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Electron spectral functions of two-dimensional high-T_c superconductors in the model of fermion ocndensation

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Spectral functions of strongly correlated two-dimensional (2D) electron systems in solids are studied on the assumption that these systems undergo a phase transition, called fermion condensation, whose characteristic feature is flattening of the electron spectrum $\epsilon(\mathbf{p})$. Unlike the previous models in the present study, the decay of single-particle states is properly taken into account. Results of our calculations are shown to be in qualitative agreement with ARPES data. The universal behavior of the ratio $\mathrm{Im}\,\Sigma(\mathbf{p},\varepsilon,T)/T$ as a function of $x=\varepsilon/T$, uncovered in [3] for the single-particle states around the diagonal of the Brillouin zone, are found to be reproduced reasonably well. However, in our model this behavior is destroyed in vicinities of the van Hove points where the fermion condensate resides.

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The single-particle (SP) dynamics of Fermi systems at near zero temperatures T is known to depend crucially on the index ν, that characterizes the imaginary part of the mass operator, $\mathrm{Im}\,\Sigma(\varepsilon\to 0)\sim\varepsilon^{\nu}$, the energy ε being measured from the chemical potential μ. In ordinary homogeneous Fermi liquids such as nuclear matter and liquid ^{3}He, where the exclusion principle "leads the dance", the index ν equals 2, and the Fermi liquid can be treated as a gas of interacting "immortal" quasiparticles, the cornerstone of standard Fermi liquid theory (SFLT) [1]. After many successful years, SFLT is currently encountering serious difficulties in treating normal states of 2D high-T_c superconductors. The analysis of ARPES data shows that even around the diagonals of the Brillouin zone, the index ν is unity [2, 3], while in the immediate vicinity of the van Hove points (vHP), the sharp ARPES peaks disappear altogether [4 – 6].

We propose that solution of this challenging problem is associated with fermion condensation [7 – 17], a novel phase transition that generates a domain C of dispersionless states, called the fermion condensate (FC), whose energies $\epsilon(\mathbf{p})$ coincide with μ. As a rule, in strongly correlated anisotropic electron systems of high-T_c superconductors, the FC occupies vicinities of the vHP [8, 18], the region, where the Fermi liquid approach just fails. States with the FC have been uncovered [7] as unconventional solutions of equations of Landau theory at $T=0$. However, in dealing with spectral functions of strongly correlated Fermi systems, the basic equation of the fermion condensation $\epsilon(\mathbf{p}\in \mathrm{C};n)=\mu$ should be rewritten as [18]

$$\epsilon^0_{\mathbf{p}}+\Sigma(\mathbf{p},\varepsilon=0;n)=\mu,\qquad \mathbf{p}\in \mathrm{C}. \tag{1}$$

Beyond the FC phase transition point, this equation does determine a new momentum distribution $n(\mathbf{p})$ differing from the conventional one $n_F(\mathbf{p})=\theta(\mu-\epsilon(\mathbf{p}))$. The degeneracy of the SP spectrum at $T=0$, a salient feature of the solution given by Eq. (1), is lifted by pairing correlations which are ignored in writing this relation. In doing so, the BCS occupation numbers $v^2(\mathbf{p})$ coincide with $n(\mathbf{p})$ evaluated from Eq. (1) provided the BCS coupling constant is rather small [13]. For this reason, superfluid systems with and without the FC look more alike than normal ones, since in normal states of conventional Fermi liquids, the damping makes no difference, whereas in normal states of systems with the FC, the damping becomes a real "weathermaker". Indeed, the relevant contribution to $\mathrm{Im}\,\Sigma_R(\mathbf{p},\varepsilon)$ is given by [19]

$$\mathrm{Im}\,\Sigma_R(\mathbf{p},\varepsilon)\sim\sum_{\mathbf{q},\mathbf{p}_1}\iint d\omega\, d\varepsilon_1 F(\varepsilon,\omega,\varepsilon_1,T)\times$$
$$\times|\Gamma(\mathbf{p},\varepsilon,\mathbf{p}_1,\varepsilon_1,\mathbf{q},\omega;n)|^2\mathrm{Im}\,G_R(\mathbf{p}-\mathbf{q},\varepsilon-\omega)\times$$
$$\times\,\mathrm{Im}\,G_R(-\mathbf{p}_1,-\varepsilon_1)\,\mathrm{Im}\,G_R(\mathbf{q}-\mathbf{p}_1,\omega-\varepsilon_1)\;, \tag{2}$$

