Pseudogaps: A third peak in the fermion spectral function.

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Abstract

I present an exactly solvable model of a pseudogap with two zero-energy fermion modes coupled to each other by a classical source of frequency \( \omega_0 \) and strength \( |\Delta| \). A suitably defined fermion propagator has an infinite number of poles at frequencies that are multiple integers of \( \omega_0 \). In the adiabatic limit, \( \omega_0 \ll |\Delta| \), the situation is *qualitatively* different from the static case \( \omega_0 = 0 \): the residue of the pole at \( \omega = 0 \) (a remnant of the bare fermion) vanishes linearly with \( \omega_0 \), a result that could not be anticipated by perturbation theory; the multiple poles of the propagator coalesce into a continuum instead of forming two single poles at \( \pm|\Delta| \), which should be interpreted as inhomogeneous broadening of the Bogoliubov quasiparticles.
The notion of a pseudogap is relevant to physics of fermionic systems with slowly fluctuating excitations of the Bose type. In a state with long-range order, fermions are strongly scattered by a condensate of these excitations, which splits the Landau quasiparticle peak into two and thus creates a gap in the fermion energy spectrum. In the disordered state, slow fluctuations can produce a qualitatively similar effect. Underdoped cuprate superconductors offer an example of such behavior. Without carrier doping, the cuprates are antiferromagnetic (AFM) insulators. Although hole doping destroys the AFM long-range order, slow spin fluctuations create a remnant of the Mott-Hubbard energy gap (a few tenths of an electronvolt [1]). There is very little spectral weight at lower energies, which makes these materials rather poor conductors.

By using a low-level approximation to estimate the fermion self-energy (a bare intermediate fermion and a reasonably guessed particle-particle susceptibility), Kampf and Schrieffer [2] have found an interesting feature in the fermion spectral function in a pseudogap regime. In addition to two peaks at energies $\pm \tilde{\epsilon}_k \equiv \pm \sqrt{\epsilon_k^2 + |\Delta|^2}$ (as expected in the ordered state), they found a small third peak at the old location $\epsilon_k$, a remnant of the Fermi-liquid state. As the fluctuations slow down, the third peak gradually disappears. If true, this finding could give an insight into the formation of coherent spectral features (i.e., fermionic quasiparticles) in the cuprates upon doping.

Deisz, Hess, and Serene [3] have attempted to verify these results in the conserving FLEX approximation [4] and found no midgap peak. In our opinion, this negative result is related to a particular form of the self-consistently calculated spin susceptibility: while in [2] it was assumed that magnons have a typical real frequency $\omega_0$, the self-consistently calculated susceptibility [3] clearly has a diffusing form. Whether or not propagating magnons can exist in the pseudogap regime is certainly an open question. Even if they can, it is far from clear whether the midgap band is a robust feature or an artifact of a low-level approximation.

With this in mind, I have studied a toy model which contains the essential features of the Kampf–Schrieffer theory, yet permits an exact solution. Basing on the results obtained within this model, one can make the following conclusions.

(a) The approximation of Kampf and Schrieffer gives reliable results in the limit of fast fluctuations $\omega_0/|\Delta| \gg 1$, which corresponds to a Fermi-liquid state.

(b) The quasiparticle peak at $\omega = 0$ persists well into the pseudogap state ($\omega_0/|\Delta| \ll 1$). Its spectral weight vanishes as $\omega_0/|\Delta|$, which is a non-perturbative result.

(c) In the adiabatic limit $\omega_0 \to 0$, the two quasiparticle peaks at $\pm \tilde{\epsilon}_k$ are strongly broadened. Broken ergodicity is necessary to restore their sharpness.

(d) When the energies of the coupled fermion modes are not equal, the spectral function in the adiabatic limit is a continuum with three peaks, none of which is a pole of the fermion propagator.

