Renormalization group analysis of electrons near a Van Hove singularity

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(April 1, 2022)

A model of interacting two dimensional electrons near a Van Hove singularity is studied, using renormalization group techniques. In hole doped systems, the chemical potential is found to be pinned near the singularity, when the electron-electron interactions are repulsive. The RG treatment of the leading divergences appearing in perturbation theory give rise to marginal behavior and anisotropic superconductivity.

75.10.Jm, 75.10.Lp, 75.30.Ds.

The relevance of a Van Hove singularity for the high-$T_c$ compounds was pointed out shortly after their discovery [1–5], and a more refined “Van Hove scenario” was proposed afterwards [6]. In addition there is mounting numerical evidence that such a singularity arises in studies of strongly correlated 2D systems [7–9]. This fact is in agreement with photoemission studies in hole doped high-$T_c$ materials [10].

The dynamics of interacting two dimensional electrons near a van Hove singularity are anomalous, as a standard perturbative treatment is plagued by logarithmic divergences. The study of these divergences requires a renormalization group treatment. The feasibility of such an approach in condensed matter systems has been analyzed in ref. [11]. In the following, we apply a suitably generalized version of the scheme proposed in [11] to the problem at hand.

\[
\mathcal{H} = \sum_{i,j=A,B} - \int \Psi_i(\vec{r}) \left[ \frac{\hbar^2}{2m_{x,i}} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{y,i}} \frac{\partial^2}{\partial y^2} \right] \Psi_i(\vec{r}) dxdy + u_{i',j'} \int \Psi_i(\vec{r}) \Psi_{i'}(\vec{r}) \Psi_j(\vec{r}) \Psi_{j'}(\vec{r}) dxdy
\]  

(1)

where \(m_{x,A} = m_{y,B}\) and \(m_{y,A} = m_{x,B}\) (see figure 1). In the following, we will use the parameters \(\bar{m} = (m_{x,A} + m_{y,B})/2\) and \(\Delta m = (m_{x,A} - m_{y,B})/2\). We have omitted spin indices for simplicity. The number of possible (isotropic) interactions is restricted by symmetry. An umklapp interaction of the type \(u_{A1, A2; B1, B2}\) is allowed. A term like this transfers a pair of electrons from the vicinity of one of the singularities to the vicinity of the other. The total momentum transfer coincides with a lattice reciprocal vector.

The couplings in (1) are expressed in units of \(\text{energy} \times \text{area}\). For instance, for a local Hubbard-like interaction, \(U\), the parameters in (1) are proportional to \(U\times\text{the area of the unit cell}\). By scaling units in (1), all couplings can be made dimensionless, that is, \(\tilde{u} = u \bar{m}^2/\hbar^2\). When (1) is a low energy approximation to a Hubbard like hamiltonian, these dimensionless parameters are proportional to \(U/\bar{m}\), where \(U\) is the Hubbard interaction and \(\bar{m}\) is the bandwidth.

We first consider the electrons near a given van Hove singularity. An anisotropic scaling of lengths leads to
\[ \Delta m = 0. \] The fact that the interaction is dimensionless implies that perturbative corrections should depend logarithmically on the remaining scales implicit in \( \Delta m \): the high energy cutoff, and the low energy scale, that is, the temperature or the external frequency in the diagram.

\[ \text{FIG. 2. Diagrams calculated in the text. Full and broken lines correspond to propagators of electrons near the two inequivalent singularities. Thin and thick wavy lines denote intra- and inter-singularity scattering.} \]

For instance, the particle hole polarizability is shown in fig. 2(b). Using a cutoff in energies, such that the filled states in the Fermi sea have energies \(-\epsilon_c < \epsilon < 0\), we obtain:

\[
\text{Re} \chi(\vec{q}, \omega) = \frac{1}{2\pi^2} \left[ \log \left( \frac{4\epsilon_c \epsilon_q}{\omega^2 - \epsilon_q^2} \right) - \frac{\omega}{\epsilon_q} \log \left( \frac{\omega + \epsilon_q}{\omega - \epsilon_q} \right) + 2 \right]
\]

\[
\text{Im} \chi(\vec{q}, \omega) = \frac{2}{\pi \epsilon_q} \left( |\omega + \epsilon_q| - |\omega - \epsilon_q| \right)
\]

