Self-energy of a nodal fermion in a d-wave superconductor.

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We re-consider the self-energy of a nodal (Dirac) fermion in a 2D d-wave superconductor. A conventional belief is that $\text{Im } \Sigma(\omega, T) \sim \max(\omega^3, T^2)$. We show that $\Sigma(\omega, k, T)$ for $k$ along the nodal direction is actually a complex function of $\omega, T$, and the deviation from the mass shell. In particular, the second-order self-energy diverges at a finite $T$ when either $\omega$ or $k - k_F$ vanish. We show that the full summation of infinite diagrammatic series recovers a finite result for $\Sigma$, but the full ARPES spectral function is non-monotonic and has a kink whose location compared to the mass shell differs qualitatively for spin-and charge-mediated interactions.

The physics of nodal quasiparticles in a 2D d-wave superconductor attracted a considerable attention since the early days of high $T_c$ era [1, 2, 3] because of its universality [3] and a relation to field theoretical studies of Dirac fermions [4]. In the normal state of the cuprates, ARPES and other studies have found that the imaginary part of the fermionic self-energy along the nodal direction, $\text{Im } \Sigma(\omega, T)$, is roughly linear in both frequency and temperature [2, 3, 4]. In the superconducting state, a generic belief is that $\text{Im } \Sigma(\omega, T)$ should become smaller as whatever the mechanism is for the quasiparticle scattering in the normal state, it must be weakened in the superconducting state due to the gap opening [3]. Recent ARPES results do show indeed that once bilayer splitting is resolved, the measured $\text{Im } \Sigma(\omega, T)$ decreases below $T_c$ faster than linear [3, 4, 10].

In an s-wave superconductor, $\text{Im } \Sigma(\omega, T)$ at $\omega < 3\Delta$ vanishes at $T = 0$ and is exponentially small at finite $T$ [11]. In a $d_{x^2-y^2}$-superconductor, the gap vanishes along the diagonal directions in the Brillouin zone. Hence the scattering into low-energy states near the nodes gives rise to power-law $\omega$ and $T$ dependences of $\text{Im } \Sigma(\omega, T)$ at the lowest $\omega$ and $T$.

Several groups have previously computed [12, 13, 14] the quasiparticle lifetime of a nodal fermion in a BCS $d$-wave superconductor at $T = 0$ and at $k = k_F$, and found the cubic frequency dependence $\text{Im } \Sigma(\omega, T = 0) \propto \omega^3$. A common belief was that (i) this dependence survives at arbitrary ratio of $\omega$ and $\epsilon_k = v_F(k - k_F)$ along the nodal direction, and (ii) for a clean system, the temperature dependence is the same as the frequency dependence, i.e., $\text{Im } \Sigma(\omega, T)$ scales as $\omega^3$ or $T^2$, whichever is larger.

In the present communication, we dispute this common belief. We show that the perturbative self-energy for a nodal fermion actually scales as $T^{7/2}/\sqrt{\omega}$ at $T >> \omega$ and generic $\omega/\epsilon_k$ and logarithmically diverges at the mass shell, $\omega = \epsilon_k$. This singular behavior has been largely missed in earlier studies (with the exception of [15]), where $T^{7/2}/\sqrt{\omega}$ has been reported. We show that the origin of this singular behavior is the same as of the mass-shell singularity in a 2D Landau Fermi liquid (LFL) [16, 17]. Like in a LFL, the singular behavior of the self-energy for a Dirac fermion is eliminated once infinite series of divergent terms are summed up, but the resulting spectral function has a kink at some finite $\omega - \epsilon_k$. We found that the kink is located at $0 > \omega > \epsilon_k$, or at $0 > \epsilon_k > \omega$ depending on whether the effective interaction is in the spin or in the charge channel. From this perspective, detailed ARPES studies of nodal spectral function can qualitatively distinguish between the theories for the cuprates based on spin or charge fluctuations.

We consider a model of a $d$-wave superconductor with a quasiparticle dispersion $E_k = \sqrt{\epsilon_k^2 + \Delta_F^2} = |k|$, where $k = (v_F k_\perp, v_\Delta k_\parallel)$, and $k_\perp$ and $k_\parallel$ are deviations from the nodal point transverse to and along the Fermi surface, respectively ($\epsilon_k = v_F k_\perp$). The fermion-fermion interaction has both charge and spin components, $U_c(q)$ and $U_s(q)$. We explicitly verified in lengthy calculations that only intra-nodal interactions, governed by $U_c(0)$ and $U_s(0)$ contribute to the self-energy along the nodal direction, and we consider only these terms. Inter-nodal interactions do contribute to the self-energy away from the nodal direction, which we did not consider.

