Abstract

We consider the symmetric single-impurity Anderson model in the presence of pairing fluctuations. In the isotropic limit, the degrees of freedom of the local impurity are separated into hybridizing and non-hybridizing modes. The self-energy for the hybridizing modes can be obtained exactly, leading to two subbands centered at $\pm U/2$. For the non-hybridizing modes, the second order perturbation yields a singular resonance of the marginal Fermi liquid form. By multiplicative renomalization, the self-energy is derived exactly, showing the resonance is pinned at the Fermi level, while its strength is weakened by renormalization.
The unusual normal state of the high-$T_c$ cuprate superconductors has been interpreted as a kind of non-Fermi liquid (FL) behavior, but so far there have been no fully convincing microscopic justifications of such a state in quasi-two-dimensional systems with short range interactions. A phenomenological marginal FL approach was suggested by Varma et al. [1] as the “gentlest” departure from the conventional FL theory to describe the anomalous properties. The central hypothesis is that over a wide range of momenta the charge and spin polarizabilities do not contain any intrinsic low energy scales, depending only on temperature and external frequency:

$$\text{Im} \chi_{\nu \sigma}(q, \omega) \sim \begin{cases} -N(0) \frac{\omega}{T}, & \omega \ll T \\ -N(0), & T \ll \omega \ll \omega_c, \end{cases}$$

where $N(0)$ is the density of states at the Fermi level, and $\omega_c$ is a high-energy cut-off of the order of 0.5 eV. Apart from cuprates, the anomalous behavior observed in the normal state of some heavy fermion superconductors can also be interpreted in terms of such a marginal FL [2]. A number of serious attempts have been made to provide a microscopic justification for this phenomenological theory, beginning with the three-body resonance [3], followed by a detailed study of related quantum impurity models [4-8], and the most recent interpretation is based on local fluctuations of the order parameter near the quantum critical point using a two-band model for cuprates [9]. As far as we understand, the issue is still open.

On the other hand, a large body of experimental data in NMR, $\mu$SR, specific heat, transport, tunneling, neutron scattering, and photoemission measurements in most underdoped cuprate superconductors can be interpreted as due to the presence of a pseudo-gap (depleted density of states at the Fermi level) above $T_c$ [10-12]. There have been various proposals for the origin of such a pseudo-gap, and one of them is due to precursor pairing fluctuations [10]. However, a possible connection of such pairing fluctuations with marginal FL behavior has not yet been explored so far.

In this Letter, we, following the experience in the heavy fermion studies, consider the hybridization of a strongly localized electron with an uncorrelated conduction electron band, in terms of an impurity model [13]. Encouraged by the recovering of non-FL behavior in the single-impurity two-channel Kondo model [14,15], we explore a generalized symmetric Anderson model with particle-particle mixing on top of the standard particle-hole mixing. This model can be justified in the presence of pairing fluctuations between the local impurity and conduction electrons. When the two types of hybridizations have the same strengths, the local impurity degrees of freedom are separated into hybridizing and non-hybridizing modes, and the anomalous polarizability (1) emerges naturally as due to the impurity contribution in the non-interacting limit. The self-energy for the hybridizing modes can be obtained exactly, and the corresponding density of states forms two subbands centered at $\pm U/2$, with
as the Hubbard repulsion. Meanwhile, the self-energy for the non-hybridizing modes is calculated in the second order perturbation, giving rise to a singular resonance at the Fermi level, of the marginal FL type. Using the multiplicative renormalization method, the exact self-energy can be derived self-consistently in the weak coupling limit and extended then to strong coupling. We find that the non-FL resonance is pinned at the Fermi level and it is described by the X-ray edge type of singularity.

