

Robustness of the Van Hove Scenario for High- T_c Superconductors

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The pinning of the Fermi level to the Van Hove singularity and the formation of flat bands in the two-dimensional $t - t'$ Hubbard model is investigated by the renormalization group technique. The “Van Hove” scenario of non-Fermi-liquid behavior for high- T_c compounds can take place in a broad enough range of the hole concentrations. The results are in qualitative agreement with the recent angle-resolved photoemission spectroscopy data on La_2CuO_4 .

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The nature of the normal state and the mechanisms of superconductivity in copper-oxide high- T_c compounds are still a subject of hot discussions [1–6]. A number of experimental data on transport properties and angle-resolved photoemission spectroscopy (ARPES) give evidence of a non-Fermi-liquid (NFL) character of the normal state in an underdoped regime and, as a consequence, of a strict confinement of current carriers in the CuO_2 planes. The latter results in an anomalously weak sensitivity of normal-phase and superconducting properties to the impurities outside the planes, hopping character of the transport along c axis, etc. Anderson [1] has put forward the idea that a 2D system can demonstrate a NFL behavior at arbitrarily small interelectron repulsion U owing to a finite phase shift at the Fermi energy. In this scenario, the confinement of current carriers is explained by “quantum protection” [2] owing to charge-spin separation and incoherent (non-quasiparticle) character of electron (or hole) motion. However, theoretical understanding of a NFL state in quasi-2D electron systems turned out to be very difficult. Modern field-theoretical investigations [7] show that such a state probably does not occur in general 2D and quasi-2D cases.

At the same time, peculiarities of the electron spectrum can lead to NFL behavior. In the presence of Van Hove singularities (VHS) near the Fermi level, the marginal Fermi-liquid [8] or NFL behavior [9] can be naturally derived. Already in the leading order of the perturbation theory in U the marginal dependences of the electron scattering rate and specific heat take place, $\text{Im}\Sigma(\mathbf{k}_F, \varepsilon) \propto |\varepsilon| \ln|1/\varepsilon|$ at $|\varepsilon| \gg |\mu|$ and $\delta C \propto T \ln^3[t/\max(|\mu|, T)]$, and the resistivity demonstrates the behavior $\rho \propto T \ln^2[t/\max(|\mu|, T)]$ [10] (T is the temperature, ε is the energy, μ is the chemical potential calculated from VHS, and t is the hopping integral). Closeness of the VHS to the Fermi level results in a 1D-like behavior of the perturbation expansion [11], but does not lead to the Luttinger-liquid fixed point since the system turns out to be unstable with respect to formation of magnetic or superconducting ground state [11–13].

This “Van Hove scenario” (for a review of early considerations, see, e.g., Ref. [14]) seems to be very attractive

since various data demonstrate the closeness of VHS to the Fermi level in high- T_c compounds at optimal doping or pressure. Recent ARPES data demonstrate that the Fermi level of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ is close to VHS in the range $x = 0.20\text{--}0.30$ [15], which corresponds to an overdoped regime. One of the two bands, which occur due to bilayer splitting (antibonding band) in the $\text{Bi}2212$ system, is also close to VHS [16]. A significant and still unsolved question is why the Fermi level should be close to VHS in a broad doping range. Although some considerations were performed [17,18], they did not take into account the renormalization of the electron spectrum, e.g., the formation of the flat part of the spectrum, which should change substantially the results of these approaches.

The flattening of the spectrum was first studied theoretically for a single hole in an antiferromagnetic background [19]. The flat region leads to some peculiarities of electron properties near the metal-insulator transition [20], in particular, to the pinning of the chemical potential. While the above-mentioned approaches describe correctly the situation at small hole doping (the doped Mott insulator regime), these approaches meet with difficulties near the optimal doping where the concentration of holes is not small. In this Letter we argue that besides antiferromagnetic fluctuations there is another factor which results in occurrence of the flat part of electron spectrum, namely, the critical fluctuations that occur near the Van Hove band filling. We also reconsider the issue of the pinning of the Fermi surface to Van Hove singularities by proposing a new scheme of renormalizations of the energy- and momentum-dependent electron Green’s function. We show that the pinning of the Fermi surface to VHS is a universal feature of 2D systems which is connected with the formation of a flat region of the electron spectrum near the $(\pi, 0)$ point. Both the phenomena, the pinning and the flattening, will be described within the same renormalization group (RG) approach.