We first re-analyzed the self-energy to the second order in the perturbation. We carried out calculations both in the Nambu formalism and using normal and anomalous Green’s functions, and obtained identical results in both approaches. In the Nambu formalism, the mean field action near a given pair or node at $k_F$ and $-k_F$ is described by the four-component massless Dirac fermions (Nambu spinors) and has the following Lorentz invariant form:

$$\mathcal{L} = i\bar{\psi}(\gamma_0 \partial_\tau + v_F \gamma_1 \partial_x + v_\Delta \gamma_2 \partial_y)\psi$$

where $\psi^+(k) = \left(\psi^+_\uparrow(k), \psi^+_\downarrow(-k), \psi^\downarrow_\uparrow(k), \psi^\downarrow_\downarrow(-k)\right)$, $\bar{\psi} = \psi^+\gamma_0$, $\gamma_0 = I \otimes \sigma^0$, $\gamma_1 = I \otimes \sigma^1$, $\gamma_2 = \sigma^2 \otimes \sigma^2$ and $\sigma^\alpha$ are the Pauli matrices. The free-fermion Green’s function is $G = \langle \psi \bar{\psi} \rangle = \gamma_0 m + p^2/p^2$. The fermion-fermion interaction is the sum of the bilinear products of charge density and spin density operators $\bar{\psi}_\alpha^\dagger \psi_\alpha$ and $\bar{\psi}_\alpha^\dagger \sigma_{\alpha\beta} \psi_\beta$, respectively.
The perturbation theory is constructed in the same way as in LFL.

In the conventional formalism, which we will follow below, the self-energy is obtained by summing up contributions from normal and anomalous Green’s functions of intermediate fermions. The expression for \( \text{Im} \Sigma(\omega, k, T) \) obtained in this formalism is presented in [2, 4]. We verified and confirmed their result. The authors of [2] analyzed the self-energy numerically and argued that it follows \( \max(\omega^3, T^3) \) behavior. We evaluated the self-energy analytically and found new, singular behavior at \( \omega \approx \epsilon_k \) at \( T = 0 \), and at \( \omega, \epsilon_k \ll T \) at a finite \( T \). To understand the origin of the singularity and to establish connection to the earlier work on the mass-shell singularity in LFL, it is convenient to view the self-energy as a convolution of the fermionic and particle-hole propagators:

\[
\text{Im} \Sigma(\omega, k, T) \propto U^2 \int d^2q d\Omega \left( \frac{\Omega}{2T} \coth \frac{\omega + \Omega}{2T} \right) \text{Im} \chi_0(\Omega, q) \text{Im} G_0(\omega + \Omega, k + q)
\]

where \( G_0 \) is the BCS fermionic Green function. In non-Nambu notations, the polarization bubble is the sum of normal and anomalous components, and is given by

\[
\chi_0(\Omega, q) \propto \int d^4l \frac{E_+ + E_-}{E_+ E_-} \left( \frac{q^2}{4} - l^2 + E_+ E_- \right) (E_+ + E_-)^2 - (\Omega + i\delta)^2
\]

where \( E_{\pm} = \left| \pm q/2 \right| \). At small \( \Omega \ll q \), \( \text{Im} \chi_0(\Omega, q) \propto \Omega \), as has already been established before [24]. The convolution of this form with the linear frequency dependence of the fermionic density of states in a \( d \)-wave superconductor gives rise to \( \text{Im} \Sigma(\omega, \epsilon_k, T) \propto (\omega^3) \) at \( \omega \sim T \) and generic \( \epsilon_k/\omega \), in agreement with [3]. The behavior of the self-energy near the mass shell is, however, determined by \( |\Omega| \approx q \), where \( \chi_0(\Omega, q) \) is singular. The singularity originates from the integration in [3] over \( l < q/2 \), and over directions of \( l \) which are nearly parallel to \( q \). In this range, \( E_+ + E_- \approx q \), i.e., the denominator almost vanishes in a finite range of internal \( l \), while the numerator in [3] remains finite. Expanding \( E_+ + E_- \) in the angle \( \theta \) between \( l \) and \( q \) as \( E_+ + E_- \approx q \left[ 1 + i\frac{\theta^2}{(q^2 - 4l^2)} + \ldots \right] \), substituting into [3] and integrating over \( \theta \), we obtain

\[
\chi_0(\Omega, q) \propto A \frac{q^2}{\sqrt{q^2 - (\Omega + i\delta)^2}}
\]

where \( A > 0 \). We see that \( \text{Im} \chi_0(\Omega, q) \) is nonzero when \( |\Omega| > q \), and it diverges at \( |\Omega| \to q \).

