Fermi surface truncation from thermal nematic fluctuations

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We analyze how thermal fluctuations near a finite temperature nematic phase transition affect the spectral function $A(k, \omega)$ for single-electron excitations in a two-dimensional metal. Perturbation theory yields a splitting of the quasi-particle peak with a $d$-wave form factor, reminiscent of a pseudogap. We present a resummation of contributions to all orders in the Gaussian fluctuation regime. Instead of a splitting, the resulting spectral function exhibits a pronounced broadening of the quasi-particle peak, which varies strongly around the Fermi surface and vanishes upon approaching the Brillouin zone diagonal. The Fermi surface obtained from a Brillouin zone plot of $A(k,0)$ seems truncated to Fermi arcs.

The concept of nematic order in interacting electron liquids has attracted considerable interest over the last decade, mostly in the context of (quasi) two-dimensional systems.\textsuperscript{1, 2} In a nematic state an orientational symmetry of the system is spontaneously broken, without breaking however the translation invariance. One route toward a nematic state is via partial melting of stripe order in a doped antiferromagnetic Mott insulator.\textsuperscript{3} Alternatively, a nematic state can be obtained from a Pomeranchuk instability generated by forward scattering interactions in a normal metal.\textsuperscript{4, 5} On a square lattice, the most natural candidate for a Pomeranchuk instability has $d_{x^2-y^2}$ symmetry.

Signatures of nematic order with a $d_{x^2-y^2}$ symmetry have been observed in several strongly interacting electron materials. A nematic phase with a sharply defined phase boundary has been established for Sr$_3$Ru$_2$O$_7$ in a strong magnetic field.\textsuperscript{6} Nematic order has also been observed in the high temperature superconductor YBa$_2$Cu$_3$O$_y$ in transport experiments and neutron scattering.\textsuperscript{7} Due to the slight orthorhombicity of the CuO$_2$ planes one cannot expect a sharp nematic phase transition in YBa$_2$Cu$_3$O$_y$. However, the strong temperature dependence of the observed in-plane anisotropy indicates that the system develops an intrinsic electronic nematicity, which drastically enhances the in-plane anisotropy imposed by the structure.\textsuperscript{10, 11}

Nematic fluctuations close to a continuous nematic quantum phase transition naturally lead to non-Fermi liquid behavior.\textsuperscript{12, 14} For a $d$-wave Pomeranchuk instability on a square lattice, the decay rate of electronic excitations is strongly momentum dependent along the Fermi surface. At the quantum critical point, the decay rate for single-particle excitations is proportional to $d^2_k |\omega|^{2/3}$, where $\omega$ is the excitation energy and $d_k$ is a form factor with $d$-wave symmetry, such as $d_k = \cos k_x - \cos k_y$.\textsuperscript{13, 15} Landau quasi-particles are thus unstable everywhere on the Fermi surface except at the Brillouin zone diagonals, where $d_k$ vanishes. The temperature dependence of the decay rate in the quantum critical regime near the quantum critical point also differs strongly from Fermi liquid behavior.\textsuperscript{16, 17}

Previous works on non-Fermi liquid behavior caused by nematic fluctuations focussed on the quantum critical point and the quantum critical regime at finite temperature. In this paper we analyze the spectral function for single-particle excitations in the thermal fluctuation regime near a nematic phase transition at finite temperatures. We show that a perturbative calculation of the self-energy in that regime leads to a splitting of the quasi-particle peak with a $d$-wave form factor in the single-particle excitation spectrum, reminiscent of a pseudogap. However, in a self-consistent calculation the split peak in the spectral function is replaced by a single broad peak.

In the Gaussian fluctuation regime, a summation of vertex corrections to all orders is possible and confirms the self-consistent result. The Fermi surface obtained from the peak of the spectral function at zero excitation energy is thus smeared by a smooth broadening, which is most pronounced near the points $(\pi, 0)$ and $(0, \pi)$ of the Brillouin zone, while it gradually decreases toward the Brillouin zone diagonal.

