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Extremely Correlated Fermi Liquids: Self consistent solution of the second order theory

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We present detailed results from a recent microscopic theory of extremely correlated Fermi liquids, applied to the t - J model in two dimensions, developed in recently by Shastry in Ref. (1) and Ref. (2). The second order theory in the parameter λ , related to the density, is argued to be quantitatively valid in the overdoped regime for $0 \leq n \lesssim 0.75$, with n denoting the particle density. The calculation involves the self consistent solution of equations for an auxiliary Fermi liquid Greens function, and an adaptive spectral weight. We present numerical results at low as well as high T , at various low to intermediate densities in the normal phase, using a minimal set of band parameters relevant to the cuprate superconductors. We display the momentum space occupation function m_k , energy dispersion curves locating the peaks of spectral functions, the optical conductivity, relaxation rates for quasiparticles, and the electronic spectral functions on an *absolute scale*. The line-shapes have an asymmetric shape and a broad background that is also seen in experiments, and our calculations validate approximate recent versions of the theory. The results also display the experimentally noted high energy kink, and provide an in depth understanding of its origin and dependence on band parameters.

I. INTRODUCTION

The t - J model describes the physics of very strongly interacting electrons, made especially difficult by the requirement of (at most) single occupancy of the lattice sites. It is the subject of many recent works in the context of the cuprate superconductors, and also other correlated systems such as sodium cobaltates. This problem is very hard since it precludes the application of standard perturbative methods. This conundrum has motivated a new strong coupling approach, resulting in the theory of *extremely correlated Fermi liquids* (ECFL)^{1,2}. Previous applications of the methodology of Ref. (1) to the cuprates has given encouraging results. These include spectral functions that compare very well with the experimental angle resolved photoemission spectroscopy (ARPES) data³⁻⁵, providing a natural explanation of the “high energy kink”, and also the more subtle “low energy kink” seen in experiments. The theory also has led to interesting predictions for the asymmetry of lineshapes⁵.

The formalism initiated in Ref. (1) charted out an approach to the problem of the t - J model using basic insights from Schwinger’s powerful approach to field theory, using source fields to write down exact functional differential equations for the propagator. In the next crucial step, it was recognized that complexity arising from the non canonical nature of the (projected) electrons can be circumvented by a product *ansatz*. This involves decomposing the propagator as the space time convolution of a *canonical electron propagator*, and an adaptive spectral weight factor termed *the caparison factor* satisfying coupled equations of motion. A recent work² develops this idea in a systematic fashion, emphasizing the role of expanding in a parameter λ ($0 \leq \lambda \leq 1$), related to the particle density, or more closely to $\lambda \sim (1 - \frac{4}{n^2}d)$, where

d is the double occupancy ($0 \leq d \leq \frac{n^2}{4}$). It further explores the implications of a novel set of identities for the t - J model, termed the *shift identities*. These simple but crucial identities provide an important constraint on the λ expansion. A method for generating a systematic set of equations for the propagator to any orders in λ is given, along with explicit equations to second order in λ that manifestly obey the shift identity constraints. We will refer to this theory as (I) here and prefix equations of that paper with (I). A detailed numerical solution of this $O(\lambda^2)$ ECFL propagator is the main focus of this work. We obtained and benchmark the results of these equations against known results, and thereby provide a solid platform for further developments of the method, as well as a validation of the phenomenological versions of ECFL. With the confidence gained by the benchmarking, we further study and report the hopping parameter sensitivity of the kink effect.

Broadly speaking, the $O(\lambda^m)$ equations resemble the fully self consistent m^{th} order skeleton diagram expansion of the standard Feynman diagram based theory, as described in standard texts⁶⁻⁸, but generalize to the case of extreme correlations. Summarizing the arguments in Ref. (2) and Ref. (1), a low order theory in λ is already expected to capture features of extreme correlations. This, perhaps initially surprising expectation, arises in view of the non Dysonian representation of the Greens function, in terms of two self energies Φ and Ψ , within the ECFL formalism. The self energy Ψ resides in the numerator of the Greens function, as in Eq. (1) and Eq. (2). It plays the role of an adaptive spectral weight that balances the somewhat opposing requirements of the “high energy” weight $1 - \frac{n}{2}$ and the low energy Luttinger theorem. The latter requires a greater magnitude of the numerator than $1 - \frac{n}{2}$, to accommodate the particles into a Fermi surface (FS) with the same volume as in the Fermi gas. A further tactical advantage of this method is due to the finite

range of variation of λ , namely $0 \leq \lambda \leq 1$ that suffices to interpolate between the Fermi gas and the extreme correlation limit. This is in contrast to controlling the double occupancy d using a repulsive energy U , with its range of values $0 \leq U \leq \infty$. Experience shows that U must be tuned to a very large value $U \gg |t|$ in order to achieve the same end, thereby invalidating low order expansions in U . In summary, within the present formalism, a low order theory in λ seems well worth examining in detail, this is our task here.

We note that apart from a few exact solutions in 1-dimension, and some calculations for finite sized systems (see below), we are aware of no systematic analytical calculations in higher dimensions, for the dynamics of the physically relevant spin $\frac{1}{2}$ version of the t - J model, working directly in the thermodynamic limit. An earlier body of work in Ref. (9) shares some of the objectives and features of our approach, but is technically very different. It relies on an expansion in the inverse number of components $\frac{1}{N}$ and is thus somewhat removed from the physical case of interest, where $N = 2$. Therefore while the importance of the t - J model was understood many years ago, there has been little detailed comparison with the ARPES experiments until recently³. This gap is one of the main motivations for this (and our related) work. In this paper, we present a controlled calculation for the spectral functions of the t - J model, by solving the above $O(\lambda^2)$ equations. We evaluate thermodynamical variables, the spectral functions, ARPES lineshapes and optical conductivity of the t - J model. The ECFL formalism and the λ expansion method provides an in-built criterion to judge the validity of the expansion at any order. Using this criterion we argue that our present $O(\lambda^2)$ calculations are valid in the high hole doping limit, known as the overdoped regime. Clearly this corresponds to low and intermediate *electron density* since the hole doping is related to the particle density as $x = 1 - n$. Future work will be aimed at higher order calculations in λ , in order to enable us to address densities closer to optimal doping ($n \sim .85$). The results are compared with other approximations as well as a few experiments. Needless to say, even in such an overdoped regime, experimental evidence points to the important role of strong correlations^{10,12}.

While analytical methods beyond crude mean field theories have been in short supply, there is a valuable body of numerical results for the t - J model from exact diagonalization¹⁴, high temperature series expansions¹⁵, variational wave functions^{16–18}, and finite temperature Lanczos methods^{19–22}. Noteworthy are the results of Ref. (20) from Prelovsek and co workers, who handle the series expansion in inverse temperature in a stochastic fashion, thereby obtaining results down to fairly low temperatures. Owing to finite size effects and the inherent nature of the high T expansion, the results from this theory, although broadly comparable to ours, seem more grainy.

The Hubbard model for large on-site coupling U tends

to the t - J model (apart from $O(t^2/U)$ correction terms), so the large U studies of this model are of interest. Quantum Monte Carlo methods, despite the difficulties associated with the sign problem, yield some valuable insights into the spectral features such as kinks²³. We note that the dynamical mean field theory (DMFT) for the Hubbard model^{24,25} gives a numerically exact solution in high enough dimensions of the Hubbard model. Although the strong coupling (i.e. $U > W$) relevant to the t - J model results is challenging, there is impressive progress overall. A recent DMFT study²⁶ at strong coupling obtains detailed spectral functions that are roughly comparable to what we find here for the t - J model.

The ECFL formalism has several advantages, since it is essentially an analytical method with a computational aspect that is lightweight, in comparison with other methods listed above. The only present limitation is the density attainable with the second order theory. When possible, we present absolute scale results that are encouragingly close to experimental data with no other fitted parameters.

We finally note that the present $O(\lambda^2)$ results for the location of the energy peaks has been recently tested in Ref. (27), against an independent theory with overlapping validity. Ref. (27) studied the infinite coupling Hubbard model in 2-dimensions, by using a highly efficient computer program to generate a series expansion in hopping of the exact Greens function and its various moments to high order. The locations of the dispersion peaks can be estimated from these. These dispersion relations match *quantitatively* the ones found from the present theory, with $J \rightarrow 0$ for the densities quoted in this paper. This suggests a high degree of reliability of the spectral functions discussed herein.