We start from the $t - t'$ Hubbard model on the square lattice,

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

with the bare electron spectrum

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t'(\cos k_x \cos k_y + 1) - \mu.$$

Hereafter we assume $t > 0$, $t' < 0$ (which is the case for hole-doped systems), $0 \leq |t'|/t < 1/2$. For arbitrary t'/t this spectrum contains VH singularities connected with the points $A = (\pi, 0)$, $B = (0, \pi)$. The chemical potential μ measures the distance between VHS and the Fermi energy, so that at $\mu = 0$ VHS lie at the Fermi level. We suppose that t'/t is not too small, and therefore the Fermi surface is not nested. It was argued [9,12,13] that, provided that the band filling is close to the Van Hove one, the vicinity of the Van Hove points gives a dominant (most singular) contribution to electronic and magnetic properties. Thus we can use the expansion of the spectrum near $A(B)$ Van Hove points

$$\varepsilon_{\mathbf{k}}^A = -2t(\sin^2 \varphi \bar{k}_x^2 - \cos^2 \varphi k_y^2) - \mu, \quad (2)$$

$$\varepsilon_{\mathbf{k}}^B = 2t(\cos^2 \varphi k_x^2 - \sin^2 \varphi \bar{k}_y^2) - \mu, \quad (3)$$

$$\begin{aligned} \text{Re}\Sigma_1(\mathbf{k}, \varepsilon) &= -(2g_0/\sin 2\varphi)^2 [A_1 \varepsilon + B_1^x \bar{k}_x^2 + B_1^y \bar{k}_y^2] \ln^2(\Lambda/v), \\ \text{Re}\Sigma_{2,3}(\mathbf{k}, \varepsilon) &= -2(g_0/\sin 2\varphi)^2 [A_{2,3} \varepsilon + B_{2,3}^x \bar{k}_x^2 + 2C_{2,3} \bar{k}_x \bar{k}_y + B_{2,3}^y \bar{k}_y^2] \ln(\Lambda/v), \end{aligned} \quad (5)$$

where $\bar{k}_x = \bar{k}_x \sin \varphi$, $\bar{k}_y = k_y \cos \varphi$, $g_0 = U/(4\pi^2 t)$ is the dimensionless coupling constant, $v = \max(\bar{k}_x^2, k_y^2, |\varepsilon|/2t, |\mu|/2t)$, $A_1 = \ln 2$, and $B_1^x = -B_1^y = 1/2 - \ln 2$. The analytical expressions for the coefficients A_i , B_i , and C_i with $i = 2, 3$, which are some regular functions of t'/t , will be published elsewhere. We perform a summation of logarithmically divergent terms which depend on $\lambda = (1/2) \ln(\Lambda/v)$ within the RG approach. To separate effects of the electron spectrum renormalization and multiplicative renormalization of the Green's function, we perform the renormalization procedure in two steps. At the first step we introduce the \mathbf{k} -dependent mass renormalization factors $Z_{mi}^a(v)$ ($a = x, y$), and at the second step all the other divergences are absorbed into the energy-dependent quasiparticle residue $Z(\varepsilon)$,

$$G(\mathbf{k}, \varepsilon) = \frac{Z(\varepsilon)}{\varepsilon + 2tZ_{xm}^{-1}(v)\bar{k}_x^2 - 2tZ_{ym}^{-1}(v)\bar{k}_y^2 + \tilde{\mu} + i\Gamma(\varepsilon)}, \quad (6)$$