We consider a one-band system of electrons on a square lattice with a tight-binding dispersion $c_k$ and an effective interaction of the form\textsuperscript{13}

$$H_I = \frac{1}{2L} \sum_{\mathbf{q}} g(\mathbf{q}) n_d(\mathbf{q}) n_d(-\mathbf{q}),$$

where $n_d(\mathbf{q}) = \sum_{\mathbf{k},\sigma} d^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k+q},\sigma}^c c_{\mathbf{k+q},\sigma}$ are $d$-wave density fluctuation operators, and $L$ is the number of sites. The function $g(\mathbf{q})$ is negative and peaked at $\mathbf{q} = 0$, so that forward scattering dominates. An effective interaction of the form $H_I$ can be obtained from microscopic models such as the Hubbard or $t$-$J$ model.\textsuperscript{5, 6}

For sufficiently negative values of $g = g(0)$ the interaction generates a $d$-wave Pomeranchuk instability leading to a nematic state with a spontaneously broken orientation symmetry.\textsuperscript{13, 18, 20} A suitable order parameter
characterizing the symmetry breaking is provided by the expectation value \( \langle n_d(0) \rangle \). Close to the transition (if continuous), strong \( d \)-wave density fluctuations with a long wavelength develop, which lead to a singular effective interaction. In the quantum critical regime the effective interaction is dynamical and of the form

\[
D_{kk'}(q, \nu_n) = -\frac{g \, dq \, dq'}{(\xi_0/\xi)^2 + \xi_0^2 |q|^2 + |\nu_n|/(u|q|) ^2},
\]

where \( \nu_n = 2\pi n T \) is a bosonic Matsubara frequency; \( \xi \) is the nematic correlation length, while \( \xi_0 \) and \( u \) are non-universal parameters determined by the momentum dependence of \( g(q) \) and the band structure. In the thermal fluctuation regime near the finite temperature phase transition, quantum (\( \nu_n \neq 0 \)) fluctuations are cut off by temperature, such that only the classical part of the effective interaction,

\[
D_{kk'}(q) = D_{kk'}(q, 0) = -\frac{g \, dq \, dq'}{\xi^2 + |q|^2},
\]

with \( \tilde{g} = g/\xi_0^2 \), is important.

The nematic transition on a square lattice belongs to the two-dimensional Ising universality class. A thermal phase transition at a critical temperature \( T_c > 0 \) is possible, since the dimensionality of the system is above the lower critical dimension (one). The correlation length \( \xi \) diverges at \( T_c \). Approaching the critical temperature, one first passes through a Gaussian fluctuation regime, where order parameter interactions are not important. Moving closer to \( T_c \), one enters the Ginzburg region, where order parameter interactions become relevant, and the fluctuation propagator acquires an anomalous scaling dimension \([21]\). Close to the quantum critical point, the width of the Ginzburg region is of order \( T_c/\log T_c \) \([22]\).

The momentum resolved spectral function for single-particle excitations can be written as

\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\omega - (\epsilon_k - \mu) - \Sigma(k, \omega)},
\]

where \( G(k, \omega) \) and \( \Sigma(k, \omega) \) are the retarded Green function and self-energy, respectively. We first compute the self-energy perturbatively to first order in the effective interaction. The contribution from classical fluctuations is given by \([16]\)

\[
\Sigma(k, \omega) = -T \int \frac{d^2 q}{(2\pi)^2} D_{kk'}(q) G(k - q, \omega).
\]

In a non-selfconsistent evaluation of Eq. \((5)\) one approximates \( G \) by the non-interacting Green function \( G_0(k, \omega) = [\omega - (\epsilon_k - \mu) + i0^+]^{-1} \). The self-energy can then be computed analytically. The imaginary part has been obtained already previously \([16]\). For momenta close to the Fermi surface and small frequencies one finds

\[
\text{Im} \Sigma(k, \omega) = -\frac{g \, dq \, dq'}{4\pi q} T \xi^2 \left( \frac{l(\kappa)}{1 + \kappa l(\kappa)} \right),
\]

where \( v_k = |\nabla \epsilon_k| \) is the velocity of the electrons, \( \kappa = |\omega - (\epsilon_k - \mu)|/v_k \), and \( l(\kappa) = (1 + \kappa^4)^{-1/2} \). We assume that the Fermi surface does not cross van Hove points, such that \( v_k \) is finite. The real part of the self energy is obtained either by a direct evaluation of Eq. \((3)\) or by a Kramers-Kronig transformation of the imaginary part as

\[
\text{Re} \Sigma(k, \omega) = \frac{\tilde{g} q^2}{4\pi v_k^2} T \xi^2 \left( \frac{1 - \kappa l(\kappa)}{1 + \kappa l(\kappa)} \right).
\]

In Fig. 1 we show results for the spectral function as obtained from the non-selfconsistent first order calculation of the self-energy. Here and in all further numerical results we have chosen a dispersion \( \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) \) with hopping amplitudes \( t = 1 \), \( t' = -0.3 \), and \( t'' = 0.15 \). The lattice constant is one, and the chemical potential \( \mu \) has been chosen such that the electron density is fixed at \( n = 0.9 \). The corresponding Fermi surface is closed around \((\pi, \pi)\). The coupling constant is \( \tilde{g} = -1.2 \) and the temperature \( T = 0.15 \). We have not attempted to compute the correlation length, since it depends on model details such as the momentum dependence of \( g(q) \). Instead we show results for various choices of \( \xi \). One can see that a pronounced splitting of the quasi-particle peak develops for increasing \( \xi \), which could be interpreted as a fluctuation precursor of the symmetry-broken state. However, we now show that the splitting disappears in a self-consistent calculation, and it is not restored by vertex corrections, at least in the Gaussian fluctuation regime.