where the factor

$$F(\varepsilon,\omega,\varepsilon_1,T)=\cosh\left(\frac{\varepsilon}{2T}\right)\times$$
$$\times\left[\cosh\left(\frac{\varepsilon_1}{2T}\right)\cosh\left(\frac{\varepsilon-\omega}{2T}\right)\cosh\left(\frac{\omega-\varepsilon_1}{2T}\right)\right]^{-1},$$

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$|\Gamma|^2$ is the absolute square of the scattering amplitude, properly averaged over spin variables, and G_R is the retarded Green function with $\mathrm{Im}\, G_R(\mathbf{p},\varepsilon) = -\gamma(\mathbf{p},\varepsilon)[(\varepsilon - \sigma(\mathbf{p},\varepsilon) - s(\mathbf{p}))^2 + \gamma^2(\mathbf{p},\varepsilon)]^{-1}$, where $\sigma(\mathbf{p},\varepsilon) = \mathrm{Re}\,\Sigma_R(\mathbf{p},\varepsilon) - \mathrm{Re}\,\Sigma_R(\mathbf{p},\varepsilon=0)$ and $s(\mathbf{p}) = \epsilon^0_{\mathbf{p}} + \mathrm{Re}\,\Sigma_R(\mathbf{p},\varepsilon=0) - \mu$.

We restrict ourselves to temperatures T markedly lower than the characteristic temperature T_f of destroying the FC that allows one to ignore the T-dependence of η, the fraction of the Brillouin zone occupied by the FC. To simplify the problem, we replace the function $\gamma(\mathbf{p},\varepsilon)$ by a set of functions of the single variable ε, e.g. in the FC region, $\gamma(\mathbf{p}\in \mathrm{C},\varepsilon)$ is reduced to $\gamma_{\mathrm{C}}(\varepsilon)$. The complementary region of momentum space, in which the dispersion of the spectrum $\epsilon(\mathbf{p})$ has a nonzero value, is composed of two subregions. The first, adjacent to the FC domain and henceforth denoted by T, is a transition region, in which the same decay processes, as in the FC region, are still kinematically allowed. The second subregion, denoted by M, is located around diagonals of the Brillouin zone. Here some of these processes are either kinematically forbidden or at least strongly suppressed. Correspondingly, $\gamma(\mathbf{p}\in \mathrm{T},\varepsilon) \to \gamma_{\mathrm{T}}(\varepsilon), \gamma(\mathbf{p}\in \mathrm{M},\varepsilon) \to \gamma_{\mathrm{M}}(\varepsilon)$. To close the set of equations of the problem, the amplitude $\Gamma(n)$ should somehow be specified. Bearing in mind that η is small, we neglect the FC contributions to Γ, replacing it by $\Gamma(n_F)$. In this article we continue to examine a scenario of [18] when the fermion condensation precedes the antiferromagnetic phase transition and employ the same amplitude $\Gamma(\mathbf{p},\mathbf{p}_1;n_F)$ as in [20, 18], $\Gamma(\mathbf{p},\mathbf{p}_1;n_F) \sim [\beta^2 + \kappa^2(\mathbf{p}-\mathbf{p}_1-\mathbf{Q})^2]^{-1}$, where $\mathbf{Q} = (\pi,\pi)$, is taken.