The plan of the paper is as follows. In Section (II), we present a summary of the equations solved here from (I). In Section (III), we discuss the computational strategy and explain the scheme, using the fast Fourier transform method (FFT), so that the spectral functions can be computed efficiently. Section (IV) presents the detailed results of the calculation. Section (V) contains a summary and concluding comments. The supplementary material in Ref. (28) details the results for thermodynamics and the wave function renormalization Z_k , and also gives further details of the computational method employed.

II. SUMMARY OF THE $O(\lambda^2)$ THEORY

In the ECFL formalism developed in (I) the physical Greens function \mathcal{G} can be factored in the momentum space as

$$\mathcal{G}(k) = \mathbf{g}(k) \mu(k), \quad \text{where } (k) \equiv (\vec{k}, i\omega_k). \quad (1)$$

Here the caparison factor $\mu(k)$ plays the role of an adaptive spectral weight, while $\mathbf{g}(k)$ is the auxiliary canonical Fermion propagator. These objects objects are expanded

in powers of a parameter λ , relating to density, and finally we set $\lambda \rightarrow 1$. As shown in equations (I-83, I-84,

I-85), the second order equations for the ECFL Greens function are:

$$\mu(k) = 1 - \lambda \frac{n}{2} + \lambda^2 \frac{n^2}{4} + \lambda^2 \Psi(k), \quad (2)$$

$$\Psi(k) = - \sum_{p,q} (\varepsilon_p + \varepsilon_{k+q-p} + \varepsilon_k + \varepsilon_q + J_{k-p} - u_0) \mathbf{g}(p) \mathbf{g}(q) \mathbf{g}(q+k-p) \quad (3)$$

$$\mathbf{g}^{-1}(k) = i\omega_n + \boldsymbol{\mu}' - \bar{\varepsilon}_k - \lambda^2 \bar{\Phi}(k) \quad (4)$$

$$\bar{\varepsilon}_k = \left(1 - \lambda \frac{n}{2} + \lambda^2 \frac{3n^2}{8} \right) \varepsilon_k + \lambda \sum_q \frac{1}{2} J_{k-q} \mathbf{g}(q) \quad (5)$$

$$\begin{aligned} \bar{\Phi}(k) = & - \sum_{q,p} \mathbf{g}(q) \mathbf{g}(p) \mathbf{g}(k+q-p) \\ & \times (\varepsilon_k + \varepsilon_p + \varepsilon_q + \varepsilon_{k+q-p} + J_{k-p} - u_0) \left\{ \varepsilon_k + \varepsilon_p + \varepsilon_q + \varepsilon_{k+q-p} + \frac{1}{2} (J_{k-p} + J_{p-q}) - u_0 \right\}, \end{aligned} \quad (6)$$

where $\sum_k \equiv \frac{1}{\beta N_s} \sum_{\vec{k}, \omega_n}$ with N_s being the number of lattice sites and β is inverse temperature. These expressions for the Greens function satisfy the “shift invariances” described in Ref. (2), i.e. any uniform shift in ε_k or J_k can be absorbed in $\boldsymbol{\mu}'$ and u_0 such that the spectral function is invariant. These second order equations are the lowest order ones where non-trivial frequency dependence arises, and will be the focus of this work. Below we discuss in detail the criterion for the quantitative validity of the present second order expansion.

As written here, $\mu(k)$ and $\mathbf{g}(k)$ have acquired a variety of static terms as well as frequency dependent terms called Ψ and $\bar{\Phi}$, respectively. This is written with slight change of notation $[\Phi(k)]_1 \rightarrow \bar{\Phi}(k)$ from (I-85), and we have introduced the effective band energy $\bar{\varepsilon}_k$ in Eq. (5) that gets a static contribution from shrinking of the bare energies ε_k , as well as from the exchange energy J . The role of the parameter u_0 as a second chemical potential will be described below. All terms are understood to be correct up to $O(\lambda^2)$, and hence possess corrections of $O(\lambda^3)$ that are ignored here.

The number of the physical electrons is fixed by the number sum rule,

$$\frac{n}{2} = \sum_k \mathcal{G}(k) e^{i\omega_n 0^+}. \quad (7)$$

In order that \mathcal{G} satisfy the Luttinger volume theorem, the auxiliary Fermions described by \mathbf{g} must be equal in number, and therefore satisfy a *second* sum rule:

$$\frac{n}{2} = \sum_k \mathbf{g}(k) e^{i\omega_n 0^+}. \quad (8)$$

In contrast to canonical theories, here we have two independent sum rule constraints requiring two Lagrange multipliers. The first Lagrange multiplier $\boldsymbol{\mu}'$, is a standard chemical potential in that it sits next to the band energies, $\bar{\varepsilon}_k$, in the denominator of \mathbf{g} . A second Lagrange

multiplier u_0 arises naturally in the ECFL formalism, thanks to the role of the shift identities, as shown in (I). The u_0 term has a role similar to that of the Hubbard U in the effective Hamiltonian in (I). It controls the broadening of the spectral function through the magnitude of Φ and Ψ . Neither of these Lagrange multipliers is the physical thermodynamic chemical potential of the Grand Canonical Ensemble. The physical chemical potential μ_{phys} , denoted by $\boldsymbol{\mu}$, can be obtained as a function of $\boldsymbol{\mu}'$ and u_0 as shown in Eq. (179) of (I):

$$\begin{aligned} \boldsymbol{\mu} = & \boldsymbol{\mu}' + u_0 \frac{\lambda n}{2} \left(1 - \frac{\lambda n}{4} \right) \\ & - \left(J_0 \frac{\lambda n}{4} \left(1 - \frac{\lambda n}{2} \right) + 2\lambda \left(1 - \frac{\lambda n}{8} \right) \sum_q \varepsilon_q \mathbf{g}(q) \right) + O(\lambda^3). \end{aligned} \quad (9)$$

We now discuss the criterion for validity of equations to a second order in λ . As stated above, dropping terms of $O(\lambda^3)$ in Eq. (2) - Eq. (6) limits the regime of validity of these calculation to densities not too close to unity. To see this, note from Eq. (2) that this theory would give a high frequency behavior of $\mathcal{G} \sim \frac{c_0}{i\omega}$ with $c_0 = 1 - \frac{n}{2} + \frac{n^2}{4}$, rather than the exact value $c_0 = 1 - \frac{n}{2}$, and thus introducing an error. This slight error in the high frequency physics is a result of keeping a few terms in the expansion in λ . Note however that the low frequency physics encoded by the Luttinger Ward sum rule is untouched by this, and is exactly obeyed to each order in λ . Thus at $n \sim .78$ we have an error of $\frac{n^2}{4-2n} \sim 25\%$ in the high frequency spectral weight in this theory, a value somewhat beyond where we can push this approximation. The $O(\lambda^3)$ terms are expected to extend the range of this approximation to higher particle densities.

III. COMPUTATION OF SPECTRAL FUNCTIONS

A. Definitions

Computationally it is expedient to employ a spectral function notation as described for example in Ref. (8). The Matsubara frequency object $\mathcal{G}(k, i\omega_n)$ is analytically continued to the real axis and we define:

$$\rho_{\mathcal{G}}(k, \omega) = -\frac{1}{\pi} \text{Im} [\mathcal{G}(k, i\omega_n \rightarrow \omega + i0^+)]. \quad (10)$$

This object is the spectral function, denoted in most experimental literature by $A(k, \omega)$. The real part of the analytically continued function can be obtained by a Hilbert transform

$$\text{Re } \mathcal{G}(k, \omega) = \text{P.V.} \int_{-\infty}^{\infty} \frac{\rho_{\mathcal{G}}(k, \nu)}{\omega - \nu} d\nu. \quad (11)$$

An analogous definition is given for spectral representation $\rho_{\mathbf{g}}(k, \nu)$, $\rho_{\bar{\Phi}}(k, \nu)$, $\rho_{\Psi}(k, \nu)$ used for \mathbf{g} , $\bar{\Phi}$, Ψ , etc, and hence, the full set of equations above can be rewritten in terms of these spectral functions. Since \mathcal{G} is a product as

in Eq. (1), we note that within the $O(\lambda^2)$ theory

$$\rho_{\mathcal{G}}(k, \omega) = \rho_{\mathbf{g}}(k, \omega) \left(1 - \frac{n}{2} + \frac{n^2}{4} + \text{Re } \Psi(k, \omega) \right) + \rho_{\Psi}(k, \omega) \text{Re } \mathbf{g}(k, \omega), \quad (12)$$

so the two sum rules Eq. (7) and Eq. (8) can be written as

$$\begin{aligned} \frac{n}{2} &= \sum_k \int d\omega \rho_{\mathbf{g}}(k, \omega) f(\omega) \\ \frac{n^2}{4} \left(1 - \frac{n}{2} \right) &= - \sum_k \int d\omega f(\omega) \\ &\times \left(\rho_{\mathbf{g}}(k, \omega) \text{Re } \Psi(k, \omega) + \text{Re } \mathbf{g}(k, \omega) \rho_{\Psi}(k, \omega) \right) \end{aligned} \quad (13)$$

where $f(\omega) = (1 + \exp(\beta\omega))^{-1}$ and $\bar{f}(\omega) = 1 - f(\omega)$. The auxiliary spectral function is in the usual Dysonian form

$$\rho_{\mathbf{g}}(k, \omega) = \frac{\rho_{\bar{\Phi}}(k, \omega)}{\left\{ \omega + \boldsymbol{\mu}' - \bar{\varepsilon}_k - \text{Re } \bar{\Phi}(k, \omega) \right\}^2 + (\pi \rho_{\bar{\Phi}})^2}. \quad (14)$$