Substituting \( \text{Im} \chi_0(\Omega, q) \) and \( \text{Im} G_0(\omega + \Omega, k + q) \propto |\omega + \Omega| \delta(|\omega + \Omega|^2 - (k + q)^2) \) into [2], we find that on the mass shell (i.e., when \( \omega = k \)), the position of the branch cut singularity in \( \text{Im} \chi_0(\Omega, q) \) and the location of the \( \delta \)-function in \( \text{Im} G(\omega + \Omega, k + q) \) coincide provided \( k \) and \( q \) are either parallel (for \( \omega' > 0 \)) or antiparallel (when \( \omega' < 0 \)). Integrating near these directions, we obtain the singular part of the self-energy. At \( T = 0 \), we find that \( \text{Im} \Sigma(\omega, \epsilon_k, T = 0) \) is non-zero only when \( \omega < \epsilon_k \) (in conventional variables where \( E_k = |\epsilon_k| \), and for \( \omega < 0 \), relevant to ARPES experiments), and is discontinuous at \( \omega = \epsilon_k \) (\( \text{Re} \Sigma \) diverges logarithmically at this point).

Explicitly,

\[
\text{Im} \Sigma(\omega \approx \epsilon_k, T = 0) = \frac{2\pi^3}{105} \frac{E_F}{v_F} \frac{v_F^2}{v_D^2} \frac{\omega^3}{E_F^2} \theta(|\omega - |\epsilon_k||)
\]

where \( E_F = v_F k_F/2 \) and \( u_{c,s} = nU_{c,s}(0)/(2\pi) \).

At a finite \( T \), we obtained in three limits:

\[
\text{Im} \Sigma(\omega = 0, k, T) \sim \frac{T^{\frac{7}{2}}}{\sqrt{|\epsilon_k|}}, \quad |\epsilon_k| \ll T,
\]

\[
\text{Im} \Sigma(\omega, k = 0, T) \sim \frac{T^{\frac{7}{2}}}{\sqrt{|\omega|}}, \quad |\omega| \ll T,
\]

\[
\text{Im} \Sigma(\omega \approx \epsilon_k, T) \sim |\omega|^3 \theta(\epsilon_k - |\omega|) + \frac{T^{\frac{3}{2}}}{\sqrt{aT^2 + b\omega^2}} \log \frac{|\epsilon_k|}{|\epsilon_k - \omega|}, \quad |\omega| \approx T.
\]

where \( a, b = O(1) \). We see that at finite \( T \), the second-order self-energy diverges logarithmically on the mass shell, and also diverges as \( 1/\sqrt{|\omega|} \) when both \( \omega \) and \( \epsilon_k \) tend to zero [15]. This result is very different from a simple \( T^3 \) behavior. The latter is only recovered when \( |\omega| \approx T \), and the system is at some distance away from the mass shell.

As we have said, the singularity in the self-energy for a Dirac fermion is similar to the mass-shell singularity in the fermionic self-energy a 2D LFL [16, 17]. In both cases, the singularity originates from the fact that the pole in the fermionic Green’s function almost coincides with the branch-cut in the polarization bubble [17]. There exists, however, an important distinction between the two cases, which makes the singularity for Dirac fermions stronger than in a Fermi liquid. In a liquid, the quasiparticle dispersion changes sign at the Fermi surface, i.e., \( \epsilon_{k_F+q} = q \cos \theta \) can be both positive and negative. Accordingly, \( \text{Im} \Sigma(\omega, T) \propto \int d^2q d\delta d\omega' q \delta(\omega' + (\omega - k) - q \cos \theta)/\sqrt{(\omega')^2 - q^2} \) and the angular integration reduces the \( \delta \) function to another square-root, so that the subsequent momentum integral only logarithmically depends on the \( \omega - k \), i.e., on the distance from the mass shell. For Dirac fermions, the dispersion \( E_k = |k| \) is \textit{positive}, and \( E_{k_F+q} \propto |q| \gg 0 \). The angle integral still accounts for the logarithmic singularity at \( \omega = E_k \), but in addition, the combination of the \( \delta \) function from the fermionic propagator and the square-root singularity in the polarization operator gives rise to the extra \( (T/|\omega|)^{3/2} \) factor in the self-energy.
The discontinuity of the self-energy on the mass shell at $T = 0$ and the divergence at $T > 0$ imply that higher-order diagrams for the self-energy may also be relevant. Evaluating higher-order self-energy diagrams with extra particle-hole bubbles, we find that they actually diverge at the mass shell already at $T = 0$, and the divergences proliferate with the order of perturbation. Like in a LFL, the most divergent diagrams form ladder (RPA) series \[ \Sigma^{	ext{ch}}(\omega, \mathbf{k}) \] such that the full self-energy can be still represented by Eq. (2), but now $\chi(\Omega, q)$ has to be replaced by the full susceptibility $\chi(\Omega, q)$. This computational procedure is justified when $u_{c,s} \ll 1$.