We start with the case $\varepsilon \gg T$, and set $T=0$ in the integral (2), thus dropping all T-dependent contributions. First we evaluate $\gamma_{\mathrm{C}}(\varepsilon\to 0)$. In this case, (i) contributions from processes involving only the FC states prevail (see below), (ii) the quantity $|\Gamma(n_F)|^2 \sim \beta^{-4}$ can be factored out of the integral (2), and (iii) the quantity $s(\mathbf{p}\in \mathrm{C},T)$, which vanishes over the FC region at $T=0$, can be verified to remain small compared to leading terms in Eq. (2), and thus can be neglected. As a result, the energy and momentum integrations in Eq. (2) separate. Taking for certainty $\varepsilon > 0$ and omitting numerical factors, we are left with

$$\gamma_{\mathrm{C}}(\varepsilon\to 0) \sim \qquad (3)$$

$$\sim \beta^{-4}\eta^2 \int\limits_0^{\varepsilon}\int\limits_0^{\omega} A_{\mathrm{C}}(\varepsilon-\omega)\, A_{\mathrm{C}}(-\varepsilon_1)\, A_{\mathrm{C}}(\omega-\varepsilon_1)\, d\omega\, d\varepsilon_1,$$

where $A_{\mathrm{C}}(\varepsilon) = \mathrm{Im}\, G_R(\mathbf{p}\in \mathrm{C},\varepsilon)$. To proceed, we insert $\gamma_{\mathrm{C}}(\varepsilon\to 0) \sim \varepsilon^{\nu_{\mathrm{C}}}$ into the Kramers-Krönig relation to obtain $\sigma_{\mathrm{C}}(\varepsilon\to 0) \sim \varepsilon^{\nu_{\mathrm{C}}}$. We then substitute γ_{C} and σ_{C} into A_{C} and find $A_{\mathrm{C}}(\varepsilon\to 0) \sim \varepsilon^{-\nu_{\mathrm{C}}}$. Finally, upon inserting this result into Eq. (3), we arrive at $\nu_{\mathrm{C}} = 1/2$ [16]. More precisely, one obtains $\gamma_{\mathrm{C}}(\varepsilon\to 0) \sim \beta^{-1}(\eta\varepsilon^0_F\varepsilon)^{1/2}$ and

$$G_R(\mathbf{p}\in \mathrm{C},\varepsilon\to 0) \sim e^{-i\pi/4}[\gamma_{\mathrm{C}}(\varepsilon\to 0)]^{-1} \sim$$

$$\sim e^{-i\pi/4}\beta(\eta\varepsilon^0_F\varepsilon)^{-1/2}\ . \qquad (4)$$

This result can be shown to hold even if the momentum dependence of the quantities $\gamma_{\mathrm{C}}(\mathbf{p},\varepsilon)$ and $\sigma_{\mathrm{C}}(\mathbf{p},\varepsilon)$ is properly taken into account to ensure the correct momentum distribution $n(\mathbf{p})$. We see that in the FC region, the conventional structure of the Green function is destroyed, the familiar pole being replaced by a branch point at $\varepsilon = 0$.

Now we are in position to discuss the impact of the damping on the topological charge N of a system with the FC, introduced by Volovik [8]. Recall, that in 2D systems, this charge is given by the integral

$$N = \oint\limits_L \frac{dl}{2\pi i}\, G(\mathbf{p},\varepsilon{=}i\Omega)\, \partial_l G^{-1}(\mathbf{p},\varepsilon{=}i\Omega)\ , \qquad (5)$$

taken along the contour L, embracing the Fermi line in the 3D space (p_x,p_y,Ω). If one neglects the ε-dependence of $\Sigma(\mathbf{p},\varepsilon)$, then the FC Green function $G(\mathbf{p}\in \mathrm{C},\varepsilon) = [\varepsilon + \mu - \epsilon^0_{\mathbf{p}} - \Sigma(\mathbf{p},\varepsilon)]^{-1}$ becomes $1/\varepsilon$, and upon inserting this expression for G into the integral (5), one finds $N = 1/2$, implying that systems with the FC form a separate class of normal Fermi liquids [8]. What happens to the topological charge N, if the energy dependence of the mass operator is incorporated and $G = 1/\varepsilon$ is replaced by the Green function (4)? After performing simple integration, we are again led to the previous result $N = 1/2$ [8], in spite of the dramatic alteration of the Green function itself that occurs in the FC region.