Using Eq. (1) to Eq. (6), we express the spectral functions for Ψ and $\bar{\Phi}$ as:

$$\begin{aligned} \rho_{\bar{\Phi}}(k, \omega) &= \frac{1}{N_s^2} \sum_{pq} \int d\nu_1 d\nu_2 \rho_{\mathbf{g}}(p, \nu_1) \rho_{\mathbf{g}}(q, \nu_2) \rho_{\mathbf{g}}(p+q-k, \nu_1 + \nu_2 - \omega) \times \\ &\{ f(\nu_1) f(\nu_2) \bar{f}(\nu_1 + \nu_2 - \omega) + \bar{f}(\nu_1) \bar{f}(\nu_2) f(\nu_1 + \nu_2 - \omega) \} \times \\ &(\varepsilon_p + \varepsilon_{k+q-p} + \varepsilon_k + \varepsilon_q + J_{k-p} - u_0) \{ \varepsilon_k + \varepsilon_p + \varepsilon_q + \varepsilon_{k+q-p} + \frac{1}{2} (J_{k-p} + J_{k-q}) - u_0 \} \end{aligned} \quad (15)$$

$$\begin{aligned} \rho_{\Psi}(k, \omega) &= \frac{1}{N_s^2} \sum_{pq} \int d\nu_1 d\nu_2 \rho_{\mathbf{g}}(p, \nu_1) \rho_{\mathbf{g}}(q, \nu_2) \rho_{\mathbf{g}}(p+q-k, \nu_1 + \nu_2 - \omega) \times \\ &\{ f(\nu_1) f(\nu_2) \bar{f}(\nu_1 + \nu_2 - \omega) + \bar{f}(\nu_1) \bar{f}(\nu_2) f(\nu_1 + \nu_2 - \omega) \} \times \\ &(\varepsilon_p + \varepsilon_{k+q-p} + \varepsilon_k + \varepsilon_q + J_{k-p} - u_0). \end{aligned} \quad (16)$$

These frequency integrals are solved by discretizing frequency over a finite window that is wide enough to capture the finite support of the spectral functions. In Ref. (28) we outline how this is accomplished efficiently with Fast Fourier Transforms (FFTs) and implemented in an iterative process.

IV. RESULTS

A. Physical Variables

The computational program has several parameters that can be varied. These include the tight binding bandstructure (through hopping parameters t , t' etc.), the spin coupling J , density, and temperature. For

the parameters of the model, we focus on a minimal model with the nearest neighbor hopping $t \sim 3000\text{K}$ and $J \sim 900\text{K}$ and all longer range hopping parameters are zero. These values are chosen to match the bandwidth of the Cuprates. However at the bare level, this produces an electron like Fermi surface near half filling, remaining closed around the $\Gamma = (0, 0)$ point in the Brillouin zone (BZ). This is in contrast to the ARPES reconstructed FS of, say, *BiSSCO* displaying a hole like surface. Nonetheless, this minimal parameter set exhibits a variety of features in common with the cuprates, most notably a broad incoherent spectrum at high negative frequency. Interestingly, we find that the distribution of incoherent weight at high frequencies is very sensitive to the bare hopping parameters. For this reason, when we look the high energy features, we will explore their dependence in the

second neighbor hopping parameter t' , also including a fine tuned tight binding fit of *BISSCO* from Ref. (29).

B. Other parameters in the programs

The program can be implemented on lattices of various size and spatial dimension. For a given choice of these parameters an appropriate choice must be made for computational grid. This includes the lattice size as well as the discretized frequency grid. We look at converged spectral functions for a wide variety of these parameters.

The majority of the following results were performed on a square lattice with dimension $L \times L$ with $L=36$, and periodic boundary conditions are imposed. We therefore work in a momentum representation with an $L \times L$ sized k -grid of points $k_{i,j} = \frac{\pi}{aL}(i,j)$ where $1 \leq i, j \leq L$ and the lattice parameter is $a = 3.82\text{\AA}$. The spectral functions have compact support, extending to $|\omega| \lesssim 8 \times t$. We choose a frequency range $-\frac{1}{2}\omega_c \leq \omega \leq \frac{1}{2}\omega_c$, with $\omega_c = 30 \times t$, a range that is sufficient to capture the full range of the spectral functions. We discretize this frequency range in $N_\omega = 3000$ bins each of width $\Delta\omega = \frac{\omega_c}{N_\omega} = .01t = 30K$. $\Delta\omega$ is the lowest resolvable frequency scale in the calculation so it is prudent to disallow any spectral features from becoming any sharper than this scale. Therefore, we introduce the convergence factor $\eta_{min} = \Delta\omega$. It serves as a lower limit on the width of spectral features. Thus in the Dysonian form of $\rho_{\mathbf{g}}$ Eq. (14) we set $\rho_{\mathbf{g}} \rightarrow \rho_{\mathbf{g}} + \frac{\eta}{\pi}$.

C. Frequency independent Variables

We now proceed to study the FS in this theory, starting with the momentum occupation function m_k of the Gutzwiller projected Fermions:

$$m_k \equiv \langle \hat{C}_{k\sigma}^\dagger \hat{C}_{k\sigma} \rangle = \int_{-\infty}^{\infty} \rho_{\mathcal{G}}(\vec{k}, \omega) f(\omega) d\omega. \quad (17)$$

A sharp drop in this function helps to locate the FS at low T . This can be compared with the Luttinger - Ward surface defined by a sign change in $\text{Re } \mathcal{G}(k, 0)$, also given in terms of the spectral function by

$$\text{Re } \mathcal{G}(\vec{k}, 0) = P.V. \int_{-\infty}^{\infty} \frac{\rho_{\mathcal{G}}(\vec{k}, \omega) d\omega}{\omega} \quad (18)$$

At $T = 0$ the FS in \vec{k} space is traced out by $\text{Re } \mathcal{G}^{-1}(\vec{k}, 0) = 0$, as dictated by the Luttinger Ward sum rule. The momentum distribution m_k is plotted in Fig. (1) at $T = 130K$ and $T = 605K$ for various densities along three principle directions of the BZ. The Luttinger Ward zero crossings $\text{Re } \mathcal{G}^{-1}(\vec{k}, 0) = 0$ are depicted by dashed vertical lines. There is a close correspondence between these crossings and the point where $m_k = .5$, similarly to that noted previously by Stephan

and Horsch¹⁴ in an exact diagonalization study. Since this correspondence is not on any rigorously firm basis, it is difficult to do more than to list the conditions for its approximate validity. Using high temperature expansions for the t - J model Singh and Glenister¹⁵ found the FS to be that of the Fermi gas by various criteria, and noted that the condition $m_{k_F} \sim 0.5$ is only satisfied approximately at high T . At higher temperature where the QP near the FS have been significantly broadened, we find that the condition $m_{k_F} \sim 0.5$ is still reliable in agreement with Ref. (14). In Fig. (1), a point of consid-