where \( \epsilon_q = \frac{\hbar^2 (\vec{q} - \vec{q}_0)^2}{2m} \) (note that \( \vec{q} \) is measured from the singularity). The angular dependence on \( q \) is determined by the SO(1,1) symmetry of the dispersion relation. Other choices of cutoff, which break this symmetry, do not change the low energy behavior of the polarizability, given by (2). This expression agrees with previous estimates of the polarizability of electrons near a van Hove singularity \( [12-14] \). The imaginary part of the susceptibility is consistent with the “marginal Fermi liquid” hypothesis \( [8] \).

The inter-singularity polarizability (also shown in fig. 2(b)) diverges as:

\[
\text{Re} \chi'(\vec{q}, \omega) \sim \log \left( \frac{\pi \pi}{\Delta m} \right) \log \left[ \frac{\epsilon_c}{\max \left( \omega, \frac{\hbar^2 (\vec{q}_0^2 + \vec{q}_0^2)}{2m} \right)} \right]
\]

\[
\text{Im} \chi'(\vec{q}, \omega) \sim \log \left( \frac{\pi \pi}{\Delta m} \right) \min \left[ 1, \frac{\pi \pi \omega}{\hbar^2 (\vec{q}_0^2 + \vec{q}_0^2)} \right]
\]

The electron-hole polarizabilities screen the bare interactions. This flow of the effective couplings makes the problem similar to the 1D Luttinger liquid \( [16] \). An unrelated renormalization scheme was proposed in \( [17] \), on the basis of the marginal Fermi liquid phenomenology \( [13] \). The \( q \) dependence of the diagrams derived from (2), and the electron-electron scattering channels are, however, totally different from those proposed in \( [14] \).

The intra-singularity effective interaction, to lowest order, is:

\[
u_{\text{eff}}(q) = \frac{u_q}{1 + \frac{u_q}{\pi} \log \left( \frac{\epsilon_q}{\epsilon_c} \right) + 2}
\]

This result implies that the system is unstable against any distortion with a (small) wavevector along the Fermi line. Repulsive interactions favor a spin density wave, while attractive interactions lead to a charge density wave. Using the same argument for the effective inter-singularity interactions, screened by \( \chi' \), we also find instabilities for the wavevector \((\pi, \pi)\) which connects the two special points.

To lowest order, we need also consider the renormalization of the self-energy, given by the Hartree diagram shown in fig. 2(b). In a conventional Fermi liquid, the integrating out of the states in a given energy shell leads to a constant contribution, which uniformly shifts the one electron levels. The present case differs, in that each new energy shell contains more and more states, and the shift increases as the renormalization proceeds towards the van Hove singularity. For instance, let us define the Fermi energy, \( \epsilon_F \), referred to the singularity. In dimensionless units, the flow of \( \epsilon_F \) is given by:

\[
\frac{\partial \epsilon_F}{\partial l} = \epsilon_F - \bar{u} \log \left( \frac{1}{1 - \epsilon_F} \right)
\]

where \( l = -\log(\epsilon_c) \).

The first term in (\( \ref{eq:qflow} \)) is determined by dimensional arguments. The Fermi energy seems larger when measured in terms of the reduced cutoff. The second term gives the shift due to the interaction with the high energy part of the Fermi sea. We assume that the high energy states which are removed lie at energy \( \epsilon_c \) below \( \epsilon_F \). Unlike in normal metals, the second term does not scale in step with the first \( \epsilon_F \). Thus, for repulsive interactions and \( \epsilon_F > 0 \), there may be a non trivial, stable, fixed point, at which the flow in (\( \ref{eq:qflow} \)) is arrested. As \( \epsilon_c \) is further reduced, \( \epsilon_F = \epsilon_F^* \) remains unchanged. In dimensionful units, it means that the Fermi energy gets pinned at the van Hove singularity.
A sketch of the physics involved is shown in fig. (3). The chemical potential at the CuO planes is fixed by the other planes (fig. 3 a). We know that, for hole doped systems, a mean field treatment of the interaction places the singularity above the Fermi level (fig. 3 c). It implies that, in the absence of the (repulsive) interaction, the singularity should be at lower energies (fig. 3 b). Let us assume that the singularity is below the Fermi level when the interaction is switched off. Then, if the Hartree diagram is treated using renormalization group techniques, starting from the previous situation, the Fermi energy will get pinned at the singularity (fig. 3 d).

