov de Gennes equations. While this approach has provided many useful insights to the problem, it is however specifically designed for studying ND junctions. We have developed a different approach based on the non-equilibrium Keldysh-Green's function formalism which enables one to construct systematically higher order corrections from the mean-field lattice Green's functions[4–6]. The merit of this approach is that it allows us to deal with the mid-gap states in other systems in a unified fashion. In this paper, we shall apply it to analyzing the mid-gap states in systems which exhibit particle-hole pairing; an example will be the DDW state in (110) direction.

Considering a junction consisting of a 2D normal metal on the left (L) hand side ($-\infty < x \leq -a$, a is the lattice constant of the metal side) and a state X ($0 \leq x < \infty$) to be probed on the right (R) hand side. Each side is governed by the Hamiltonian H_L and H_R, respectively. The tunneling Hamiltonian connects the interface points at $x = -a$ and $x = 0$, and is given by $H_T = \sum_y t(|y_L - y_R|)(c_L^\dagger c_R + c_R^\dagger c_L)$, where the summation is over lattice points along the interface, which is chosen as the y direction. For definiteness, we take the left hand side a square lattice; other types of lattice can also be considered in our formulation. The total grand Hamiltonian is then given by $K = H_L - \mu_L N_L + H_R - \mu_R N_R + H_T \equiv K_0 + H_T$. Here μ_L and μ_R are the chemical potentials and their difference $\mu_L - \mu_R$ is fixed to be the voltage drop eV across the junction. In the non-equilibrium Keldysh-Green's function formalism, H_T is adiabatically turned on[4,6]. As a result, in the lowest order, one obtains that the differential conductance is proportional to the local density of states at $x = 0$

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$$\mathrm{d}I/\mathrm{d}V \propto -\sum_{y,y'} \mathrm{Im}\{\bar{G}(\mathbf{r},\mathbf{r}',eV)\}\Big|_{x=x'=0}, \qquad (1)$$

where $\bar{G}(\mathbf{r},\mathbf{r}',eV)$ is the half-space Green's function of the state X defined only on a half plane. Note that in the zeroth order of H_T, the two half-spaces are disconnected, hence $\bar{G}(\mathbf{r},\mathbf{r}',eV)$ has to vanish near the boundary. In the simplest case, $\bar{G}$ has to vanish at the hard wall $x=-a$ [5]. To impose the boundary condition, a Fourier transform in the y direction is performed first. For each k_y, the problem is then reduced to one dimension (1D), and the hard wall becomes a point. Eq.(1) thus becomes

$$\mathrm{d}I/\mathrm{d}V \propto -\sum_{k_y} \mathrm{Im}\{g(x=0,x'=0,k_y,eV)\} \qquad (2)$$

with $g(x,x',k_y,eV)$ being the half-space Green's function of the reduced 1D Hamiltonian. The most general form of this 1D Hamiltonian is (with n sites per unit cell)

$$H_R = -\sum_{i=1}^{\infty} \big[t_1 (c_i^{A_1})^\dagger c_{i+1}^{A_2} + t_2 (c_{i+1}^{A_2})^\dagger c_{i+2}^{A_3} + \cdots + t_n (c_{i+n-1}^{A_n})^\dagger c_{i+n}^{A_1}\big] + h.c. \qquad (3)$$

Here A_1 ($i=1$) is the boundary point $x=0$, t_i depends on k_y; we will consider half-filled configurations where $\mu_R = 0$. For DDW in (110) direction, only t_1 and t_2 are needed. We find $t_{1,2} = 2(\chi_R \cos k_y a/\sqrt{2} \mp \chi_I \sin k_y a/\sqrt{2})$ with $\chi_R + i\chi_I$ being the hopping amplitude over the bond. To make g vanishes at $x=-a$, we construct $g(x=0,x'=0,k_y,eV) \equiv g(V) = G(0,0) - G(0,-2a)G^{-1}(-a,-2a)G(-a,0)$, where G is the bulk Green's function (with k_y and eV dependence suppressed)[5]. It is clear that whenever the bulk Green's function $G(-a,-2a)$ has zeros, there will be poles in $g(V)$ which appear as peaks in the $\mathrm{d}I/\mathrm{d}V$ curve. Since, in general, $g(x,x',k_y,eV)$ can be expressed as eigenfunction expansions $g = \sum_n \phi_n^*(x)\phi_n(x')/(eV-E_n)$, any extended state will have vanishing contribution at the interface due to the normalization factor $1/\sqrt{\text{volume}}$; the states corresponding to the conductance peak must be localized surface states. Furthermore, because there is no degeneracy for any bound states in 1D systems, only one state corresponds to each conductance peak.

The bulk Green's function can be obtained by first expressing Eq.(3) in the Fourier space, resulting in an $n \times n$ Hamiltonian h_k. The retarded Green's function is then the Fourier transform of $(\omega + i\eta - h_k)^{-1}$. At $\omega = 0$, the Fourier integral can be evaluated analytically by substituting $z = \exp(inka)$ and performing contour integration. For the case $n=2$ and $t_1 < t_2$, the Green's function has anomalous behavior: starting from any point over the A_2 sublattice, the electron only propagates to the right with decaying length $\frac{\ln t_2/t_1}{2}$. As a result, $G(-a,-2a)$ has a zero at $\omega=0$ for $t_1 < t_2$, leading to a peak at $eV=0$. For finite μ_R, $\omega=0$ is shifted to $\omega=\mu_R$ so that the peak shifts to $eV=\mu_R$. The condition $t_1 < t_2$ determines the range of k_y where the mid-gap peak in the DDW state arises. As mentioned, this peak would correspond to a localized surface state. In the $n=2$ case, the wavefunction can be easily constructed. We find that $\Psi \approx (1,0,-\epsilon,0,\epsilon^2,0,-\epsilon^3,0,\cdots)$ with $\epsilon \equiv t_1/t_2$. The condition $t_1 < t_2$ is thus connected with the decay of the wavefunction away from the surface.

For general n with $\mu_R = 0$, the bulk energy dispersion consists of n energy bands. If n is odd, the middle band crosses the zero energy; therefore, there is no mid-gap state at $\omega=0$. Indeed, because at $\omega=0$ one finds that $G(-a,-2a) \approx \oint_{|z|=1} z/[z^2+1-i\eta \mathrm{sgn}(t_1 t_2 \cdots t_n)]\, dz$ always has poles inside $|z|=1$, so that $G(-a,-2a) \neq 0$; hence there is no mid-gap state at $\omega=0$. Similarly, for even n, we obtain that at $\omega=0$, $G(-a,-2a) \approx \oint_{|z|=1} 1/[z \pm t_2 t_4 t_6 \cdots / t_1 t_3 t_5 \cdots]\, dz$, which vanishes when $|t_2 t_4 t_6 \cdots / t_1 t_3 t_5 \cdots| > 1$. Therefore, mid-gap states at $\omega=0$ exist for even n under the condition $|t_2 t_4 t_6 \cdots| > |t_1 t_3 t_5 \cdots|$. The above only concerns the mid-gap near $\omega=0$. In general, because the energy dispersion consists of n bands, mid-gap states could arise in other gap regimes at finite ω. This indeed happens as one can easily check for a simple example with $n=3$ and $t_1=1$, $t_2=1.5$, and $t_3=2$. In this case, even though there is no mid-gap state at $\omega=0$, at finite $\omega \approx 2.0$, all the poles when calculating $G(-a,-2a)$ lie outside $|z|=1$, resulting in mid-gap states at finite energy.

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