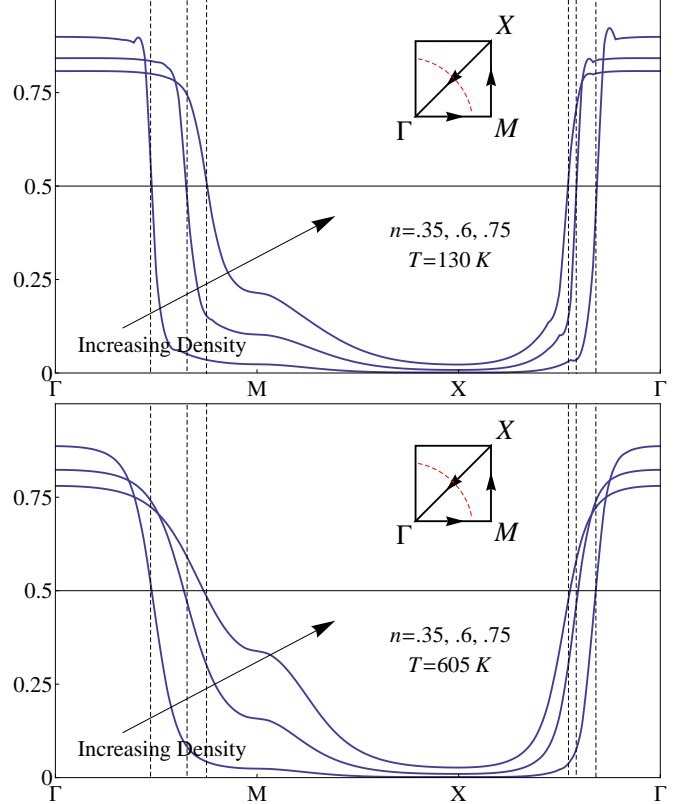


FIG. 1. The momentum distribution function m_k is plotted along three principle lines of the BZ. The left and right figures are at 130K and 605K respectively. In each case the FS is the same as in the non-interacting problem. The Luttinger Ward crossing $\text{Re } \mathcal{G}^{-1}(\vec{k}, 0) = 0$ is indicated for each density by the vertical dashed lines. For each density and each temperature the Luttinger Ward crossings correspond well with the condition $m_k = \frac{1}{2}$.

erable interest is the spillover of the occupation to the regions in k space that are unoccupied in the Fermi gas as noted in various variational wave function studies of the t - J model already¹⁶⁻¹⁸. From Eq. (17) we note that the magnitude of m_k for momenta $k > k_F$, provides an estimate of the spectral weight $\rho_{\mathcal{G}}(k, \omega)$ at occupied energies at low T . In early analyses of ARPES data, the significance of this piece of information was not always realized, and often substantial spectral weight were discarded as belonging to some unspecified background.

Only recent studies such as Ref. (3) have taken note of the significance of the background.

D. Various excitation energies

The spectra obtained here contain sharp peaks as well as substantial incoherent background due to extreme correlations. The QP weight Z_k is discussed in the supplemental material Ref. (28). To understand the effect of the many body renormalizations, it is fruitful to study three dispersion relations defined in Ref. (4),

$$\begin{aligned}\bar{\epsilon}_k &= \left(1 - n + \frac{3n^2}{8}\right) \epsilon_k + \frac{1}{2} \sum_q J_{k-q} m_q, \\ E_k &= \bar{\epsilon}_k - \mu' + \text{Re } \bar{\Phi}(k, E_k), \\ E_k^* &= \max[\rho_G(k, \omega) : \omega].\end{aligned}\quad (19)$$

Here $\bar{\epsilon}_k$ defines the bare energy times its static renormalization, while E_k locates the vanishing point for the real part of the auxiliary Greens function \mathbf{g} , thereby defining the Luttinger Ward surface through a change of sign. E_k^* locates the highest peak of the physical Greens function \mathcal{G} , and hence defines QP excitations provided they are sufficiently sharp. ARPES experiments performed with constant k , termed the energy distribution curves (EDC)'s, locate E_k^* as the peak locations; thus $E_{EDC}(k) \leftrightarrow E_k^*$. On the other hand, the momentum distribution curves (MDC's) are obtained by fixing ω , and by scanning k . The so obtained peak locations yield the fourth dispersion spectrum E_{MDC} . To obtain E_{MDC} in practice, one may invert the MDC peak locations through:

$$k^*(\omega) = \max[\rho_G(k, \omega) : k], \quad E_{MDC}(k) = \text{Inverse of } k^*(E). \quad (20)$$

It is worth mentioning that the high energy kink (or the waterfall) is experimentally defined as the the peeling off of the $E_{MDC}(k)$ from the $E_{EDC}(k) = E_k^*$ spectra³⁰.

In Fig. (2) we illustrate the density dependence of the three dispersions in Eq. (19). The inset shows the bandwidths, $W(n)$, of the three dispersions as a function of the density. Note that the bare bandwidth of ϵ_k is 2eV for both cases. Near the FS we see that $E_k \approx E_k^*$ but they differ near the Γ -point where E_k^* and E_{MDC} are also split off from each other, satisfying the above operational definition of the high energy kink. We now discuss the origin of these splittings.

Although E_k is not directly experimentally relevant, it plays a significant role in the theory so we first comment on the splitting between E_k and E_k^* near the Γ point. Since E_k is defined as the root of $\text{Re } \mathbf{g}^{-1}(k, E_k) = 0$, we plot $\omega + \mu' - \bar{\epsilon}_k - \text{Re } \bar{\Phi}(k, \omega)$ at various k as a function of ω in the inset of Fig. (2). A strong ω dependence of $\text{Re } \bar{\Phi}(k, \omega)$ causes a flattening of the curves near the zero crossing between -0.6 and -0.3 eV, and this causes the E_k to fall rapidly with k in the main figure Fig. (2). Just as E_k breaks away from E_k^* , so also does E_{MDC} , resulting

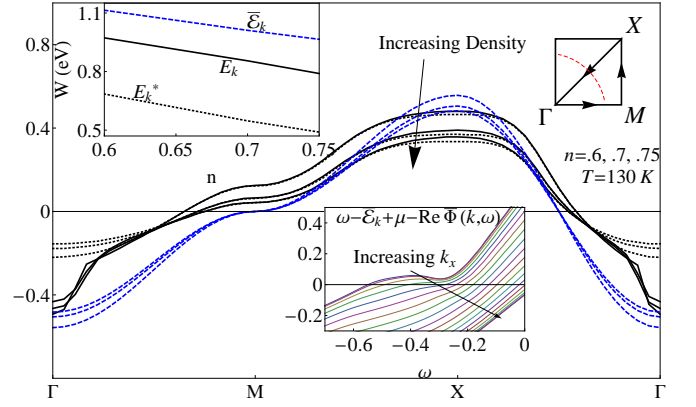


FIG. 2. $T = 130K$. The three dispersions defined in Eq. (19) are plotted along principle directions for three different densities. The upper insets show the bandwidth of the dispersions as a function of the density. The bare bandwidth is 2eV but each of these dispersions shrinks compared to that scale. The bandwidth renormalization due to $\text{Re } \bar{\Phi}$ in Eq. (19) is k -dependent, and so E_k has a different shape than ϵ_k . Note that $E_k \sim E_k^*$ near the FS. However, E_k^* differs from E_k near the Γ -point for each of the densities. The **lower inset** shows the evolution of real part of the denominator of $\mathbf{g}(k, \omega)$ with ω to illustrate the origin of the difference between E_k and E_k^* . In the **inset** E_k is determined by the zero crossings of the curves. At low k notice that a relatively flat feature develops with a shallow minimum near $\omega = -0.3$ eV. The minimum corresponds to the peak E_k^* . For increasing k , the flat feature quickly disappears and the zero crossing move quickly upward in frequency producing the observed kink in E_k .

in the kink. This is shown most clearly in the left panel of Fig. (3) where the spectral function is depicted as a color density plot with the dispersions (E_k, E_k^*, E_{MDC}) overlaid. Near the Γ -point where $k = (0, 0)$ the QP becomes incoherent and the bulk of its spectral weight is spread out to high negative frequencies. In this region E_{MDC} differs considerably from E_k^* , and recovers the scale of the bare dispersion ϵ_k . The right panel of Fig. (3) shows the spectral function as calculated using the tight binding parameters of *BISSCO* given in Ref. (29). These parameters result in a hole like FS around the Γ point, unlike the minimal model with an electron like FS. However, we observe in Fig. (3) that the high energy kink occurs for both sets of parameters.

The occurrence of the high energy kink is understandable as a straightforward consequence of additional broad peaks in the spectral function, separated from the quasi-particle type peaks. In an energy range where they exist, these are particularly effective in dominating E_{MDC} and less prominent in E_{EDC} , therefore resulting in the separation between these dispersions.