At this stage, it becomes essential whether the effective interaction is in the charge or in the spin channel, as the RPA renormalizations in charge and spin channels have opposite signs. Summing up the bubble and the ladder diagrams, we obtain the following expressions for the full $\chi_c(\Omega, q)$ and $\chi_s(\Omega, q)$

$$\chi_c(\Omega, q) = \frac{\chi_0(\Omega, q)}{1 + U_c \chi_0(\Omega, q)} \quad \chi_s(\Omega, q) = \frac{\chi_0(\Omega, q)}{1 - U_s \chi_0(\Omega, q)} \tag{7}$$

where $\chi_0(\Omega, q)$ is given by (4) (recall that $U_{c,s} > 0$ and $Re \chi_0(\Omega, q) > 0$). For a charge-mediated interaction, there is no pole outside the particle-hole continuum. Accordingly, the RPA renormalization only eliminates the square-root singularity in $Im \chi(\Omega, q)$ at $\Omega = q$. The full $Im \chi(\Omega, q)$ then behaves as in Fig. 1: it initially follows $Im \chi_0(\Omega, q)$ and increases at approaching $\Omega = q$, but passes through a maximum and vanishes at $\Omega = q$.

For $\chi_s(\Omega, q)$, the sign of the renormalization is different, and the interaction not only eliminates the square-root divergence at $\Omega = q$, but also generates a zero-sound-type pole outside the particle-hole continuum, at $\Omega = q(1 - Bu_c^2 q^2)$, $B \sim 1/k_F^2 > 0$, as on Fig. 1b.

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The different forms of $\chi_c$ and $\chi_s$ lead to different results for the full self-energy. We illustrate this for the $T = 0$ case. For charge-mediated interaction, the softening of the square-root singularity in $\chi_s$ just implies that $Im \Sigma(\omega, k)$ becomes continuous. However, it still vanishes at $0 > \omega > \epsilon_k$. We found

$$Im \Sigma(\omega, k) \propto \left| \omega \right|^3 \theta(\epsilon_k - \omega) f \left( \frac{c^2 u_c^2 \left| \omega \right|^3}{(\epsilon_k - \omega)E_F^2} \right), \tag{8}$$

where $c \sim v_F/\nu_A$, and $f(x)$ subject to $f(0) = 1$ decreases with increasing $x$ and scales as $1/x$ at large $x$. This $1/x$ behavior implies that very near the mass shell, $Im \Sigma(\omega, E_k) \propto (\epsilon_k - \omega) \theta(\epsilon_k - \omega)$. The behavior of the spectral function for this case is shown in Fig. 2a. For experimental comparison, we added a constant impurity scattering. The spectral function is anisotropic with respect to $\omega - \epsilon_k$, and has a kink at $\omega - \epsilon_k \sim u_c^2 \omega^3/E_F^2 < 0$, when the renormalization of the susceptibility becomes relevant.

For a spin-mediated interaction, the situation is different. Due to the presence of the zero-sound pole in $\chi_s(\Omega, q)$, $Im \Sigma(\omega, E_k)$ is non-zero at the mass shell, and only vanishes at $\omega - \epsilon_k > u_c^2 \left| \omega \right|^3/E_F^2 > 0$, when the Cherenkov-type absorption becomes impossible. The spectral function now has the form of Fig. 2b. It again has a kink (more precisely, a square-root non-analyticity), but now the kink is located at $\omega - \epsilon_k > 0$, i.e., on the other side of the mass shell. We see therefore that interactions in the charge or in the spin channel lead to qualitatively different results for the spectral function.