where $\tilde{\mu} = \mu + \text{Re}\Sigma(\mathbf{k}_{\text{VH}}, -\mu)$ is the renormalized

chemical potential, and the damping $\Gamma(\varepsilon) = Z(\varepsilon)\text{Im}\Sigma(\mathbf{k}_{\text{VH}}, \varepsilon)$ is determined by analytical continuation. The coefficients $Z_{am}(v) = Z_{m1}^a(v)Z_{m2}^a(v)Z_{m3}^a(v)$ satisfy the RG equations

$$\rho_0(\varepsilon) = (\pi^2 \sqrt{t^2 - (2t')^2})^{-1} \ln(\Lambda t/|\varepsilon + \mu|), \quad (4)$$

which diverges logarithmically at $\varepsilon = -\mu$. We show that the renormalized density of states contains a much stronger divergence, which results in the pinning of the Fermi surface to VHS. To this end we calculate the electron self-energy $\Sigma(\mathbf{k}, \varepsilon)$ for \mathbf{k} near the VH point $\mathbf{k}_{\text{VH}} = (\pi, 0)$. In the second order in U this contains three contributions that arise from intermediate quasimomenta which are close to the same or another VH point (cf. Refs [9,10]), $\Sigma^{(2)}(\mathbf{k}, \varepsilon) = \sum_{i=1}^3 \Sigma_i(\mathbf{k}, \varepsilon)$,

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$$\begin{aligned} d \ln Z_{m1}^a(\lambda)/d\lambda &= (B_1^a - A_1) \lambda \gamma_4^2 / \sin^2 2\varphi, \\ d \ln Z_{m2}^a(\lambda)/d\lambda &= (B_2^a - A_2) (\gamma_1^2 + \gamma_2^2 - \gamma_1 \gamma_2) / \sin^2 2\varphi, \\ d \ln Z_{m3}^a(\lambda)/d\lambda &= (B_3^a - A_3) \gamma_3^2 / \sin^2 2\varphi. \end{aligned} \quad (7)$$

Here γ_i are four-electron vertices determined from

$$\begin{aligned} d\gamma_1/d\lambda &= 4d_1(\lambda)\gamma_1(\gamma_2 - \gamma_1) + 4d_2\gamma_1\gamma_4 - 4d_3\gamma_1\gamma_2, \\ d\gamma_2/d\lambda &= 2d_1(\lambda)(\gamma_2^2 + \gamma_3^2) + 4d_2(\gamma_1 - \gamma_2)\gamma_4 \\ &\quad - 2d_3(\gamma_1^2 + \gamma_2^2), \\ d\gamma_3/d\lambda &= -4d_0(\lambda)\gamma_3\gamma_4 + 4d_1(\lambda)\gamma_3(2\gamma_2 - \gamma_1), \\ d\gamma_4/d\lambda &= -2d_0(\lambda)(\gamma_3^2 + \gamma_4^2) \\ &\quad + 2d_2(\gamma_1^2 + 2\gamma_1\gamma_2 - 2\gamma_2^2 + \gamma_4^2), \end{aligned} \quad (8)$$

where

$$d_0(\lambda) = \lambda(1 - R^2)^{-1/2}, \quad d_1(\lambda) = \min\{\lambda, \ln[(1 + \sqrt{1 - R^2})/R]\}, \quad d_2 = (1 - R^2)^{-1/2}, \quad d_3 = \tan^{-1}(R/\sqrt{1 - R^2})/R, \quad (9)$$

with $R = -2t'/t$. Equations for $Z(v) = Z_1(v)Z_2(v)Z_3(v)$ are obtained by the replacement $B_i^a - A_i \rightarrow A_i$ in (7). It was argued in Ref. [13] that Eqs. (8) reproduce correctly the solutions of the parquet equations which take into account the complete momentum dependence of the vertices. Numerical solution of Eqs. (7) demonstrates that the vertices γ_i increase with decreasing v and diverge at the critical value $v = v_c(t'/t)$ [13]. We have $Z_{am}(v) \rightarrow \infty$ at $v \rightarrow v_c$ while $Z_a(v) \rightarrow 0$. This divergence signals a

transition into a magnetically ordered or superconducting state at $|\mu| < \mu_c = 2tv_c$. The equations (7) and (8) are valid in the weak- and intermediate-coupling regime $\gamma_i < 1$, i.e., at $|\mu|$ not too close to μ_c .