While the qualitative picture of the kinks is reasonably clear, it is not immediately clear what accounts for the slightly different magnitude of the scale of the high energy kink in Fig. (3). In Fig. (4) we show density plots of the spectral function with $t'/t = \pm 4$. The case $t' = .4 \times t$ on left, has greater curvature at the

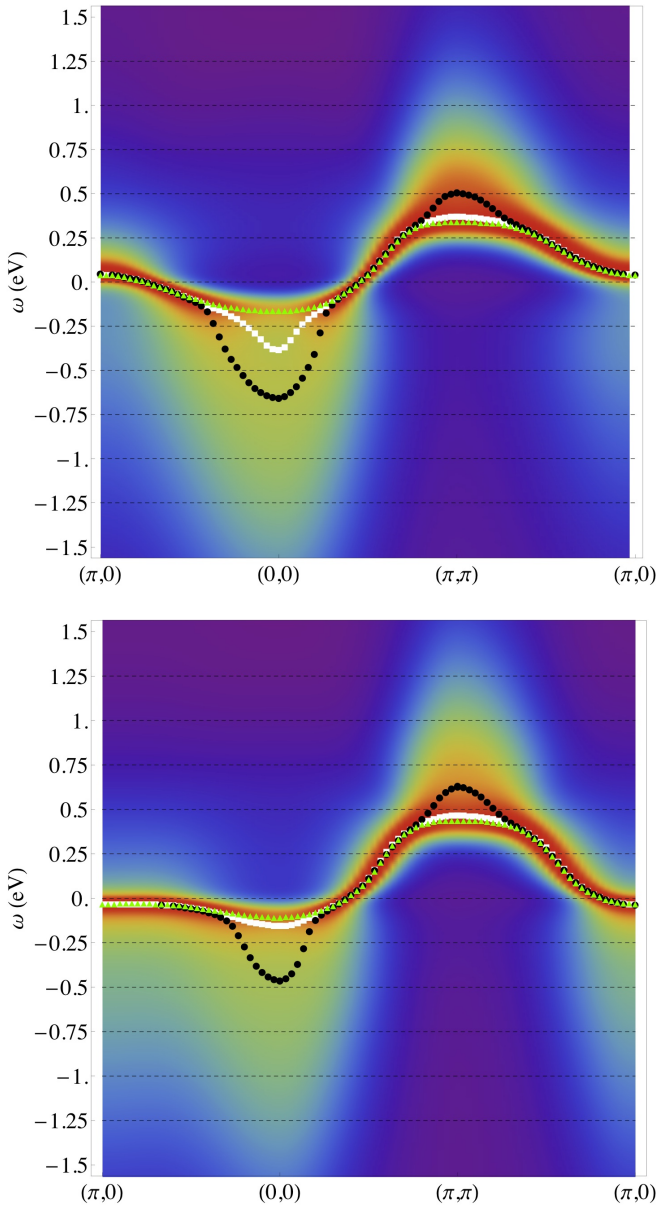


FIG. 3. $L = 60$, $(n, T) = (.75, 300K)$. Density plot of $A(k, \omega)$ of the minimal model (top) and the refined model Ref. (29) (bottom). (Here and below we red denotes high intensity and blue denotes low intensity). E_k , E_k^* , and $E_{MDC}(k)$ spectra are white, green and black, respectively. Near k_F we see that the three spectra coincide. In the region near $k = (0, 0)$ $E_{MDC}(k)$ is at a significantly higher energy scale than E_k or E_k^* , signifying the high energy kink (waterfall) effect. Also the EDC peak loses weight in this regime. A new feature arises at near $k = (\pi, \pi)$ resembling an inverted waterfall.

band bottom, and is identified with the phenomenology of the electron doped cuprates³¹ and²³. The QP peaks lose most of their weight, unlike in the minimal case. The resulting scale of the drop in the waterfall is bigger than in the minimal case, and correlates well with experimental observations in Ref. (32).

We note in Fig. (4) (right), that the case $t'/t = -.4$ has no measurable waterfall near the Γ -point. The background at negative frequency is essentially featureless, and the QP peaks maintain their spectral weight. However, at positive frequencies, an inverted waterfall like feature develops near $k = (\pi, \pi)$. This particular parametrization is often invoked to rectify the electron like curvature of the minimal model ($t' = 0$), but ends up giving a very flat band bottom at Γ . This is unlike the more sophisticated band parameters in Ref. (29), where the curvature is also hole like, and now the band regains significant curvature at its bottom, resulting in the observed kink.

E. Detailed Spectral Lineshapes (EDCs)

In this section, we present detailed line-shapes for the spectral function. In an earlier work³, we have compared the results of the simplified ECFL formalism. These included some phenomenological inputs, with the experimental data at somewhat higher particle densities $n \sim 0.85$, and found remarkably good agreement with the line-shapes. We are content in this work to present the results at lower particle densities, but *from a microscopic calculation* of ECFL. This is made possible by solving the $O(\lambda^2)$ equations in Eq. (6) numerically. The line-shapes obtained here have a similar general nature as the ones in Ref. (3), giving support to that work. However, as one expects from a lower density situation, we find somewhat less dynamical asymmetry about zero energy. More detailed comparison with data near optimal doping with the microscopic ECFL theory must await the solution of the third or higher order equations where the criterion for validity discussed above (see para following Eq. (8)) is satisfied more closely than here.

Let us first examine the local density of states (LDOS) at $n = 0.75$ for both cases at low T in Fig. (5). A prominent feature is that the main peak is much narrower than in the bare LDOS. There is furthermore a long tail extending to (negative) frequencies, much greater than those seen in the bare LDOS. Finally we note that the LDOS acquires a second peak at positive frequency. This peak arises due to some k-dependent features in the self energy (discussed below) resulting in sharper QP at positive frequency.

We next discuss Fig. (6) displaying the nodal spectral function at three different temperatures. The lines are quite sharp near k_F but broaden out rapidly away from k_F . The insets give an idea of the change of spectral density with temperature. Notably, there is a secondary local maximum for k near the Γ -point near $\omega = -.4$ eV. This second peak is responsible for the waterfall discussed above, and is also contained in the models used in Ref. (4) and Ref. (3). As discussed above in connection with kinks, its microscopic origin is sensitive to tight binding parameters. It is also noteworthy that lines with $k > k_F$, though broader than at k_F , are sharper than

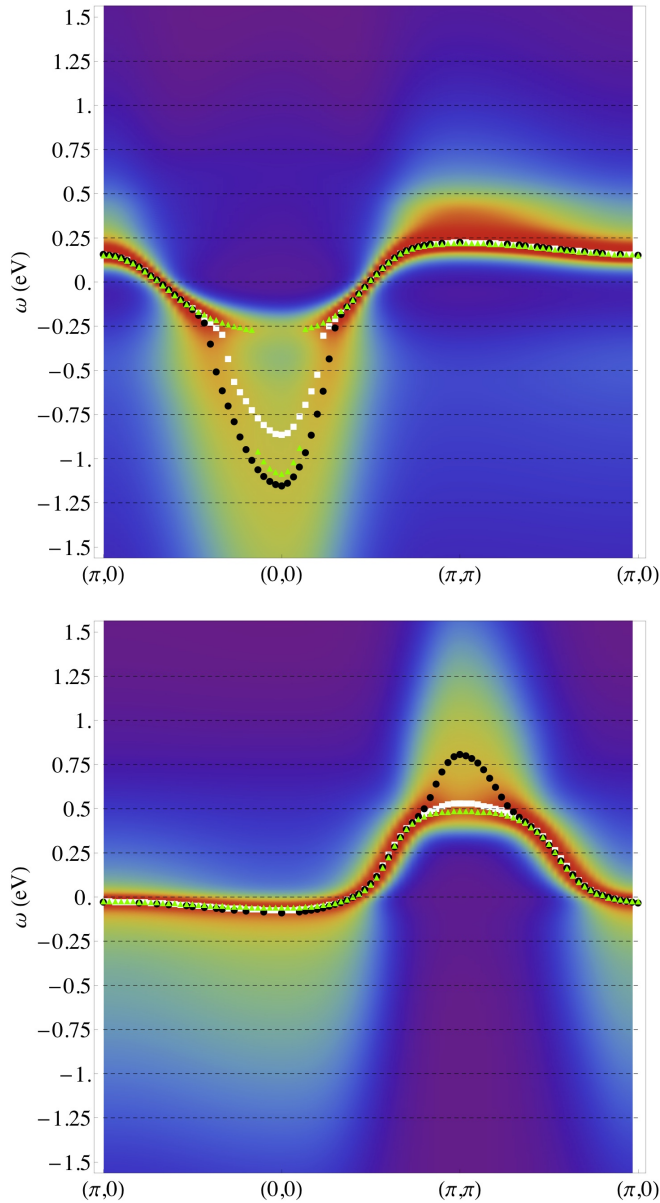


FIG. 4. $L = 60$, $(n, T) = (.75, 300K)$. (Top) $t'/t = .4$ is used to model electron doped High Tc superconductors. The kink features is prominent here. (Bottom) uses $t'/t = -.4$, to crudely model a hole like FS. In this case the kink near $(0,0)$ is lost, unlike in Fig. (3), correlating with a flat (bare) band dispersion.

those with $k < k_F$.