The toy model is defined as follows. Two fermion modes $a_1$ and $a_2$ interact with each other via a classical, time-dependent external source whose frequency equals $\omega_0$; the Hamiltonian of this system is

$$H = (\Delta a_1^\dagger a_2 + \Delta^* a_2^\dagger a_1) \cos \omega_0 t. \quad (1)$$

By an appropriate unitary transformation, $\Delta$ can always be made positive, $\Delta = \Delta^* = |\Delta|$. It should be noted that a similar model of two fermion modes interacting with a single (quantum) boson mode of frequency $\omega_0$ has been considered by Schrieffer [5].
If the external source is static, $\omega_0 = 0$, the Hamiltonian is readily diagonalized: there are two eigenmodes $a_\pm \equiv (a_1 \pm a_2)/\sqrt{2}$ with energies $\mp|\Delta|$. When $\omega_0 \neq 0$, symmetry with respect to time translations is broken and the time-ordered propagator matrix $G_{\alpha\beta}(t,t') = -i\langle \psi|T[a_\alpha(t)a_\beta^\dagger(t')]|\psi \rangle$ becomes a function of two time variables. In order to restore this symmetry (and conservation of energy with it), I perform translations $t \to t + \tau$, $t' \to t' + \tau$ and average $G(t + \tau, t' + \tau)$ with respect to $\tau$. This process is similar to restoring translational invariance in the impurity problem by averaging over impurity positions throughout the crystal. The resulting propagator

$$\overline{G}(t-t') = \langle G(t + \tau, t' + \tau) \rangle_{\tau}$$

(2)
is a function of $t - t'$ only. Treating $H$ as a perturbation, one can write out a series for $G(t,t')$ by iterating the matrix Dyson equation

$$G(t,t') = G^{(0)}(t - t') + |\Delta| \int dt'' G^{(0)}(t - t'') \sigma_1 \cos \omega_0 t'' G(t'', t').$$

Upon averaging over time shifts, diagrams with an odd number of cosine factors vanish, making the series for $\overline{G}$ diagonal (this would not be so in the static case):

$$\overline{G}(t-t') = G^{(0)}(t-t')$$

$$+ \frac{|\Delta|^2}{2} \int dt_1 dt_2 G^{(0)}(t-t_2) G^{(0)}(t_2-t_1) \cos \omega_0 (t_2-t_1) G^{(0)}(t_1-t')$$

$$+ \ldots$$

(3)

A generic term of the perturbation series for $\overline{G}$ can be readily written out, most easily for the Fourier transform of $\overline{G}$ $\overline{G}(\omega)$ — see Fig. 11. Note that the effective coupling constant is $g \equiv |\Delta|^2/4$.

To second order in $|\Delta|$, the self-energy is

$$\Sigma^{(2)}(\omega) = \frac{|\Delta|^2}{4(\omega - \omega_0)} + \frac{|\Delta|^2}{4(\omega + \omega_0)} = \frac{|\Delta|^2}{2(\omega^2 - \omega_0^2)} \omega.$$  

It is similar to $\Sigma$ of Kampf and Schrieffer in that it vanishes with a negative slope at $\omega = 0$. Therefore, to this order, $\overline{G}(\omega) = 1/[\omega - \Sigma(\omega)]$ has three poles, at $\omega = \pm \sqrt{\omega_0^2 + |\Delta|^2/2}$ and at $\omega = 0$, the latter with the residue

$$z_0 = \frac{\omega_0^2}{\omega_0^2 + |\Delta|^2/2},$$

(4)

which apparently vanishes as $2\omega_0^2/|\Delta|^2$ in the limit of slow fluctuations. Simultaneously, the other two poles are approaching $\pm |\Delta|/\sqrt{2}$ and their residues tend to 1/2, as in the static case. When fluctuations are fast, the dominant pole is at $\omega = 0$. Thus a picture of a smooth crossover from one to two peaks in the spectral function emerges.

This smoothness is, however, misleading. As has already been noted, there are off-diagonal contributions to the propagator matrix in the static case, but not in the fluctuating case. Therefore, the adiabatic limit ($\omega_0 \to 0$) is not expected to resemble the static situation ($\omega_0 = 0$). In addition, higher powers of $|\Delta|$ in the self-energy can be neglected only when $|\Delta|$
is small, which for low fermion frequencies $\omega$ translates into $|\Delta| \ll \omega_0$. Another indication of a nonperturbative character of the adiabatic limit comes from the exact expression for the residue of the $\omega = 0$ pole obtained below. As $g \equiv |\Delta|^2/4 \to \infty$, the behavior of $z_0$ is nonanalytic: $z_0 \sim \text{const} g^{-1/2}$.

