Pseudogap effects induced by resonant pair scattering

Boldizsári Jankó, Jiri Maly and K. Levin

The James Franck Institute, The University of Chicago, 5640 S. Ellis Avenue, Chicago IL 60637

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We demonstrate how resonant pair scattering of correlated electrons above \( T_c \) can give rise to pseudogap behavior. This resonance in the scattering T-matrix appears for superconducting interactions of intermediate strength, within the framework of a simple fermionic model. It is associated with a splitting of the single peak in the spectral function into a pair of peaks separated by an energy gap. Our physical picture is contrasted with that derived from other T-matrix schemes, with superconducting fluctuation effects, and with preformed pair (boson-fermion) models. Implications for photoemission and tunneling experiments in the cuprates are discussed.

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Effects it was shown [15] that the fluctuation gap above applied to conventional superconducting fluctuation effects tend to diminish leading order features [21], it is straightforward to demonstrate using the more general criteria introduced by Kadanoff and Baym [20] that this theory preserves all conservation laws.

It has been shown that the results of the full “mode-coupling” scheme of Fig. 1(a) are qualitatively captured by the lowest order conserving approximation of Fig. 1(b) [18]; this approximation, nevertheless, goes beyond the original work of Nozières and Schmitt-Rink. Unlike other T-matrix approaches, where higher order self-consistency effects tend to diminish leading order features [2], it is found [18] that within the present framework the inclusion of “mode-coupling” effects amplify these first order (pseudogap) features. For simplicity, we, therefore, focus on the lowest order approximation. The discussion of feedback effects is deferred to a future publication.

In our scenario the physical process which generates the pseudogap is resonant pair scattering (above \( T_c \)), arising from the condition that the real part of the inverse T-matrix, \( \text{Re} [T_{q=0}^{-1} (\Omega)] \), is sufficiently small. This resonant behavior is manifested as a sharp peak in \( \text{Im} [T_{q=0}^{-1} (\Omega)] \). This peak is in turn reflected in the electronic self-energy and the spectral function. The pair resonance condition is illustrated in the insets of Fig. 2, where the behavior of \( \text{Re} [T_{q=0}^{-1} (\Omega)] \), as a function of frequency is contrasted for weak \( (g/g_c < 1) \) (2a) and intermediate \( (g/g_c \approx 1) \) (2b) couplings. Each series of curves corresponds to varying temperature. The dashed lines indicate the form of \( \text{Im} [T_{q=0}^{-1} (\Omega)] \) at \( T_c \) in each of the two cases. The critical value \( g_c \) establishes the approximate dividing point between resonant and non-resonant scattering. As can be seen, there is a finite frequency zero crossing of \( \text{Re} [T_{q=0}^{-1} (\Omega)] \) for \( T > T_c \), corresponding to resonant scattering, only in the stronger coupling limit. The resonance energy increases as a function of temperature \( T \) and \( q \) until it disappears at a cross-over wave vector \( q^* \) or temperature \( T^* \).
The associated spectral functions \( A_k(\omega) \) for each of the two cases considered in the insets are numerically computed from the self-energy using Eq. (2) and plotted for the case \( k = k_F \) in the main portion of Fig. 3 as a function of \( \omega \), for varying \( T \). (Throughout the unit of energy is \( E_F \).) Although the numerical integrations involved are computationally intensive, the integrated spectral weight is unity to several significant digits for each spectral curve presented. In the stronger coupling limit and at sufficiently low \( T \) (Fig. 3(b)), the two peaked structure characteristic of a pseudogap appears and becomes more pronounced with larger \( g/g_c \). In the more weakly coupled limit (\( g/g_c = 0.6 \)), the single peak behavior characteristic of a normal Fermi liquid is recovered, as shown in Fig. 3(a). In general, the two peaked structure correlates with the presence of a resonance in the \( T \)-matrix. For \( g \) slightly greater than \( g_c \), the two maxima are resolvable up to \( T^* \) of the order of several \( T_c \).