Finally we note that while the self energy is strongly k-dependent it is not anisotropic. Consequently, the EDC lineshapes look similar at different parts of the FS, at least to $O(\lambda^2)$. In the regime of validity of this theory, namely the (hole) overdoped region, the Cuprates do not display a strong anisotropy either.

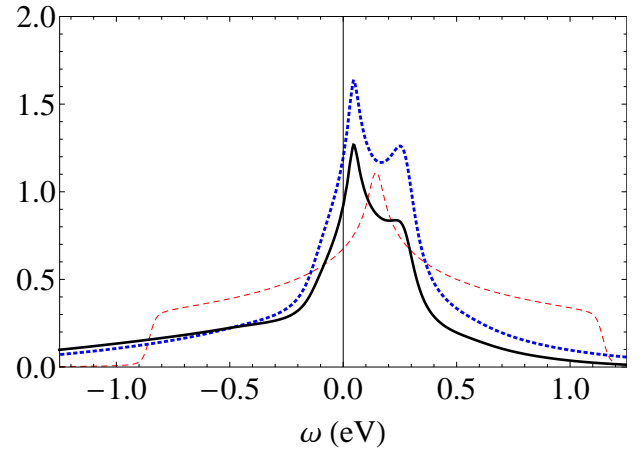


FIG. 5. $n = .75$. The LDOS of the physical \mathcal{G} (auxiliary \mathbf{g}) is in black (dotted blue), the bare DOS is the dashed red curve. The renormalized band displays narrowing, and a long tail at $\omega < 0$. The LDOS develops a second spectral peak for $\omega > 0$ from a strongly k-dependent feature in the self energy.

F. Optical conductivity

The optical conductivity, $\sigma(\Omega)$, is computed within the lowest approximation of (I) here by discarding the vertex corrections and working with the auxiliary \mathbf{g} :

$$\text{Re}\sigma(\Omega) = \frac{1}{\Omega} \sum_k v_k^2 \int \rho_{\mathbf{g}}(k, \omega) \rho_{\mathbf{g}}(k, \Omega + \omega) d\omega \times (f(\omega) - f(\Omega + \omega)) \quad (21)$$

The imaginary part of the conductivity can be obtained by a Hilbert transform of the real part. In this purely t - J calculation we must be careful how we interpret the imaginary part of σ . A more realistic calculation should include contributions from the upper Hubbard band and from charge transfer processes that are significant at high frequencies, these are discarded in the t - J model. For our current purposes we will discuss two kinds of relaxation rates. First we compute a momentum averaged rate $1/\tau_\sigma$ extracted from the low frequency behavior $\sigma(\omega)$ using:

$$\frac{1}{\tau_\sigma} = \frac{4}{\pi} \int_0^{1/\tau_\sigma} \text{Re } \sigma(\omega)/\sigma(0) d\omega, \quad (22)$$

where the prefactor is chosen to yield the usual rate for a Lorentzian shape. This convenient definition is designed to be insensitive to the shape of $\sigma(\omega)$. Secondly we look at the momentum resolved scattering lifetimes, defined as the inverse width of the ARPES lineshape at the Fermi momentum. These scattering rates are displayed in Fig. (7). We find that the $1/\tau$ curves from ARPES and the conductivity have essentially the same temperature dependence, apart from a factor of $O(1)$. The $1/\tau$ rises quadratically at low temperature in accordance with the standard FL picture, crossing over to a linear dependence at a fairly low temperature scale.

In Fig. (8), we display the computed optical conductivity $\text{Re } \sigma(\omega)$ at various T for $n = 0.75$, and also the phase angle $\theta = \text{Tan}^{-1}(\frac{\sigma''(\omega)}{\sigma'(\omega)})$ on an absolute scale. The rapid fall of the optical conductivity at low T is rapidly filled in at low ω , and the phase angle falls off with ω at about 4000 cm^{-1} . At optimum doping, the phase angle is known experimentally to be flat in ω over a much larger range¹¹, and differs from the present calculation, whose validity is confined to overdoping. Experimental measurements in the overdoped case of the phase angle would be useful in benchmarking theories in that regime—such as the present one. For the real part, such a comparison is possible. In Fig. (9) we display the $\text{Re } \sigma(\omega)$ curves along with optical conductivity measurements published by Puchkov et al¹² for an overdoped Thallium compound. We note that in the overdoped regime, the computed conductivity matches quite well with experiments (to within a factor 2 on the vertical scale).

A further interesting aspect of the resistivity obtained from this ECFL formalism lies in the high temperature limit. A lack of resistivity saturation has been observed in numerical treatments of strongly coupled models, as in a recent DMFT work²⁶. These results are in qualitative agreement with resistivity measurements in the cuprates and other strongly correlated compounds. The ECFL theory leads to a similar result, and provides a simple picture for its origin in terms of the second Lagrange multiplier u_0 . As discussed in the supplemental material, both μ' and u_0 rise linearly with T at high temperature. Due to the explicit appearance of u_0 in the expressions for Φ and Ψ , the magnitude of the self energies also grows continuously with temperature via u_0 , resulting in a monotonic broadening of the spectral function. This broadening is insensitive to the Mott Ioffe Regel (MIR) saturation expected in weakly correlated metals, and leads to a non saturating resistivity at high T , as we observe in the inset of Fig. (7).

G. Self energies

We now display the self energies that are involved in calculating the spectral functions. In Fig. (10) we display $\rho_{\bar{\Phi}}$ and ρ_{Ψ} . Both functions exhibit the ω^2 behavior close to zero, as one finds for a weakly interacting FL self energy. Unlike conventional FL's, the magnitude of the quadratic term is strongly k -dependent. From these functions and the associated real parts we can construct a Dyson-Mori self energy defined through the equation

$$\mathcal{G} = \frac{a_{\mathcal{G}}}{x - \Sigma} \quad (23)$$

where $a_{\mathcal{G}}$ is the total spectral weight of the physical \mathcal{G} and $x = \omega + \mu' - \bar{\epsilon}_k$ such that

$$\Sigma = x + \frac{a_{\mathcal{G}}}{a_{\mathcal{G}} + \Psi}(\bar{\Phi} - x).. \quad (24)$$

In Fig. (11) we plot the computed imaginary part of the D-M self energy, ρ_{Σ} . It exhibits a similar magnitude and

k -dependence at low frequency to that in $\rho_{\bar{\Phi}}$. However, large asymmetries begin to appear at intermediate frequencies. It is interesting that at positive frequency the function is considerably smaller than at negative frequencies, a feature that has already been noted for simplified versions of the ECFL^{4,5} and also in a recent DMFT study of the Hubbard model²⁶. In this calculation however, we see an interplay between the momentum and frequency dependences. In particular we see that at positive frequency $0 < \omega \lesssim 200 \text{ meV}$, ρ_{Σ} is strongly k -dependent, so that particle-like excitations near $k = (\pi, \pi)$ are long-lived while those inside the FS suffer a large damping. This is very different from weakly coupled or local theories such as DMFT, where the scattering rate is determined by *frequency alone*. We note that this self energy does not differentiate between nodal and antinodal directions, but rather, the k -dependence arises only through $\epsilon_{\bar{k}}$, so that the scattering rate is constant along the FS.

The low frequency asymmetry is usefully described as a FL like quadratic dependence modified by a cubic term. The right panel of Fig. (11) shows low frequency ($|\omega| \leq 75 \text{ meV}$) fit parameters of ρ_{Σ} as a function of k , exhibiting a marked softening of the quadratic coefficient b . The final effect on the relaxation rate $\Gamma(k) = \rho_{\Sigma}(k, E_k^*)$, displayed in Fig. (12), is summarized by the expression

$$\Gamma(k) \sim b_f \left(1 - \left| \frac{b'_f}{b_f} \right| (k - k_F) \right) V_F^2 (k - k_F)^2, \quad (25)$$

where b_f (b'_f) is the coefficient (derivative of the coefficient) at the Fermi momentum, and V_F is the Fermi velocity. The cubic term in $k - k_F$ is a significant correction to the leading term from Fermi liquid theory, resulting in longer lived quasiparticles outside the Fermi surface, as compared to quasi-holes inside the Fermi surface. Furthermore the T dependence of Γ is stronger at $k < k_F$. At the highest temperature shown, the longest lived quasiparticles drift somewhat away from k_F . In Fig. (7), we also display the T dependence of the single particle relaxation rate $\Gamma(k)$. This rate shows a crossover at a reduced scale to linear in T behavior, about $\sim 150 \text{ K}$, as compared to $T_{\mu'} \sim 400 \text{ K}$, detailed in the supplemental material Ref. (28).