The symmetric single impurity Anderson model in the presence of pairing fluctuations is given by:

\[
H = \sum_{\vec{k}, \sigma} \epsilon_{\vec{k}} C_{\vec{k}, \sigma}^\dagger C_{\vec{k}, \sigma} + \frac{V}{2} \sum_{\vec{k}, \sigma} (C_{\vec{k}, \sigma}^\dagger d_\sigma + d_\sigma^\dagger C_{\vec{k}, \sigma}) + U (d_{\uparrow}^\dagger d_{\downarrow} - \frac{1}{2}) (d_{\downarrow}^\dagger d_{\uparrow} - \frac{1}{2}) + \frac{V_a}{2} \sum_{\vec{k}, \sigma} (C_{\vec{k}, \sigma}^\dagger d_\sigma^\dagger + d_\sigma C_{\vec{k}, \sigma}),
\]

where the symmetric condition \(\epsilon_d = -U/2\) has been assumed, and the chemical potential of conduction electrons is set to zero. It is worthwhile to note that the \(V_a\) term is similar to the transverse interaction term for the second channel in the effective two-channel Kondo Hamiltonian obtained in the abelian bosonization approach [14]. We will focus on the case of \(V_a = V\), corresponding to the isotropic case of the model. As justification of this model we would mention that Varma has emphasized the importance of the potential scattering at the impurity \(V_0 \sum_{\vec{k}, \vec{k}', \sigma} c_{\vec{k}, \sigma}^\dagger c_{\vec{k}', \sigma} d_\sigma d_\sigma\) [16], and the renormalization group analysis showed that the unitarity limit for this potential scattering is being approached, while the opposite-spin scattering is renormalized to zero [7]. A mean field decoupling of this quartic term allowing “anomalous average” \(\langle d_\sigma c_\sigma\rangle\) due to pairing fluctuations would lead to the particle-particle mixing term in Eq. (2). Such a pairing is of triplet character, and whether it is related to the “odd frequency” pairing discussed earlier [17] is not considered here. Nor we are going to discuss the self-consistency issue of the pairing per se. We will rather focus on the physical consequences of the above well-defined model.

In order to reveal the characteristics of this generalized model, it is very useful to introduce the Majorana fermion representation [15]: \(d_\uparrow = (d_1 - id_2)/\sqrt{2}, \quad d_\downarrow = (-d_3 - id_0)/\sqrt{2}\). The model Hamiltonian can then be rewritten as \(H = H_0 + H_I\), where

\[
H_0 = \sum_{\vec{k}, \sigma} \epsilon_{\vec{k}} C_{\vec{k}, \sigma}^\dagger C_{\vec{k}, \sigma} + \frac{V}{\sqrt{2}} \sum_{\vec{k}} \left[ (C_{\vec{k}, \uparrow}^\dagger - C_{\vec{k}, \uparrow}) d_1 - (C_{\vec{k}, \downarrow}^\dagger - C_{\vec{k}, \downarrow}) d_3 \right],
\]

\[
H_I = Ud_1 d_2 d_3 d_0.
\]

Now it is clear that the pairing fluctuation terms have changed the structure of the model: one half degrees of freedom of the local impurity \((d_1, d_3)\) hybridize with the conduction electrons, while another half degrees of freedom \((d_0, d_2)\) decouple. The former will be referred
to as hybridizing modes, whereas the latter as non-hybridizing modes. These two types of
modes are correlated through the Hubbard interaction. We emphasize that this change is
non-perturbative in nature and makes the non-interacting limit nontrivial.

In the $U = 0$ limit, $H_0$ is solved exactly. The Green’s functions for the hybridizing and
non-hybridizing modes are calculated as $G_h^{(0)}(\omega_n) = \frac{1}{\omega_n + i\Delta \text{sgn}(\omega_n)}$ and
$G_{nh}^{(0)}(\omega_n) = \frac{1}{\omega_n}$, where
$\omega_n = (2n + 1)\pi/\beta$ with $\beta = 1/T$, $\Delta = \pi \rho(0)V^2$ is the hybridization width, $\rho(0)$ is the density
of states of conduction electrons at the Fermi level, and $\Delta$ will be the high energy cutoff in
the weak coupling theory. The Green’s function for the non-hybridizing modes describes a
fermionic zero mode and $G_{nh}^{(0)}(\tau) = -\text{sgn}(\tau)/2$. The total impurity density of states is thus
obtained as $A_{\delta}^{(0)}(\omega) = \frac{1}{\pi \omega^2 + \Delta^2} + \delta(\omega)$. Apart from a Lorentz distribution, a delta function
peak due to the non-hybridizing modes appears at the Fermi level. As a result, the impurity
charge and spin density fluctuations will be affected. Since the charge and spin density
operators are defined as