In the transition region T, the decay into the FC states is not kinematically forbidden. Accordingly, $\gamma_{\mathrm{T}}(\varepsilon\to 0) \sim \beta^{-1}(\eta\varepsilon^0_F\varepsilon)^{1/2}$, while the function $s(\mathbf{p}\in \mathrm{T})$ already differs from zero. Requiring it to vanish at the boundaries of the FC region along with its first derivative, one finds that in the region T, the conventional structure of the Green function is recovered, but in the vicinity of the FC domain, SP excitations appear to be ill-defined, since the pole of $G(\mathbf{p},\varepsilon)$ is located close to the imaginary energy axis.

In the region M, dominant contributions to $\mathrm{Im}\,\Sigma_R(\varepsilon)$ come from a process associated with the generation of three states: two from the FC region and one from the M region. In this case, the formula for finding $\gamma_{\mathrm{M}}(\varepsilon\to 0)$ reads

$$\gamma_{\rm M}(\varepsilon\to 0)\sim\beta^{-4}\sum_{\mathbf{p},\mathbf{p}_1}\int_0^{\varepsilon}\int_0^{\omega}A_{\rm C}(-\varepsilon_1)\,A_{\rm C}(\omega-\varepsilon_1)\times$$
$$\times\,[1-\theta(\mathbf{p})]\,P_{\rm C}(\mathbf{p}-\mathbf{p}_1)\,A_{\rm M}(\mathbf{p},\varepsilon-\omega)\,d\omega\,d\varepsilon_1, \qquad (6)$$

where $P_{\rm C}(\mathbf{q})=\sum_{\mathbf{p}}\theta(\mathbf{p})\theta(\mathbf{p}-\mathbf{q})$ and $\theta(\mathbf{p})=1$ if $\mathbf{p}\in$ C and otherwise vanishes. It is seen that in this case, the momentum and energy integrations do not separate. However, one can take advantage of the fact that the spectrum $\xi_{\rm M}(\mathbf{p})=\epsilon_{\rm M}(\mathbf{p})-\mu$ is proportional to $(p-p_F)$ and introduce $\xi_{\rm M}(\mathbf{p})$ as a new variable. Then after simple integration, we are led to the result $\nu_{\rm M}=1$ postulated in the model of a marginal Fermi liquid [21]. Evaluation of the η-dependence of relevant quantities in the M region yields $\gamma_{\rm M}(\varepsilon\to 0)\sim\beta^{-2}\eta^{1/2}\varepsilon$ and $\sigma_{\rm M}(\varepsilon\to 0)\sim\beta^{-2}\eta^{1/2}\varepsilon\ln|\varepsilon|$.

These results can be applied to the case $\varepsilon\sim T$, where according to Eq. (4), the leading term in the FC Green function has the form $G_R(\mathbf{p}\in {\rm C},\varepsilon)\sim e^{-i\pi/4}[\gamma_{\rm C}(\varepsilon,T)]^{-1}$. Upon inserting this expression into Eq. (3) one finds that the damping $\gamma_{\rm C}(x,T)$, where $x=\varepsilon/T$, can be displayed as $\gamma_{\rm C}(x,T)=\gamma_{\rm C}\sqrt{T\varepsilon_F^0}\,D(x)$ where the constant $\gamma_{\rm C}$ specifies the compound, while the dimensionless quantity $D(x)$ obeys the universal integral equation

$$D(x)=\cosh\frac{x}{2}\times \qquad (7)$$
$$\times\iint\frac{dy\,dz}{\cosh\frac{y}{2}\cosh\frac{x-z}{2}\cosh\frac{z-y}{2}\,D(-y)\,D(x-z)\,D(z-y)}.$$

With this result, the damping $\gamma_{\rm M}(x,T)$ is calculated straifghtforwardly:

$$\gamma_{\rm M}(x,T)=\gamma_{\rm M}T\cosh\frac{x}{2}\times \qquad (8)$$
$$\times\iint\frac{dy\,dz}{\cosh\frac{y}{2}\cosh\frac{x-z}{2}\cosh\frac{z-y}{2}\,D(-y)\,D(z-y)},$$

the constant $\gamma_{\rm M}$ being a characteristics of the given compound. The function $\gamma_{\rm M}(x,T)/T$ starts out of the origin as a parabolic function $\gamma_{\rm M}(x,T)/T\sim 1+0.1x^2$. The asymptotic regime $\gamma_{\rm M}(x,T)/T\sim x$, stemming from Eq. (6), is attained at $x\sim 2.5$.