V. CONCLUDING REMARKS

In summary we have presented the results of a systematic low density expansion for the t - J model, using the recently developed formalism of *extremely correlated Fermi liquids*, discussed in Ref. (1) and Ref. (2). This calculation complements the phenomenological theory in Ref. (3), where the lineshapes at optimal doping are successfully modeled, using a very small number of parameters. Here we calculate from first principles, assuming only the value of J and the hopping t , and where possible, quote results on an absolute scale. The second order in λ equations studied here, valid for $n \lesssim 0.75$, are somewhat

removed from the most interesting regime of optimal doping. Nevertheless the computed forms of the twin self energies found here indeed have the character assumed in the phenomenological ECFL studies, also the resulting spectral functions have lineshapes that are skewed towards negative ω . This feature is ultimately a consequence of Gutzwiller projection as argued in Ref. (1), and captures a striking characteristic of the experimental data.

The salient points from our study may be summarized as follows:

- The momentum occupation function $m_k = \langle \hat{C}_k^\dagger \hat{C}_k \rangle$, is calculated along the nodal direction at various T and densities, where it indicates a large spillover for $k > k_F$. This spillover quantifies the smooth part of spectral weight at $\omega < 0$ for wavevectors $k > k_F$, and is of potential use in calibrating ARPES studies.
- The spectral functions $A(k, \omega)$ at various k values and different temperatures displays a non Lorentzian form, with a pronounced skew towards occupied energies $\omega < 0$. This results in spectra resembling those seen in most experiments in cuprates, and emerges as a natural consequence of the Gutzwiller projection, i.e. very strong correlations.
- The dispersion relations $E_{MDC}(k)$ and $E_{EDC}(k)$ are deduced from the peaks of $A(k, \omega)$, and display considerable band narrowing due to correlations. They further split apart near $\vec{k} \sim (0, 0)$ i.e. the Γ point, resulting in a high energy kink, quite similar to that seen in experiments. The splitting between these peaks is due to a prominent broad second

maximum in the spectral function, away from the quasiparticle peak. A high sensitivity of the high energy kink to the bare band parameters is found, with flat band dispersions eliminating the kinks.

- The ECFL results for the optical conductivity and the phase angle are reported on an absolute scale, and the real part is in quite reasonable proximity of experimental data. Better agreement should be possible with tuning the available band parameters, although we have not explored this here.
- The resistivity is calculated as a function of T at various densities and found to be non saturating in its T dependence, analogous to the resistivity seen in experiments. The absence of saturation is easy to understand within the ECFL formalism, the magnitude of the self energy grows indefinitely due to its dependence on the second chemical potential u_0 and leads to a growing resistivity from the Kubo formula.
- The single particle decay rate $\Gamma(k, T)$ is reported at various k and T . It is smaller for $k > k_F$ than for $k < k_F$ due to a strong correction to Fermi liquid behavior, leading to spectral lines that are narrower than for $k < k_F$.

VI. ACKNOWLEDGEMENTS

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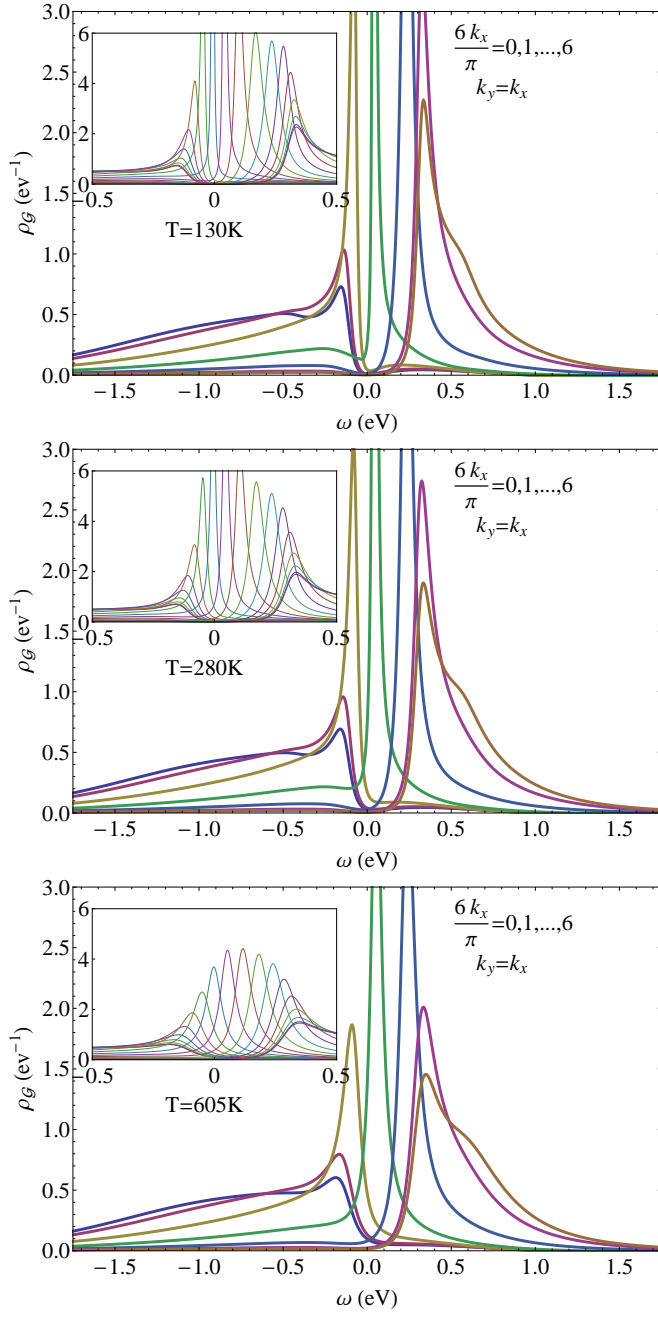


FIG. 6. $n = .75$. The spectral function $\rho_G (= A(k, \omega))$ at several k points along $\langle 11 \rangle$ direction and T . We used $L_x = 36$; the insets show all positive k_x 's and the main figures display a third of the allowed k_x 's. The inset in each case zooms out to reveal the heights. The linewidth near k_F is seen to be strongly effected by rising T , the incoherent parts has very little T dependence. The tails exhibit a secondary broad peak near $\omega = -.4\text{eV}$, giving rise to the high energy kink (waterfall).

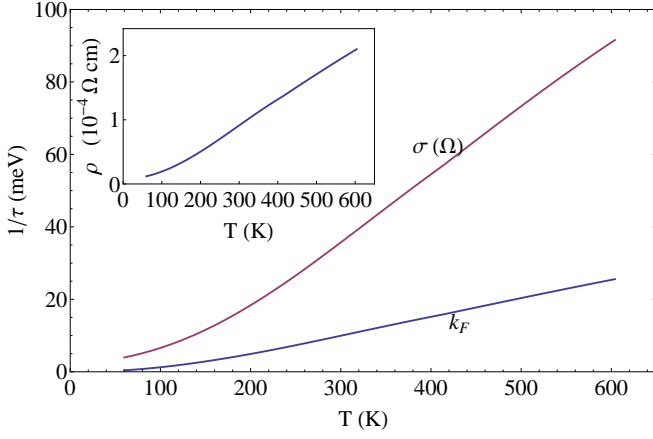


FIG. 7. $n = .75$: The QP relaxation rate at the FS along $\langle 11 \rangle$ obtained from $\rho_{\Sigma}(k, E_k^*)$, and the rate obtained from the optical conductivity as in Eq. (22). The T^2 behavior a FL is visible at low temperature, crossing over at a modest temperature ($\sim 150K$), partly due to the shrinking band width as seen directly in Fig. (2). The **inset** shows the DC resistivity obtained from the inverse of Eq. (21). It similarly displays a T^2 behavior crossing over to a linear behavior, as well as a lack of saturation that persisting to higher T than shown.