$$n_d = \frac{1}{2} (d^\dagger_1 d_1 + d^\dagger_4 d_4 - 1) = -\frac{i}{2} (d_1 d_2 + d_0 d_3),$$

$$S^z_d = \frac{1}{2} (d^\dagger_3 d_3 - d^\dagger_4 d_4) = -\frac{i}{2} (d_1 d_2 - d_0 d_3),$$

the charge and spin dynamical susceptibilities are both given by

$$\chi^{(0)}_{\rho,\sigma}(\Omega_n) = \frac{1}{2\beta} \sum_{\omega_n} G_h^{(0)}(\omega_n) G_{nh}^{(0)}(\Omega_n - \omega_n),$$

where $\Omega_n = 2n\pi/\beta$. After summation over frequency, the retarded imaginary part is ob-
tained:

$$\text{Im} \chi^{(0)}_{\rho,\sigma}(\Omega, T) = -\frac{\pi}{4} N(\Omega) \tanh \left( \frac{\Omega}{2T} \right),$$

where $N(\Omega) = \frac{1}{\pi \omega^2 + \Delta^2}$ is the density of states of the hybridizing modes. This is exactly
what has been assumed in the marginal FL phenomenology [1], of the same form as Eq.(1)!
It becomes transparent that the anomalous impurity charge and spin polarizability is due
to the delta resonance at the Fermi level, which is induced by the pairing fluctuations under
the condition $V_a = V$. An analogous situation previously appeared in the studies of the
two-channel Kondo model in the isotropic case [14,15,18].

Now consider the effects of interaction on the impurity density of states. The perturba-
tion theory in terms of Majorana fermions has been fully developed in the earlier publications
[18]. In the second order perturbation, the self-energy of the hybridizing modes is given by:

$$\Sigma_h(\tau - \tau') = N^2 \frac{\Delta}{4} G_h^{(0)}(\tau - \tau').$$

It is worthwhile to note that this self-energy is exact, which can also be obtained by means of retarded double-time Green’s functions with the help of

$$[d_2 d_0, H] = 0.$$
and the density of states is thus

\[ \text{Im}G_h(\omega) = \frac{1}{2\pi} \left[ \frac{\Delta}{(\omega - U/2)^2 + \Delta^2} + \frac{\Delta}{(\omega + U/2)^2 + \Delta^2} \right]. \] (8)

This spectral density is similar to that of the conventional symmetric single impurity Anderson model in the Hartree-Fock approximation [13].

Meanwhile, the self-energy of the non-hybridizing modes in the second order perturbation is expressed by:

\[ \Sigma_{nh}^{(2)}(\omega_n) = \frac{U^2}{\beta^2} \sum_{\omega_1,\omega_2} G_h^{(0)}(\omega_1)G_h^{(0)}(\omega_2)G_{nh}^{(0)}(\omega_n - \omega_1 - \omega_2). \] (9)

Using the spectral representation, the hybridizing Green’s functions are expressed in terms of their density of states \( N(\epsilon) \), and after the frequency summation we find

\[ \Sigma_{nh}^{(2)}(\omega_n) = \frac{U^2}{4} \int_{-\infty}^{\infty} d\epsilon_1 d\epsilon_2 \frac{N(\epsilon_1)N(\epsilon_2)}{i\omega_n - \epsilon_1 - \epsilon_2} \tanh \left( \frac{\epsilon_1}{2T} \right) \times \left[ \tanh \left( \frac{\epsilon_2}{2T} \right) + \coth \left( \frac{\epsilon_1}{2T} \right) \right]. \] (10)

Carrying out the analytical continuation \( i\omega_n \rightarrow \omega \) and approximating \( N(\epsilon) \) by its value at the Fermi level, the imaginary part of the retarded self-energy is derived as

\[ \text{Im}\Sigma_{nh}^{(2)}(\omega, T) = -\frac{\pi}{2} \left( \frac{U}{\pi \Delta} \right)^2 \omega \coth \left( \frac{\omega}{2T} \right), \] (11)

and the corresponding real part is also obtained as \( \text{Re}\Sigma_{nh}^{(2)}(\omega, T) \approx \left( \frac{U}{\pi \Delta} \right)^2 \omega \ln \left( \frac{\max(\omega, T)}{\Delta} \right) \).