![FIG. 1: (Color online) Spectral function \( A(k, \omega) \) as obtained from a non-selfconsistent perturbative calculation of the self-energy for various choices of the correlation length \( \xi \). The graphs show \( A(k, \omega) \) as a function of \( \omega \) for a fixed momentum \( k = (0.69, 2.34) \) on the Fermi surface remote from the Brillouin zone diagonal (see inset).](image-url)
acting on the fluctuation propagator $D_{kk}(q)$, yielding
\begin{equation}
\hat{D}_k(q_r) = \int \frac{dq_r}{2\pi} D_{kk}(q) = \frac{\hat{g}_{kk}^2}{2\sqrt{q_r^2 + q_f^2}}.
\end{equation}

The momentum dependence of the self-energy $\Sigma(k, \omega)$ can be parametrized by the Fermi momentum $k_F$ closest to $k$, and the oriented distance from the Fermi surface $k_r$, which carries the sign of $\hat{g}_k$. One then obtains the one-dimensional integral equation
\begin{equation}
\Sigma(k_r, \omega) = \frac{\hat{g}_{kk}^2 \left( \frac{T}{4\pi} \right)}{\sqrt{\omega^2 + \Omega^2}} \times \frac{1}{v_F(k_r - \omega - \Sigma(k_r - \omega))}.
\end{equation}

Note that $\Sigma$ does not depend on $k_r$ and $\omega$ independently, but only on the difference $\omega - v_F k_r$. The dependence of $\Sigma$ on $k_F$ enters only parametrically via $v_F$ and $d_{kF}$ and has not been written explicitly. The integral equation (9) can be solved numerically. The results for $A(k, \omega)$ differ strongly from those suggested by non-self-consistent perturbation theory. The quasi-particle splitting observed in the perturbative calculation (Fig. 1) is wiped out completely by the self-energy feedback into $G$. The spectral function exhibits only a single peak with a maximum at $\omega = v_F k_r$, even for a very large correlation length $\xi$.

We now consider higher order contributions not contained in the self-consistent one-loop approximation (6). The sum over all self-energy contributions generated by thermal fluctuations can be written as
\begin{equation}
\Sigma(k, \omega) = -T \int \frac{d^2q}{(2\pi)^2} A_{kk}(q) G(k - q, \omega) \times \Lambda(k - q/2, \omega; \nu, 0),
\end{equation}
where $\Lambda(k, \omega; q, \nu)$ is the irreducible charge vertex including all vertex corrections. We exploit the fact that dominant contributions are due to small momentum transfers $q$ of order $\xi^{-1}$, to resum vertex corrections via an asymptotic Ward identity [23, 24]. For small $q$, the charge vertex is related to the current vertex $A$ and the propagator via the Ward identity $\nu \Lambda(k, \omega; q, \nu) - \Lambda(k, \omega; q, \nu) \cdot \Lambda(k, \omega; q, \nu) = G^{-1}(k + q/2, \omega + \nu/2) - G^{-1}(k - q/2, \omega - \nu/2)$. In the Gaussian fluctuation regime, interactions between order parameter fluctuations are not important. In a diagrammatic representation of perturbation theory, these interactions are generated by fermionic loops with more than two vertices. Neglecting Feynman diagrams with such loops leads to two simplifications. First, the effective interaction [3] remains unrenormalized. Second, diagrams contributing to the charge and current vertices involve only an open fermionic line. Since contributions with small $q$ dominate, the electron velocity $v_F$ entering the current operator is almost conserved such that the current vertex can be expressed by the charge vertex as $A(k, \omega; q, \nu) = \hat{v}_k \Lambda(k, \omega; q, \nu)$. The latter relation holds for each Feynman diagram without fermionic loops. Combining this with the Ward identity one obtains, in the static limit $\nu = 0$,
\begin{equation}
\Lambda(k, \omega; q, 0) = G^{-1}(k - q/2, \omega) - G^{-1}(k + q/2, \omega),
\end{equation}

Inserting Eq. (11) into Eq. (10), and using the Dyson equation $G^{-1} = G^{-1}_0 - \Sigma$, one obtains a closed system of equations for $\Sigma$ and $G$.