The difference between a mean field and a RG treatment of the Hartree potential lies in the fact that, in the latter case, electrons near the Fermi energy experience a larger shift from “fast” electrons, which lie at high energies, than from “slow” electrons. The RG analysis allows for the correlation hole generated by the low energy electrons. The pinning discussed here is only possible in nominally hole doped systems, in agreement with photoemission experiments [10].

Because of this anomalous divergence, a straightforward approach of RG techniques is not possible. We have chosen to scale the couplings as function of \( l^2 = \log^2(\epsilon_c) \) which corresponds to summing the leading log\(^2\) divergences [2]. Defining \( v \) as the intra-singularity scattering, and \( v' \) as the inter-singularity scattering, the flow is given by:

\[
\frac{\partial v}{\partial l^2} = -v^2 - v'^2 \\
\frac{\partial v'}{\partial l^2} = -2vv'
\]  

These equations can be integrated, and the flow follows the lines \( v' = \pm (k \pm \sqrt{k^2 + v^2}) \), where \( k \) is a constant. The flow of the couplings is schematically shown in fig. (4).

Thus, the spectral weight of the quasiparticle states is energy dependent, and decreases as the Fermi energy is approached. This behavior is reminiscent of a 1D Luttinger liquid [10], and qualitatively agrees with the “marginal Ferm liquid” hypothesis [12]. In addition, the transport properties, in the normal state, of the electrons near a singularity are strongly modified by the existence of a Umklapp electron electron scattering channel [12, 18].

Finally, we analyze the BCS channels, shown in figure (2c) and (2d). These diagrams also induce logarithmic corrections to the couplings, which diverge like the logarithm of the cutoff squared. Thus, this effect dominates over the influence of the electron-hole renormalization from the diagrams in fig. (2b).

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\[
1 - Z_k = \frac{\partial \text{Re} \Sigma(k, \omega)}{\partial \omega} \sim \dot{\omega}^2 \log \left( \frac{\epsilon_c}{\epsilon_k} \right)
\]  

These equations can be integrated, and the flow follows the lines \( v' = \pm (k \pm \sqrt{k^2 + v^2}) \), where \( k \) is a constant. The flow of the couplings is schematically shown in fig. (4).

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A purely repulsive $v$ is renormalized towards $v = 0$, which is a marginal fixed point. If $|v'| > |v|$, the couplings eventually become large and attractive. The flow towards strong coupling is the renormalization group version of the BCS instability. Thus, this instability always takes place when $|v'| > |v|$, irrespective of the sign of the couplings.

The instability arises because a large $v'$ favors a coherent superposition of Cooper pairs at both singularities. A repulsive interaction ($v' > 0$) implies that the condensate amplitude has opposite signs at the two singularities, i.e. d-wave pairing.

**FIG. 5.** Kohn-Luttinger diagrams which renormalize the couplings in the BCS channel.

Usually, a repulsive interaction in $q$ space is, either constant, or decays for large $q$'s. In the present case, however, $v$ and $v'$ are screened in very different ways by the electron-hole polarizabilities calculated in (2) and (3). These processes are the equivalent to those originally discussed by Kohn and Luttinger [[8]], when studying the possibility of superconductivity from screened repulsive interactions. The physics is very much the same, except that, in the present case, the anisotropy of the screening matches well the phase space available for the formation of Cooper pairs. Thus, the instability arises in a more natural way. In addition, the existence of a van Hove singularity modifies the relation between the BCS gap and the dimensionless coupling, which now becomes $\Delta_{BCS} \sim T_c \sim \epsilon_c \exp^{-1/\sqrt{\epsilon_c - v'}}$, ($v, v' > 0$).

In summary, we have shown that a system of interacting electrons near a 2D van Hove singularity can be analyzed using renormalization group methods. The treatment presented here is still far from complete, but the derived features are independent of the details of the model, and consistent with the observed behavior of high-$T_c$ materials.

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