The electron spectrum is determined by the pole of the Green's function (6). Increasing the factors $Z_{am}(v)$ with decreasing v leads to $|\varepsilon + \mu| < 2t \min(\bar{k}_x^2, k_y^2)$ at the pole, so that $v = \max(\bar{k}_x^2, k_y^2)$

$|\tilde{\mu}|/2t$) to logarithmic accuracy. This demonstrates that the separation of momentum- and energy-

renormalization effects turns out to be self-consistent. We obtain therefore for the renormalized spectrum $E_{\mathbf{k}}$

$$E_{\mathbf{k}} = -\tilde{\mu} + 2t \begin{cases} Z_{ym}^{-1}(k_y^2)\tilde{k}_y^2 - Z_{xm}^{-1}(k_x^2)\tilde{k}_x^2 & k_{x,y}^2 > |\tilde{\mu}|/(2t), \\ Z_{ym}^{-1}(|\tilde{\mu}|/2t)\tilde{k}_y^2 - Z_{xm}^{-1}(|\tilde{\mu}|/2t)\tilde{k}_x^2 & k_{x,y}^2 < |\tilde{\mu}|/(2t). \end{cases} \quad (10)$$

For $|\tilde{\mu}| > \mu_c$ and $k \gg k_c = v_c^{1/2}$ we have $Z_{xm,ym}^{-1}(k^2) \simeq 1$, and the dispersion coincides with the bare one, while at $\tilde{k}_x, \tilde{k}_y < k_c$ the spectrum becomes more flat due to renormalization by the factors $Z_{xm,ym}^{-1}(|\tilde{\mu}|/2t)$. Although the regime $|\tilde{\mu}| \leq \mu_c$, $k < k_c$ is outside of the region of the validity of RG equations (7) and (8), we have formally $E_{\mathbf{k}} = -\tilde{\mu}$ for $k < k_c$, i.e., the spectrum is flat in this region. This is similar to the result of Dzyaloshinskii [9]. However, unlike that paper, we have taken into account all the channels of electron scattering, which gives a flat part of the spectrum already in one-loop approximation for the vertices. The flat part formation was considered earlier as one of the formally possible instability channels of Landau Fermi-liquid ("fermionic condensation" [21,22]). Here we demonstrate that similar phenomena can take place in two-dimensional systems near the Van Hove filling. The result of numerical calculation of the dispersion law $E_{\mathbf{k}}$ according to Eqs. (7) and (10) at different values of $\tilde{\mu}$ is shown in Fig. 1. One can see that even at $|\tilde{\mu}| > \mu_c$ the spectrum has a wide, almost flat region. The picture shown in Fig. 1 is in good qualitative agreement with the ARPES data for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [15]. These data give a possibility to estimate $k_c \simeq 0.6a^{-1}$ (a is the lattice constant) for this system; according to (2), this k_c value corresponds to $\tilde{\mu}_c/(2t) = v_c \simeq 0.1$. We stress once more the difference of the present approach with the approaches [23] which yield the flattening of the spectrum owing to strong antiferromagnetic correlations and therefore are reliable only at low hole concentrations.