An intuitive understanding of the splitting of the spectral peak into a pair of asymmetrically broadened peaks may be gained by examining the imaginary part of the self-energy. On the real frequency axis \( (i\zeta \rightarrow \omega + i\delta) \), \( \text{Im} [\Sigma_k(\omega)] \) is given by

\[
\text{Im} [\Sigma_k(\omega)] = -\sum_q \frac{\varphi_k^2}{q^2} \text{Im} [T_q(\omega + \epsilon_q - k)] \times \left[ f(\epsilon_q - k) + n(\omega + \epsilon_q - k) \right],
\]

(4)

where \( f(x), n(x) = (e^{x\gamma} + 1)^{-1} \). For intermediate coupling strengths, a resonance condition leads to a peak in \( \text{Im} [T_q(\Omega)] \) at small frequencies and momenta, which in turn yields a maximum in \( -\text{Im} [\Sigma_k(\omega)] \) at \( \omega + \epsilon_k \approx 0 \) (see the inset of Fig. 3(b)). The frequency weight under this peak is written as \( \pi |\Delta|^2 \varphi_k^2 \), where \( |\Delta| \) can be viewed as the pseudogap energy. This peak in \( -\text{Im} [\Sigma_k(\omega)] \) implies via the Kramers–Kronig relation – a corresponding resonance structure in \( \text{Re} [\Sigma_k(\omega)] \) at the same frequency \( \omega \approx -\epsilon_k \). In this way \( A_k(\omega) \) acquires two peaks separated by \( 2|\Delta|\varphi_k \) with

\[
|\Delta|^2 \approx \sum_q \int_{-\infty}^{+\infty} \frac{d\Omega}{\pi} n(\Omega) \text{Im} [T_q(\Omega)].
\]

(5)

The asymmetric broadening \( \Delta \) of the two spectral peaks is a generic feature of our results and is due to the interaction of correlated pairs with the Fermi sea. This asymmetry, which is contained in Eq. 3, reflects in \( \text{Im} [T_q(\Omega)] \), as a function of \( \Omega \). In Fig. 3 we plot the momentum dependence of the spectral function slightly above \( T_c \) for weak (3a) and intermediate (3b) coupling, along with typical self-energies shown in the insets. The former case shows the single peak structure which evolves with \( k \) in a fashion characteristic of a finite temperature Fermi liquid \( \Delta \). In the stronger coupling limit (Fig. 3b) the spectral weight shifts from the negative to the positive frequency peak as the momentum vector \( \mathbf{k} \) passes through the Fermi surface. Close to the Fermi momentum the peaks disperse roughly as \( E_k \sim \pm \sqrt{\epsilon_k^2 + |\Delta|^2 \varphi_k^2} \).

This dispersion provides a predictive signature for future ARPES measurements, within the precursor superconductivity scenario. Indeed, this behavior is reminiscent of the particle-hole mixing found in photoemission measurements on the superconducting state \( \Delta \).

Finally, the density of states, \( N(\omega) \), is plotted in Fig. 4 as a function of energy. This quantity may be directly related to tunneling as well as to thermodynamic measurements in the pseudogap regime. The asymmetry in the curves reflects, in part, the asymmetry of the spectral functions seen in Fig. 3(a) and 3(b). For clarity the results are represented by subtracting the “normal” state curve, obtained, for definiteness, in the very weak coupling limit. Fig. 4(a) indicates the coupling constant dependence of \( N(\omega) \) and Fig. 4(b) the corresponding temperature dependence for fixed \( g \). A depression in \( N(\omega) \) – which increases with \( g \) – develops at smaller couplings, and persists to higher temperatures, than do pseudogap effects in the spectral function (see Fig. 3).

In summary, we have demonstrated how resonant pair scattering above \( T_c \) gives rise to a splitting of the spectral function, \( A_k(\omega) \), as well as a density of states depression. Experimental observation of the former is the more significant manifestation of pseudogap behavior, providing...
strong constraints on theoretical models. Our precursor superconductivity scenario has predictive signatures: an asymmetry in the widths of the two spectral peaks and a $k$-dependent dispersion of the $T > T_c$ spectral function, qualitatively similar to that of the BCS state. A\[ d_{x^2-y^2} \] symmetry of the normal state gap will arise naturally in the present scenario, for a $d$-wave superconducting instability. This would be accompanied by a spectral peak broadening proportional to $(\cos k_x - \cos k_y)^2$. The present picture should be differentiated from preformed pair models: the correlated pairs of our picture have significant spatial extent and fail to obey Bose statistics. Furthermore, in contrast to the stripe picture of Emery and Kivelson, the amplitude and phase of this paired state is never established beyond the dimensions of a single pair. Quasi two dimensionality will enhance our pseudogap effects, which should, then, become more pronounced as the insulator is approached. Magnetic correlations may, also, ultimately play a role in the extreme underdoped regime. Nevertheless, short coherence lengths and quasi 2d features suggest that precursor superconductivity is present to some degree and must necessarily be calibrated in order to obtain a full understanding of the cuprate pseudogap.

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[17] During numerical evaluations we neglect the $f(q-k)$ in this equation, since it is insignificant in generating the pseudogap. However, this approximation overestimates the particle-hole asymmetry in spectral properties. Small variations in $\mu$ with $T$, were also neglected to avoid numerical complexity.
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