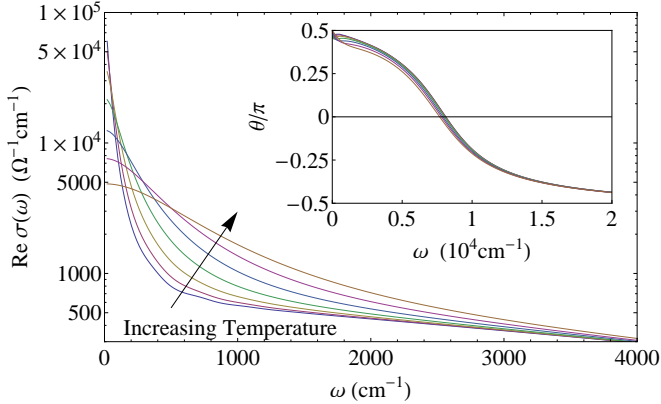


FIG. 8. $n = .75$, $T = 60, 90, 130, 190, 280, 410, 605K$. The optical conductivity is calculated on an absolute scale, and illustrates how increasing T rapidly fills up the regime $200 \leq \omega \leq 1000 \text{ cm}^{-1}$. The rise of conductivity at very low ω is also inferred from the DC resistivity displayed in Fig. (7). The phase of the complex σ falls off rapidly beyond 4000 cm^{-1} .

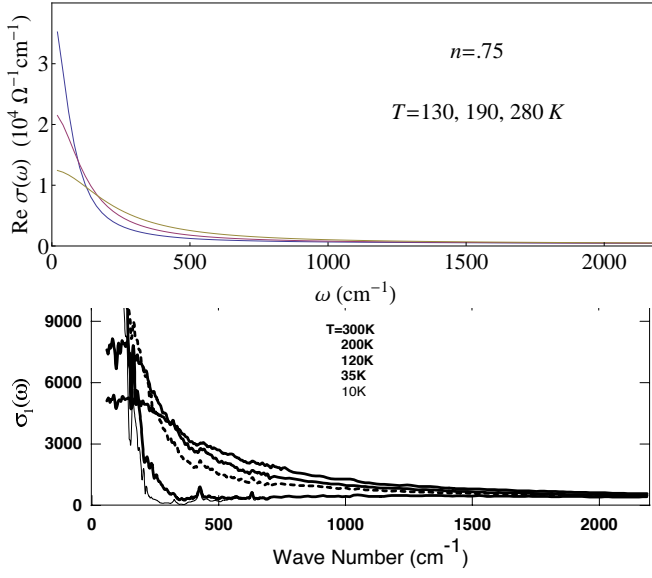


FIG. 9. An explicit comparison of optical conductivity with measurements of Puchkov et al from Ref. (12) with the authors kind permission. The data pertains to an overdoped Thallium based cuprate with $T_c = 23K$, with a density $n \approx .75$. We note the similarity of magnitude and variation with ω and T . It is worth noting (to be reported elsewhere), that the vertical scale can be brought into better agreement with an adjusted hopping, as also the Fermi velocity.

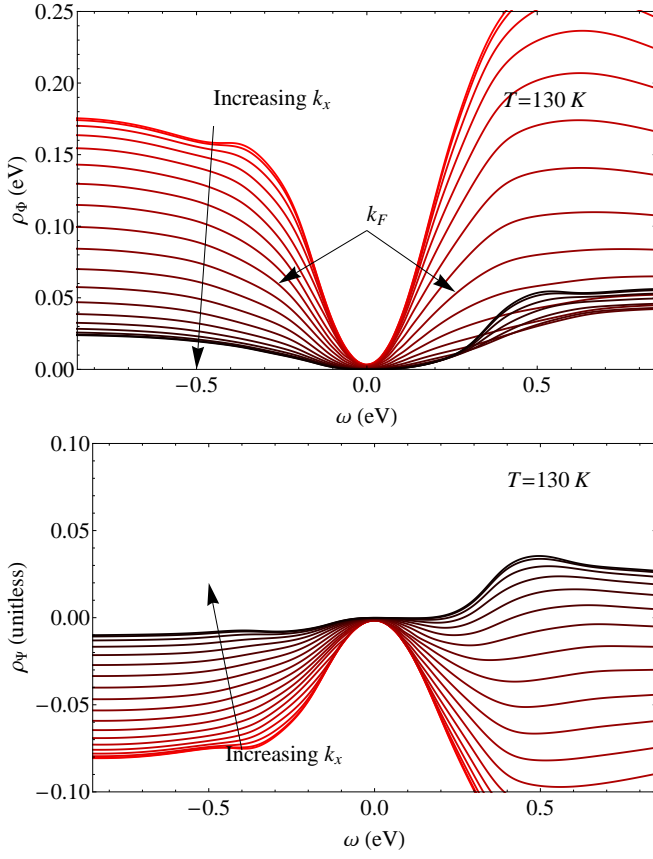


FIG. 10. $(n, T) = (.75, 130K)$. The spectral functions for the two self energies Φ and Ψ , i.e. ρ_Φ (top) and ρ_Ψ (bottom) at several k points along the $\langle 11 \rangle$ direction. Both are roughly quadratic and symmetric at low frequency, but have a strongly k -dependent curvature. In the plot of ρ_Φ , the minimum width η chops off the bottom of the low frequency minimum.

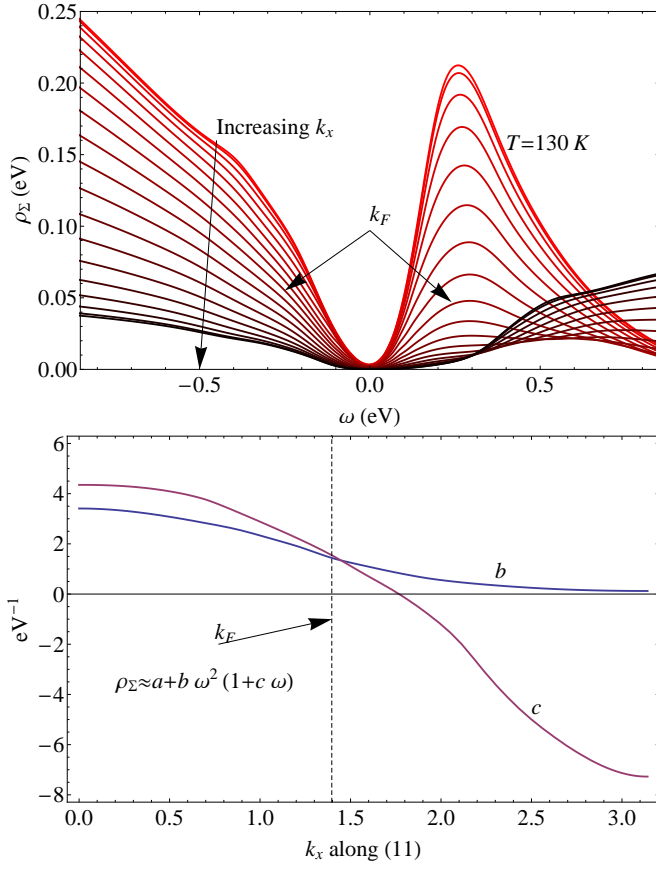


FIG. 11. $(n, T) = (.75, 130K)$. (Top) The spectral function ρ_Σ of the Dyson-Mori self energy Σ from Eq. (24), at several k points along the $\langle 11 \rangle$ direction. As with ρ_Φ , ρ_Σ has inherited a strong k dependence. (Bottom) k dependence of the fit parameters from $\rho_\Sigma = a + b\omega^2(1+c\omega)$ at low frequencies $|\omega| \leq 75$ meV. Observe the softening of the quadratic coefficient with increased k . The cubic term $\rho_\Sigma \propto \omega^3$ produces particle hole asymmetry as argued in Ref. (5), and grows in magnitude with increasing k beyond k_F .

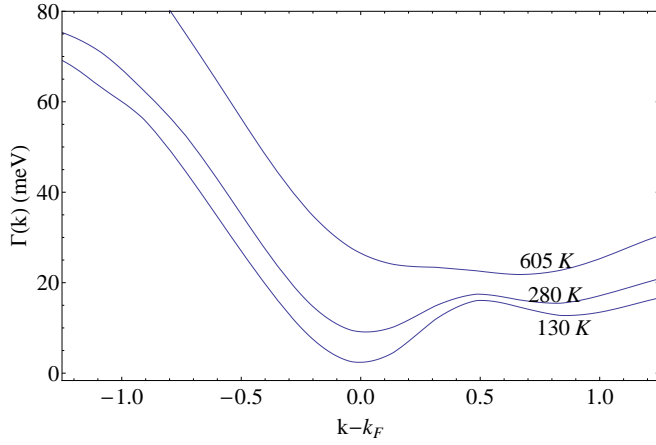


FIG. 12. $n = .75$. The decay rate of QP near k_F along the nodal line from $\Gamma_k = \rho_\Sigma(k, E_k^*)$. The strong and T dependent asymmetry makes quasiparticles longer lived at $k > k_F$. With increased T the minimum of Γ moves to $k > k_F$.