**Exact solution.** By making a unitary transformation, the Hamiltonian (1) can be diagonalized (in the same way as in the $\omega = 0$ case):

$$H = |\Delta| \cos \omega_0 t \left( a_+^\dagger a_- - a_-^\dagger a_+ \right).$$

Time dependence of the annihilation operators is given by

$$a_\pm(t) = a_\pm(0) \exp \left( \pm i \frac{|\Delta|}{\omega_0} \sin \omega_0 t \right).$$

After choosing a state vector $|\psi\rangle$, one can immediately write down the propagator $G(t,t')$. A particular choice of $|\psi\rangle$ does not affect the form of $G(\omega)$ but rather determines the integration path in the complex plane of $\omega$. If we select the state annihilated by $a_-$ and $a_+^\dagger$,

$$G_\pm(t,t') = \mp i \exp \left[ \pm i \frac{|\Delta|}{\omega_0} (\sin \omega_0 t - \sin \omega_0 t') \right] \theta(\pm t \mp t')$$

and, after averaging over time shifts,

$$\langle G_\pm(t) = \mp i J_0 \left( \frac{2|\Delta|}{\omega_0} \sin \frac{\omega_0 t}{2} \right) \theta(\pm t),$$

where $J_0(x)$ is a Bessel function. Note that $G(t,t')$ and $\langle t - t' \rangle$ behave differently in the limit $\omega_0 \to 0$. Without averaging, fermions $a_\pm$ have well-defined energies in this limit. By averaging over time, we force them to slowly sample the whole range of energies between $-|\Delta|$ and $|\Delta|$. Evidently, this would take an infinite amount of time as $\omega_0 \to 0$.

The Fourier transform $\mathcal{G}(\omega)$ can now be readily determined. In the limit $\omega_0 \to 0$, $\mathcal{G}(\omega) \to 1/\sqrt{\omega^2 - |\Delta|^2}$ with all of the spectral weight

$$\mathcal{A}(\omega) \to \mathcal{A}_0(\omega) \equiv \frac{1}{\pi \sqrt{|\Delta|^2 - \omega^2}}$$

concentrated between $-|\Delta|$ and $|\Delta|$. This result can be simply understood. On a time scale less than $1/\omega_0$, each individual fermion has a well-defined frequency $\omega$ equal to the instantaneous amplitude of the external source. Since the latter fluctuates as $|\Delta| \cos \omega_0 t$, the probability density to find a certain strength $\omega$ of this field is given precisely by (5). Thus the density of fermions whose pole is shifted from 0 to $\omega$ is (5). Similar broadening in the limit of slow fluctuations has been discussed in connection with a pairing [6] and Peierls [7] pseudogaps. This simple observation could perhaps vindicate the FLEX approximation in light of its recent criticism [9]: the strong broadening of quasiparticle peaks by slow AFM fluctuations is a natural phenomenon and not an artifact of the FLEX approximation.

When $\omega_0 \neq 0$, the spectral weight of an $a_\pm$ fermion is a superposition of sharp peaks $\mathcal{A}(\omega) = \sum_n z_n \delta(\omega - n\omega_0)$ with residues $z_n = J_n^2(|\Delta|/\omega_0)$. (This result differs markedly from
The spectral weight at $\omega = 0$ is a remnant of the bare fermion. In the fast limit,
\[ z_0 \approx 1 - \frac{|\Delta|^2}{2\omega^2}, \tag{4} \]
which agrees with the perturbative expansion for $z_0$. In the slow limit,
\[ z_0 \approx \omega_0 \left[ 1 + \sin \left( \frac{2|\Delta|}{\omega_0} \right) \right], \tag{5} \]
which certainly does not agree with (4). Apart from the oscillatory part, $z_0$ in this limit can be obtained as the area under the adiabatic density of states (5) between $-\omega_0/2$ and $\omega_0/2$, as illustrated in Fig. 2 (note that chaotic oscillations of the peak heights are absent close to $\omega = \pm|\Delta|$). Thus, unlike the perturbation theory, the picture of adiabatic evolution provides a reasonable description of the system in the limit of slow fluctuations.