Decomposing the momenta $k$ and $q$ in radial and tangential components, and integrating $D_{kk}(q)$ over $q$, as before (self-consistent solution), one finds a one-dimensional linear integral equation for $G$,
\begin{equation}
(\omega - v_{k_F} k_r + i0^+) G(k_r, \omega) = 1 + T \int \frac{dq_r}{2\pi} \frac{D_{kk}(q_r)}{v_{k_F} q_r} G(k_r - q, \omega),
\end{equation}
with $D_{kk}(q_r)$ from Eq. (8).

Note that vertex corrections cannot be summed by the above method at a nematic quantum critical point or for the related problem of non-relativistic fermions coupled to a $U(1)$ gauge field. This is because in these cases the dominant momentum transfers are almost tangential to the Fermi surface, so that the term $v_F \cdot q$ becomes subleading compared to contributions originating from fluctuations of the electron velocity [24].

The integral equation (12) can be converted to a linear differential equation by a Fourier transformation. The differential equation can be solved by standard methods. The result for the spectral function reads
\begin{equation}
A(k, \omega) = \int_{-\infty}^{\infty} dx \hat{A}(x) e^{i(\omega - v_{k_F} k_r) x/v_{k_F}},
\end{equation}
where
\begin{equation}
\hat{A}(x) = \frac{1}{2\pi v_{k_F}} \exp \left[ \int_0^x dx' \int_0^{x'} dx'' T \frac{\hat{g}_{kk}^2}{2\pi v_{k_F}^2} K_0(x''/\xi) \right].
\end{equation}

$K_0$ is a modified Bessel function. Note that $A(k, \omega)$ depends on $k_r$ and $\omega$ only via the difference $\omega - v_{k_F} k_r$.

In Fig. 2 we plot the spectral function $A(k, \omega)$ for the same parameters as in Fig. 1. The function exhibits only a single peak with no trace of a splitting. The splitting present in Fig. 1 is therefore an artefact of the perturbative expansion, at least in the Gaussian regime. Vertex corrections do not change the self-consistent one-loop result qualitatively. Quantitatively they tend to sharpen the peak in $A(k, \omega)$, but only moderately. For a large correlation length $\xi$ the width of the peak in $A(k, \omega)$ is proportional to $\sqrt{\log \xi}$, corresponding to a peak in the imaginary part of the self-energy $\text{Im}\Sigma(k, \omega) \propto \sqrt{\log \xi}$ at $\omega = v_{k_F} k_r$. The width of the peak in $\text{Im}\Sigma$ is also proportional to $\sqrt{\log \xi}$ and therefore increases with $\xi$. This is very different from the perturbative result for $\text{Im}\Sigma$, Eq. (7), where the height of the peak increases rapidly with $\xi$, while its width shrinks.
In the quantum critical regime studied previously [16] the spectral function also exhibits a single peak with a temperature dependent broadening. In that regime the width of the peak is proportional to $T \xi$, with a correlation length $\xi$ diverging as $(T|\log T|)^{-1/2}$ upon approaching the quantum critical point at $T = 0$.

It is striking that perturbation theory indicates a fluctuation precursor of the symmetry broken state at leading order, which is however not robust with respect to higher order contributions. One may compare with the case of a charge density wave with a finite wave vector, where symmetry breaking opens a gap. Perturbation theory indicates a pseudogap above the transition temperature in such systems, for example for the flux order parameter, for the specific choice of parameters. Away from the Brillouin zone diagonal, the imaginary part of the self-energy has a peak at $\omega = \epsilon_k - \mu$, in clear contrast to the conventional Fermi liquid form.

It is remarkable that the effect of Gaussian thermal fluctuations on electronic excitations could be treated non-perturbatively. The method used to sum contributions from thermal fluctuations to all orders is not restricted to nematic fluctuations, but could be applied equally well to other critical thermal fluctuations with a small wave vector, for example, close to a structural phase transition.

A continuous finite temperature phase transition is well established at the roof of the nematic dome found for Sr$_3$Ru$_2$O$_7$ in a strong magnetic field [7]. That system thus provides an opportunity to observe the fluctuation effects computed in this work, but also an experimental challenge, since the standard tool to measure the momentum resolved spectral function, that is, photoemission, is hampered by the magnetic field.

Fermi arcs have been observed in photoemission measurements of the spectral function $A(k,\omega)$ in various high-$T_c$ cuprate compounds [20]. However, the Fermi surface truncation in these materials is associated with a pseudogap formation, while we obtain only a strongly momentum dependent broadening of the spectral function. Although experiments indicate electronic nematicity at least in some cuprates [1], our results thus show that another mechanism needs to be invoked to explain the photoemission data.

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