This self-energy gives rise to a quasiparticle weight depending logarithmically on frequency or temperature, namely,

\[ z_{nh}^{(2)} \approx 1 + \left( \frac{U}{\pi \Delta} \right)^2 \ln \left( \frac{\max(\omega, T)}{\Delta} \right). \] (12)

In the corresponding Green’s function, the pole \( \omega = 0 \) is preserved and the resonance is characterized by a marginal FL origin. To some extent, the non-hybridizing modes may represent the low energy excitations of the model.

Since there is a logarithmic correction to the self-energy for the non-hybridizing modes, we have to examine the higher order expansions carefully. Moreover, the logarithmic singularity in the reducible interaction vertex diagrams can be proved to cancel each other, so one has to consider the \textit{irreducible} interaction vertex \( \Gamma_{1,2,3,0}(0, \omega_n; 0, \omega_n) = \Gamma(\omega_n) \), which
can not be severed into separate diagrams by cutting a pair of lines, one of which is the propagator of $G_{nh}$ and the other is $G_h$. The lowest order correction to $\Gamma(\omega_n)$ is given by

$$\frac{U^3}{\beta^2} \sum_{\omega_1, \omega_2} G_h^{(0)}(\omega_1) G_h^{(0)}(\omega_2) \left[ G_{nh}^{(0)}(\omega_n - \omega_1 - \omega_2) \right]^2.$$  

It is interesting to note that this lowest order correction can be related to $\Sigma_{nh}^{(2)}(\omega_n)$ by the relation $\Gamma^{(3)}(\omega_n) = -U \frac{\partial \Sigma_{nh}^{(2)}(\omega_n)}{\partial (i\omega_n)}$. Therefore, the correction to the irreducible vertex is also logarithmically divergent:

$$\Gamma^{(3)}(\omega, T) \approx -U \left( \frac{U}{\pi \Delta} \right)^2 \ln \left( \frac{\max(\omega, T)}{\Delta} \right).$$  

(13)

In fact, from a general consideration of the model, a Ward identity can be established [19], relating the irreducible vertex to the non-hybridizing self-energy:

$$\Gamma(\omega_n) = U \left[ 1 - \frac{\partial \Sigma_{nh}(\omega_n)}{\partial (i\omega_n)} \right],$$  

(14)

which shows that to a large extent the singularity in $\Gamma(\omega_n)$ and $\Sigma_{nh}(\omega_n)$ cancel each other. This implies that the renormalization of the self-energy in the higher order expansions must be treated on an equal footing with that of the irreducible vertex.

In the treatment of logarithmic problems, the multiplicative renormalization is an effective method [20]. In such a treatment, the temperature is fixed at zero for simplicity and only the frequency variables are retained. Since the interaction is cut off at $\Delta$ in our weak coupling theory, the Green’s functions and vertices will depend only on the ratio $\frac{\omega}{\Delta}$, and the dimensionless coupling constant $\tilde{U} \equiv \frac{U}{\pi \Delta}$ must be defined as the proper invariant coupling constant. When we express the irreducible vertex by $\frac{1}{\pi \Delta} \Gamma = \tilde{U} \tilde{\Gamma}$, it follows from the structure of the Dyson equation that the renormalization equations will have the forms

$$G_h(\omega, \Delta', \tilde{U}') = z_1 G_h(\omega, \Delta, \tilde{U}),$$

$$G_{nh}(\omega/\Delta', \tilde{U}') = z_2 G_{nh}(\omega/\Delta, \tilde{U}),$$

$$\tilde{\Gamma}(\omega/\Delta', \tilde{U}') = z_3^{-1} \tilde{\Gamma}(\omega/\Delta, \tilde{U}),$$

$$\tilde{U}' = z_1^{-1} z_2^{-1} z_3 \tilde{U}.$$  

(15)