Relations (7), (8) hold even in superfluid states as long as the gap value remains less than the damping $\gamma_{\rm C}(T)$. On the other hand, they are violated if energy attains values, at which contributions to $\gamma(\varepsilon)$ that were omitted from Eqs. (3) and (6) become comparable to the terms that were retained. A leading correction $\delta\gamma_{\rm C}(\varepsilon)$ to the integral (3) comes from final states, that involve one hole (particle) belonging to the region T. Eq. (6) can be employed to estimate this contribution, with the single replacement $s(\mathbf{p}\in{\rm M})\to s(\mathbf{p}\in{\rm T})$. We find $\delta\gamma_{\rm C}(\varepsilon\to 0)\sim\beta^{-1}\varepsilon$, which is independent of the η value. Estimation of other corrections to $\gamma(\varepsilon)$ is carried out along the same lines, justifying the identification of (3) and (6) as paramount contributions to ${\rm Im}\,\Sigma_R(\mathbf{p},\varepsilon\to 0)$ until ε exceeds the characteristic FC energy $\varepsilon_{FC}\simeq\eta\varepsilon_F^0$, evaluated by comparison of $\delta\gamma_{\rm C}(\varepsilon)$ and $\gamma_{\rm C}(\varepsilon)\sim\beta^{-1}(\eta\varepsilon_F^0\varepsilon)^{1/2}$.

At energies $\varepsilon\geq\varepsilon_{FC}$ corrections exhibit themselves in full force, so Eq. (2) should be solved numerically in conjunction with the Kramers-Krönig relation, employed to connect $\gamma(\varepsilon)$ and $\sigma(\varepsilon)$. This is performed with the aid of an iteration procedure, which converges rapidly. In Fig.1 we display results from these calculations. Two

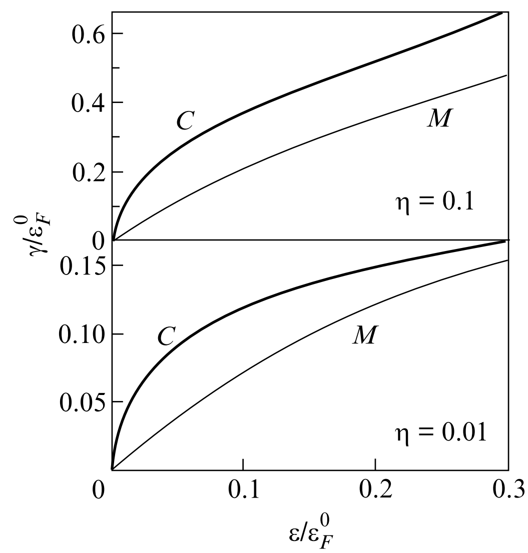

Fig.1. The damping of the SP states in the vicinity of the vHP (solid lines) and around the diagonals of the Brillouin zone (thin lines), calculated with the scattering amplitude $\Gamma(\mathbf{p},\mathbf{p}_1)=(N(0))^{-1}[\beta^2+\kappa^2(\mathbf{p}-\mathbf{p}_1-\mathbf{Q})^2]^{-1}$, where $N(0)$ is the density of states and $\beta=0.2$, for $\eta=0.1$ (upper panel) and $\eta=0.01$ (lower panel), and measured in ε_F^0

different η values, specifying the fraction of the Brillouin zone occupied by the FC, were considered: (a) $\eta=0.1$, close to the maximum η value in the model of fermion condensation driven by antiferromagnetic fluctuations [18], and (b) $\eta=0.01$. In spite of the simplicity of the interaction adopted, salient features of ARPES data [3, 6, 15] are reproduced, including the shape of the curve ${\rm Im}\,\Sigma_R(\mathbf{p}\in{\rm M},x,T)/T$ as a function of $x=\varepsilon/T$ measured in [3] for the optimally doped cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$, provided the proper nomalization of the results is done. Moreover, our theory predicts the same behavior of ${\rm Im}\,\Sigma_R(\mathbf{p}\in{\rm M},x)/T$ in different compounds. This can be seen from Fig.2, where two curves of ${\rm Im}\,\Sigma_R(\mathbf{p}\in{\rm M},x,T)/T$ evaluated at $\eta=0.1$