A similar situation holds at a finite $T$. For brevity, we list the results for a charge-mediated interaction, and set $k = k_F$. For the most interesting case $T \gg \left| \omega \right|$, we found that $T^{7/2}/\sqrt{\left| \omega \right|}$ behavior holds down to $\omega \sim \omega_0 = u_c^2 T^3/E_F^2$. Below this scale, $T^{7/2}/\sqrt{\left| \omega \right|}$ behavior crosses over to $\sqrt{T \left| \omega \right|}$. The crossover behavior is somewhat involved, but the two limiting forms of $Im \Sigma$ are captured by a simple extrapolation formula

$$Im \Sigma(\omega, T) \sim u_c \frac{T^2}{E_F} \Psi \left( \frac{\left| \omega \right|}{\omega_0} \right), \quad \Psi(x) = \frac{\sqrt{x}}{x + 1} \tag{9}$$

We display this behavior in Fig. 3. Note that at the maximum, $Im \Sigma(\omega, T)$ scales as $T^2$. This is qualitatively different behavior from $Im \Sigma \propto T^3$, which would be the case if the mass shell singularity didn’t exist.
The unusual behavior of the spectral function has a profound influence on the fermionic density of states $N(\omega) \sim \int d^2x I_m G(\omega, x)$. In particular, $N(0) \propto T^{7/3}$. It, however, makes little difference for the tunneling density of states $N_{\text{tunn}}(\omega) \propto (1/T) \int d\omega' N'(\omega')/\cosh^2(\omega + \omega')/2T$. The latter one is non-zero already in the non-interacting $d$-wave gas, where $N(\omega) \propto |\omega|$. Then $N_{\text{tunn}}(0) \propto T$. The fermionic self-energy accounts for the corrections to the linear-$T$ behavior. Typical frequencies and $\epsilon_k$ in the integral for $N_{\text{tunn}}(0)$ are of the order of $T$, hence relevant $I_m \Sigma(\omega, k, T)$ are of the order of $T^{7/2}/\sqrt{|\omega|} \sim T^3$. As a result, $N_{\text{tunn}}/T = A + BT^2$ is analytic in $T$.

To summarize, in this communication we reconsidered the self-energy of a nodal fermion in a 2D $d$-wave superconductor. We found that the $I_m \Sigma(\omega, \epsilon_k, T)$ is actually a complex function of $\omega, T$ and the quasi-particle energy $\epsilon_k$, and is qualitatively different from $I_m \Sigma(\omega, T)$, $\Sigma(\omega, \epsilon_k, T)$ suggested on general grounds. We found that the perturbative self-energy is non-analytic near the mass shell at $T = 0$. At a finite $T$, it diverges as $T^{7/2}/\sqrt{|\omega|}$, when $\omega$ tends to zero, and diverges even stronger near the mass shell. We demonstrated that the divergences in the self-energy for Dirac fermions originate from the same physics as the mass shell singularity in a 2D Landau Fermi liquid. We further demonstrated that the full summation of infinite diagrammatic series eliminates the divergences and makes $I_m \Sigma(\omega, \epsilon_k, T)$ finite, even at $\omega = \epsilon_k$. However, the full $\Sigma(\omega, \epsilon_k, T)$ at a given $T$ is non-monotonic as a function of $\omega$, and at a maximum is of order $T^2$ rather than $T^3$. We also found that the full spectral function has a kink, whose location compared to the mass shell depends on whether the dominant fermion-fermion interaction is in the spin or in charge channel. For negative $\omega$, relevant to ARPES experiments, kink is located at $\omega - \epsilon_k > 0$ for spin-mediated interaction, and at $\omega - \epsilon_k < 0$ for charge-mediated interaction. We hope that careful ARPES studies of the nodal spectral function in high $T_c$ materials below $T_c$ will be able to distinguish between charge and spin-mediated interactions.

The doping dependence of the kink strength may also provide the information about the interaction. Singular self-energy along the nodal direction is determined by intra-nodal scattering, and the magnitude of the effect is determined by $U(q = 0)$. This interaction is not enhanced if lowering the doping drives the system closer to an instability at a finite $q$ (e.g., an antiferromagnetic instability). On the other hand, if the system evolution towards half-filling is governed by low-energy fluctuations at small $q$, one should expect a strong enhancement of the kink strength at smaller doping.

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