The flat part of electron spectrum leads to drastic changes in the density of states and dependence $n(\tilde{\mu})$. The contribution of the flat part of the spectrum to the density of states can be written as

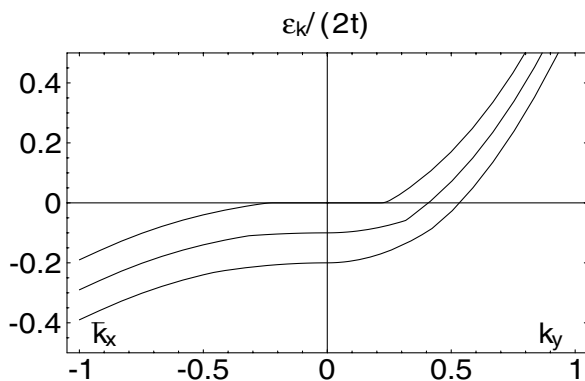


FIG. 1. Quasiparticle dispersion for $t'/t = -0.3$ and $U = 4t$ from RG approach. The values of the chemical potential are $\tilde{\mu} = 0, -0.2t, -0.4t$ (from top to bottom).

$$\delta\rho(\varepsilon) = -\frac{k_c^2}{\pi^2} \frac{\text{Im}\bar{\Sigma}(\mathbf{k}_{\text{VH}}, \varepsilon)}{[\varepsilon + \tilde{\mu} - \text{Re}\bar{\Sigma}(\mathbf{k}_{\text{VH}}, \varepsilon)]^2 + [\text{Im}\bar{\Sigma}(\mathbf{k}_{\text{VH}}, \varepsilon)]^2} = \frac{k_c^2}{\pi} A(\mathbf{k}_{\text{VH}}, \varepsilon), \quad (11)$$

where $\bar{\Sigma}(\mathbf{k}, \varepsilon) = \Sigma(\mathbf{k}, \varepsilon) - \text{Re}\Sigma(\mathbf{k}, -\mu)$ and $A(\mathbf{k}_{\text{VH}}, \varepsilon)$ is the quasiparticle spectral weight at the Van Hove momentum.

Consider first the results obtained within the second-order expression for $\Sigma(\mathbf{k}_{\text{VH}}, \varepsilon)$, Eq. (5). Note that at this stage the effects connected with the renormalization of electron dispersion are already taken into account by performing summation of \mathbf{k} -dependent logarithmically divergent terms to all orders of perturbation theory. We have at $|\tilde{\mu}| \ll |\varepsilon| \ll t$ to leading logarithmic accuracy for $\bar{\Sigma}(\mathbf{k}_{\text{VH}}, \varepsilon)$ the result

$$\delta\rho(\varepsilon) \simeq \frac{k_c^2}{\pi|\varepsilon|} \frac{C \ln(\Lambda t/|\varepsilon|)}{[1 + C \ln^2(\Lambda t/|\varepsilon|)]^2}, \quad C = \frac{g_0^2 \ln 2}{\sin^2 2\varphi}. \quad (12)$$

Therefore we obtain

$$n(\tilde{\mu}) = n_{\text{VH}} - \frac{\tilde{\mu}}{\pi^2 \sqrt{t^2 - (2t')^2}} \ln \frac{\Lambda t}{|\tilde{\mu}|} - \frac{k_c^2}{2\pi} \frac{\text{sgn}\tilde{\mu}}{1 + C \ln^2(\Lambda t/|\tilde{\mu}|)}, \quad (13)$$

where n_{VH} is the Van Hove filling. The second term in the right-hand side of Eq. (13) comes from momenta $k > k_c$ outside the flat part of the spectrum and can be calculated by using the bare density of states (4) since the renormalization of the spectrum at these momenta is not too important. For small enough $|\tilde{\mu}|$ we can neglect this term in comparison with the third term to obtain

$$n(\tilde{\mu}) = n_{\text{VH}} - \frac{k_c^2 \sin^2 2\varphi}{2\pi g_0^2 \ln 2} \frac{\text{sgn}\tilde{\mu}}{\ln^2(\Lambda t/|\tilde{\mu}|)}, \quad (14)$$

(the unity is small in comparison with the squared logarithm in the denominator). The chemical potential measured from the VHS energy is given by a nonanalytical function,

$$\tilde{\mu}(n) = \Lambda t \exp(-\text{const}/|n - n_{\text{VH}}|^{1/2}), \quad (15)$$

and is therefore practically zero in a rather wide range of electron concentrations n near n_{VH} . Note that, generally speaking, in the absence of the quadratic terms in the electronic spectrum, quartic terms may be important. However, the presence of such terms give only subleading corrections to the above results and does not change them qualitatively.