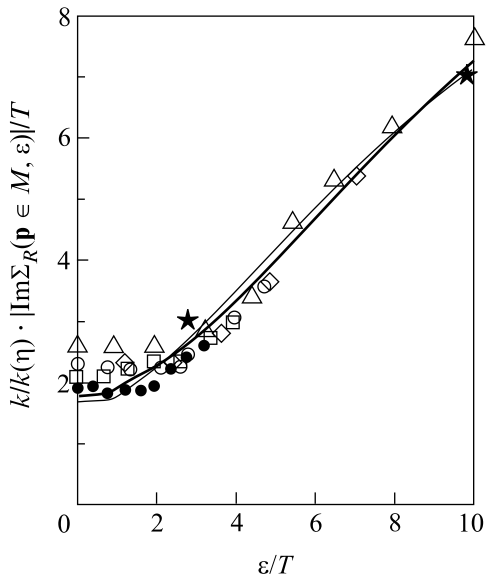

Fig.2. The ratio $|\mathrm{Im}\,\Sigma_R(\varepsilon)|/T$ around the diagonal of the Brillouin zone as a function of ε/T, calculated for $\eta = 0.1$ (solid line) $\eta = 0.01$ (thin line) and normalized to the same slope $k = 0.75$, i.e. multiplied by the factor $k/k(\eta)$, where $k(\eta) = |\partial\,\mathrm{Im}\,\Sigma_R(\mathbf{p}{\in}\mathrm{M},\varepsilon,T;\eta)/\partial\varepsilon|$. The experimental data for the optimally doped cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$ [3] are shown by open and solid circles ($T = 300$ K), triangles and squares ($T = 90$ K), and diamonds and stars ($T = 48$ K)

and $\eta = 0.01$ and normalized at $x \gg 1$ to the same slope are compared to each other and to experimental data [3]. At the same time, as seen from the above formula $\gamma_C(x,T) = \gamma_C\sqrt{T\varepsilon_F^0}\,D(x)$, the linearity of $\mathrm{Im}\,\Sigma_R(T)$ with T at a given x, uncovered in [3], is destroyed in the FC region, and instead this function displays $\sqrt{T}$-dependence.

The above scenario in which the fermion condensation precedes the antiferromagnetic phase transition does apply in the three-dimensional case, although the range of the FC region shrinks markedly. Along the same lines, one can analyze the situation with fermion condensation in the vicinity of other second order phase transitions, such as charge-density-wave instability [12]. So far the feedback of the FC on the scattering amplitude Γ has been ignored. However, the simplest FC diagram, i.e. a loop, evaluated with the FC Green function (4), diverges logarithmically. As a result, we are led to a familiar problem of the parquet-diagram summation, solution of which will be reported in a separate paper.

Summing up the results of our analysis, we infer that electron systems with a fermion condensate, irrespective of the dimensionality, do not admit Landau quasiparticles, since the renormalization factor $z = (1-\partial\Sigma/\partial\varepsilon)_F^{-1}$ that determines the quasiparticle weight in the SP state vanishes in all regions of the Brillouin zone. The model of fermion condensation presented here allows one to explain basic features of the spectral functions of normal states of high-T_c superconductors, including (i) the marginal Fermi liquid behavior of the damping of SP states around the diagonals of the Brillouin zone (the M region) and (ii) the suppression of the peaks in APRES data in the immediate vicinity of the van Hove points (the C region). And the universal behavior of the ratio $\mathrm{Im}\,\Sigma_R(\mathbf{p} \in \mathrm{M}, T, x)/T$ where $x = \varepsilon/T$, as established in the M region in [3], is also reproduced in this model. Moreover, our model predicts that all data for $\mathrm{Im}\,\Sigma_R(\mathbf{p} \in \mathrm{M}, T, x)/T$, when properly normalized, should collapse on the same curve. However, as we have seen, this universal behavior is destroyed in the C region.

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