Since its second order perturbational result is exact, the Green’s function for the hybridizing modes should remain unrenormalized and therefore $z_1 = 1$. Using the low order perturbation results for $z_{nh}$ and $\tilde{\Gamma}$, we deduce

$$z_2^{-1} = 1 + \tilde{U}^2 \ln \left( \frac{\Delta'}{\Delta} \right), \quad z_3 = 1 - \tilde{U}^2 \ln \left( \frac{\Delta'}{\Delta} \right),$$  

(16)
and $\tilde{U}' = \tilde{U}$. The invariant coupling constant is not renormalized, and this conclusion is actually valid beyond the multiplicative renormalization approximation, because it is ensured by the Ward identity!

Meanwhile, the quasiparticle weight $z_{nh}(\omega)$ is also a proper quantity satisfying the criterion of multiplicative renormalization, and has good transformation properties. When the second order perturbation result of $z_{nh}$ is taken into account, the Lie equation up to the second order can be derived as follows:

$$\frac{\partial \ln z_{nh}}{\partial \ln \omega} = \tilde{U}^2 \frac{1}{\omega}.$$  \hspace{1cm} (17)

By integrating over $\omega$ and determining the constant of integration from fitting to the second order perturbation expression, we get $z_{nh}(\omega) = \left(\frac{\omega}{\Delta}\right)^{\tilde{U}^2}$. The Green's function for the non-hybridizing modes is thus obtained

$$G_{nh}(\omega) = \frac{1}{\omega} \left(\frac{\omega}{\Delta}\right)^{\tilde{U}^2}. \hspace{1cm} (18)$$

To calculate the spectral density $\text{Im}G_{nh}$ we note that the branch cut of $G_{nh}$ extends only on one side of the branching point. Thus, $\text{Im}G_{nh}$ is a step function of the energy. The phase of the factor $\omega^\alpha$ is then completely determined: on the branch cut side it involves a factor $(-1)^\alpha$. In the weak coupling limit $\tilde{U} << 1$, we thus obtain

$$\text{Im}G_{nh}(\omega) = \pi \tilde{U}^2 \frac{1}{\omega} \left(\frac{\omega}{\Delta}\right)^{\tilde{U}^2}.$$  \hspace{1cm} (19)

The singularity of the resonance at $\omega = 0$ is weakened by renormalization, and follows a power law with an exponent proportional to the squared interaction strength. The non-FL quasiparticle weight vanishes at the Fermi level, thus there are strong similarities between the present singular resonance and the X-ray emission spectra [21], and the marginal FL resonance is actually described by a power law behavior in the low energy limit. Paralleling the asymptotically exact calculation for the X-ray edge problem [22], we believe that it is possible to develop an exact treatment of this resonance for arbitrary coupling parameter $\tilde{U}$.

This way, the above weak coupling results may be extended to strong coupling limit after replacing $\tilde{U}$ by $\delta/\pi$, where $\delta = \arctan(\tilde{U}/\Delta)$ is an s-wave phase shift at the Fermi level.

In addition, when the large $U$ limit is considered, a Schrieffer-Wolf transformation can be applied to the model Hamiltonian, generating an s-d type of model:

$$H' = \sum_{k,\sigma} \varepsilon_k C_{k,\sigma}^\dagger C_{k,\sigma} + \frac{4V^2}{U} \sigma^y(0) + \tau^y(0)]S^y_d,$$ \hspace{1cm} (20)

where $\sigma^y(0) = -i(C_{0,\uparrow}^\dagger C_{0,\downarrow} - C_{0,\downarrow}^\dagger C_{0,\uparrow})/2$, and $\tau^y(0) = -i(C_{0,\uparrow}^\dagger C_{0,\downarrow} - C_{0,\downarrow} C_{0,\uparrow})/2$, are the y-components of the spin and isospin densities of the conduction electrons at the impurity.
$S^y_d = -id_3d_1$ is the corresponding impurity spin operator. This resulting model is reminiscent of the so-called compactified two-channel Kondo model [15]. However, here is only one component in the exchange interactions, which become a genuinely marginal operator, being compatible with the renormalization analysis of the Hubbard interaction.