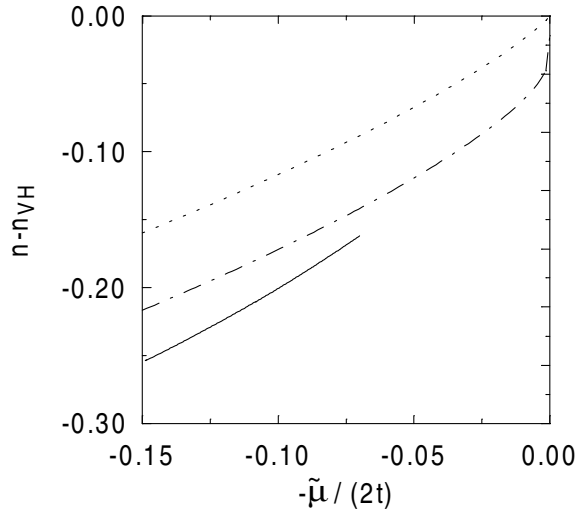


FIG. 2. The dependence $n(\tilde{\mu}) - n_{\text{VH}}$ for the same parameter values as in Fig. 1, $\tilde{\mu}$ being referred to as VHS energy. The used value of k_c is 0.6. The dashed line corresponds to a bare electron spectrum and the solid line to the result (13). The dot-dashed line is the dependence with account of renormalizations of $\Sigma(\mathbf{k}_{\text{VH}}, \varepsilon)$.

The results of numerical calculations of $n(\tilde{\mu})$ with Eq. (13) and the renormalized dependence $n'(\tilde{\mu})$ with account of renormalization of $\Sigma(\mathbf{k}_{\text{VH}}, \varepsilon)$ according to Eq. (7) are shown in Fig. 2 for $U = 4t$ and $k_c \approx 0.6$. The dependence $n_0(\tilde{\mu})$ obtained by integrating the bare density of states (4) is also shown for comparison. The result for $n'(\tilde{\mu})$ is shown at $\tilde{\mu} < -\mu_c$ only. One can see that the dependence $n(\tilde{\mu})$ yields the pinning of the Fermi surface in the concentration range about 4% above and below VH filling [in fact, in the present approach the picture is symmetric, $n(\tilde{\mu}) - n_{\text{VH}} = n_{\text{VH}} - n(-\tilde{\mu})$]. Such behavior is in qualitative agreement with the ARPES results of Ref. [15]. On the other hand, this is in contrast with the behavior of the chemical potential measured relative to its position in the insulating phase (Ref. [24]).

It is important that the condition $|n'(\tilde{\mu}) - n_{\text{VH}}| > |n(\tilde{\mu}) - n_{\text{VH}}|$ holds. This means that after account of renormalizations the pinning effect becomes even stronger than that given by Eqs. (13) and (15). Being extrapolated to the region $|\tilde{\mu}/t| < v_c$, the dependence $n'(\tilde{\mu})$ should give even larger values of critical concentrations (about 6%). One can expect that, for larger values of U/t , the critical concentrations will be larger.

To conclude, we have developed a RG approach which gives a possibility to describe the flattening of the electron spectrum and does not suppose the presence of strong antiferromagnetic fluctuations. As a result of the peculiar structure of the spectrum, the pinning of the Fermi level to Van Hove singularities in 2D systems occurs, the chemical potential being practically constant in a range of dopings near VH filling. In the pinning region the electron density of states is determined by the quasiparticle damping and

the system demonstrates essentially non-Fermi-liquid behavior. Further experimental investigations on LaSrCuO and Bi2212 systems would be of interest to verify the pinning picture proposed.

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