**Fermions with nonzero bare energy: adiabatic limit.** When the bare fermion modes $a_{1,2}$ have unequal energies $\epsilon_{1,2} = \pm \epsilon$, the problem does not admit such a simple solution for a finite $\omega_0$ because the Hamiltonian does not commute with itself at different times. However, it is still possible to find the $\tau$-averaged propagator (2) in the adiabatic limit $\omega_0 \to 0$. To do so, we first determine the propagator for a given instantaneous strength of the external source $\delta = |\Delta| \cos \omega_0 t$,
\[ G(\omega, \delta) = \frac{1}{\omega^2 - \epsilon^2 - \delta^2} \left( \omega - \epsilon \frac{\delta}{\omega + \epsilon} \right), \]
and then average it over $\delta$ using the probability density (5). As a result, off-diagonal (anomalous) components $\mathcal{G}_{12}$ and $\mathcal{G}_{21}$ vanish, while
\[ \mathcal{G}_{11}(\omega) = \int_{-|\Delta|}^{\omega_0} \frac{d\delta}{\pi \sqrt{|\Delta|^2 - \delta^2}} \frac{\omega + \epsilon}{\omega^2 - \epsilon^2 - \delta^2} = \sqrt{\frac{\omega + \epsilon}{(\omega - \epsilon)(\omega^2 - \epsilon^2)}}, \]
with a nonzero spectral weight in the two ranges $\epsilon^2 < \omega^2 < \tilde{\epsilon}^2 \equiv \epsilon^2 + |\Delta|^2$:
\[ \mathcal{A}_{11}(\omega) = \frac{1}{\pi} \sqrt{\frac{\omega + \epsilon}{(\omega - \epsilon)(\epsilon^2 - \omega^2)}}. \tag{6} \]
For $\epsilon \neq 0$, there are three peaks in the spectral function, at $\omega = \epsilon$ and $\pm \tilde{\epsilon}$. None of these is a pole of the propagator, but rather an inverse square-root branch point. In the limit $\epsilon \gg |\Delta|$, the cut near $\epsilon$ evolves into a simple pole, while the other cut vanishes (Fig. 3).

At zero temperature, the occupation number of a fermion mode with bare energy $\epsilon$ is
\[ n(\epsilon) = \int_{-\infty}^{0} \mathcal{A}_{11}(\omega) d\omega = 1/2 - (\epsilon/\pi \tilde{\epsilon}) K'(\epsilon/\tilde{\epsilon}), \]
where $K'(k)$ is a complete elliptic integral of the first kind. There is no discontinuity as $\epsilon$ crosses zero, although the slope of $n(\epsilon)$ diverges logarithmically as $\epsilon \to 0$. Assuming a constant bare density of fermion states (DOS), it is also possible to obtain the DOS in the adiabatic limit by integrating (6) over $\epsilon$. The resulting DOS is identical to that of a pure $d$-wave superconductor, it vanishes linearly with $\omega$ in the middle of the pseudogap and diverges logarithmically at its edges.
The simple model considered in this note indicates that the midgap band of Kampf and Shrieffer may in fact be inseparable from the two bands above and below the pseudogap. This effect can be ascribed to the fluctuations of the gap amplitude in this model. Calculations of the FLEX type inevitably contain such fluctuations (see, e.g., [6]) and therefore do not lead to a sharp energy gap. In principle, this adiabatic broadening of the quasiparticle peaks can be lifted if the observation time is shorter than the inverse frequency of the fluctuations $1/\omega_0$ (but still longer than $1/|\Delta|$). If fluctuations can also propagate in space, one has to limit observations to a spatial area without significant retardation. Given the speed of the propagating fluctuations $s$, the size of such an area should not exceed $s/\omega_0$.

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FIGURES

FIG. 1. Feynman diagrams for $\overline{G}(\omega)$ through second order in the coupling constant $g \equiv |\Delta|^2/4$. Broken lines: $|\Delta|/2$. Solid lines: bare propagators $G^{(0)}$ at a frequency shown on the left.

FIG. 2. Density of states for $|\Delta|/\omega_0 = 30$. Height of impulses represents spectral weight of discrete levels. The broken line is the result of an adiabatic extrapolation.

FIG. 3. Fermion spectral weight $\overline{A}(\omega)$ in the adiabatic limit for positive bare energies $\epsilon = 0 \ldots 2|\Delta|$. Dotted lines are $\omega = \pm \epsilon$ and $\omega = \pm \tilde{\epsilon}$. 
FIG. 3. Fermion spectral weight $\tilde{A}(\omega)$ in the adiabatic limit for positive bare energies $\epsilon = 0 \ldots 2|\Delta|$. Dotted lines are $\omega = \pm \epsilon$ and $\omega = \pm \bar{\epsilon}$. 
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