The total density of states of the local impurity is a sum of the hybridizing and non-hybridizing modes: $\text{Im}G_h + \text{Im}G_{nh}$. Within the present exact theory, a very interesting picture emerges in a nature way: The hybridizing modes form two subbands with Lorentz form centered at $\pm U/2$, in some sense similar to the lower and upper Hubbard bands, while the non-hybridizing modes form a singular non-FL resonance at the Fermi level. The low-energy excitations and high-energy excitations are thus separated, and only the former is strongly renormalized. More interestingly, a very similar picture with three peaks in the density of states has been suggested by Kotliar, Georges, and coworkers [23] in their studies of the symmetric $d = \infty$ one-band Hubbard model close to the metal-insulator transition, where the central peak is a FL quasiparticle resonance. It is very likely that the present model including the pairing fluctuations between the local impurity and conduction electrons could shed some light on the nature of some strongly correlated electron systems.

In conclusion, we have considered the effect of pairing fluctuations on the symmetric single impurity Anderson model. The main features of this model are very similar to those anticipated for the “three body” resonance model, considered earlier [3]. However, the difficulty due to generating a new low-energy scale, inherent in the previous model, does not appear here. This model study suggests a possible microscopic origin of the marginal FL behavior. After completing the present calculation, we saw a new preprint [24] where an attempt was made to make connection between the marginal FL behavior and a lattice of three-body bound states. However, the issue considered there is different from ours.

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REFERENCES

[1] C. M. Varma et al, Phys. Rev. Lett. 63, 1996 (1989).
[2] M. B. Maple et al, Low Temp. Phys. 95, 225 (1994).
[3] A. E. Ruckenstein and C. M. Varma, Physica C 185, 134 (1991).
[4] Q. Si and G. Kotliar, Phys. Rev. Lett. 70, 3143 (1993); Phys. Rev. B 48, 13881 (1993).
[5] I. Perakis, et al., Phys. Rev. Lett. 70, 3467 (1993).
[6] C. Sire, et al., Phys. Rev. Lett. 72, 2478 (1994).
[7] G.-M. Zhang and L. Yu, Phys. Rev. Lett. 72, 2474 (1994).
[8] G. Kotliar and Q. Si, Phys. Rev. B 53, 12373 (1996).
[9] C.M. Varma, Phys. Rev. B 55, 14554 (1997).
[10] See, a recent review, M. Randeria, cond-mat/9710223.
[11] S. Martin, et al., Phys. Rev. B 41, 846 (1990).
[12] A.V. Puchkov, et al., J. Phys. Condens. Matter 48, 10049 (1996).
[13] P. W. Anderson, Phys. Rev. 124, 41 (1961).
[14] I. Affleck and A.W.W. Ludwig, Nucl. Phys. B 360, 641 (1991); V. J. Emery and S. Kivelson, Phys. Rev. B, 46, 10812 (1992); M. Fabrizio, et al., Phys. Rev. Lett. 74, 4503 (1995).
[15] P. Coleman, et al, Phys. Rev. B, 52, 6611 (1995).
[16] C.M. Varma and T. Giamarchi, in Strongly Interacting fermions and High Tc Superconductivity, Les Houches Lectures, ed. by B. Doucot and J. Zinn-Justin (Elsevier New York, 1995).
[17] V.L. Berezinskii, JETP Lett. 20, 287 (1974); A.V. Balastky and E. Abrahams, Phys. Rev. B 45, 13125 (1992).
[18] G.-M. Zhang and A. C. Hewson, Phys. Rev. Lett. 76, 2137 (1996).
[19] G.-M. Zhang, unpublished.
[20] J. Sólyom, J. Phys. F 4, 2269 (1974).
[21] P. Nozières, et al., Phys. Rev. 178, 1084 (1969).
[22] P. Nozières and C. T. De Dominicis, Phys. Rev. 178, 1097 (1969).
[23] A. Georges et al. Rev. Mod. Phys. 68, 13 (1996).
[24] A.F. Ho and P. Coleman, cond-mat/9801004.