Role of the van Hove Singularity in the Quantum Criticality of the Hubbard Model


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A quantum critical point (QCP), separating the non-Fermi liquid region from the Fermi liquid, exists in the phase diagram of the two-dimensional Hubbard model [Vidhyadhiraja et al., Phys. Rev. Lett. 102, 206407 (2009)]. Due to the vanishing of the critical temperature associated with a phase separation transition, the quantum critical point is characterized by a vanishing quasiparticle weight. Near the quantum critical point the pairing is enhanced, since the real part of the bare $d$-wave particle-particle susceptibility exhibits an algebraic divergence with decreasing temperature, replacing the logarithmic divergence found in a Fermi liquid [Yang et al., Phys. Rev. Lett. 106, 047004 (2011)]. In this paper we explore the van Hove singularity in the dispersion, which cross the Fermi level near the quantum critical filling, and examine its role in determining the critical algebraic behavior of the bare susceptibility. We calculate the bare susceptibility to a $d$-wave pair field for the usual two-dimensional tight binding dispersion and a hypothetical quartic dispersion. We find that the usual logarithmic van Hove singularity cannot correctly describe the critical algebraic behavior and it is essential to have an extended van Hove singularity with an algebraic singularity in the density of states. The extended van Hove singularity is found to be pinned near the Fermi level for a larger range of doping when we include a negative next-nearest-neighbor hopping $t'$ in the model. Transport properties near the quantum critical point are investigated using high quality estimates of the self energy obtained by direct analytic continuation of the self energy from Continuous-Time Quantum Monte Carlo. Resistivity, thermal conductivity, the Wiedemann-Franz Law, and the thermopower are examined in the Fermi liquid, marginal Fermi liquid, and pseudo-gap regions. A negative next-nearest-neighbor hopping $t'$ increases the doping region where the marginal Fermi liquid character is found, consistent with the van Hove singularity picture. Both $T$ and negative $t'$ are relevant variables for the quantum critical point, and both the transport and the motion of the van Hove singularity with filling suggest that they are roughly isotropic in their effect.

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I. INTRODUCTION

A plausible scenario for the high temperature superconductivity in cuprates is based upon the presence of a van Hove singularity corresponding to the saddle points in the single particle energy dispersion. These flat regions in the energy dispersion are directly observed in ARPES experiments on various cuprate compounds. Recently, it was also observed in the tunneling spectra of Bi-2201. If by doping the Fermi level is made to coincide with the van Hove singularity, then the superconducting transition temperature is greatly enhanced. The van Hove scenario is also argued to be responsible for the marginal Fermi liquid behavior in which the lifetime broadening of the quasiparticles is of the order of its energy. Thus the van Hove scenario can account for the linear-$T$ resistivity, $T$-independent thermopower, anomalous isotope effect, etc.

There is numerical evidence for the presence of van Hove singularities in models of strongly correlated systems. The energy dispersion of one hole in an antiferromagnetic background has been considered in studies of the Hubbard model and $t$-$J$ model. These studies report the presence of extended saddle points. Assaad and Imada found that the dispersion has a quartic dependence with momentum near the anti-nodal point $(\pi, 0)$. A recent account of the presence of an extended saddle point in the energy dispersion, due to the electronic correlations found in graphene, argues that it leads to a superconducting instability.

These examples of extended saddle points in various correlated superconducting systems, and their proximity to the Fermi level at the doping where the maximum transition temperature occurs, demonstrate that it is extremely important to understand the role played by these singularities. A plethora of scientific efforts have been devoted towards achieving this understanding. At the simplest level, the role of the van Hove singularity may be interpreted within the BCS formalism. Here, the superconducting transition temperature, $T_c$, is determined by the condition $V \chi'_0(\omega = 0) = 1$, where $\chi'_0$ is the real part of the $q = 0$ bare pairing susceptibility, and $V$ is the strength of the pairing interaction. In a BCS superconductor, $\chi'_0(\omega = 0)$ displays a logarithmic divergence as $T \rightarrow 0$, yielding the BCS exponential form for $T_c$. The van Hove singularity enhances the divergence of $\chi'_0(\omega = 0)$, replacing the logarithm by a power law, yielding higher transition temperatures.

On the other hand, there is also strong evidence of a quantum critical point (QCP) located beneath the superconducting dome in the cuprates, and in close prox-
inity to the doping with the maximum $T_c$. Above the QCP, in a narrow range of doping associated to the marginal Fermi liquid behavior, the in-plane resistivity is known to vary linearly with $T$ over a wide range of temperatures. The resistivity increases as the doping decreases from the Fermi liquid into the pseudogap region. In the Fermi liquid region the low temperature resistivity varies as $T^2$. Moreover, the thermal conductivity $\kappa$ \cite{31,32} and the tunneling conductance \cite{33,54} have been investigated near the QCP of the cuprates. $\kappa$ is observed to be nearly independent of temperature in the marginal Fermi liquid state\cite{54} and depends on $1/T$ in the Fermi liquid region, this is consistent with the Wiedemann-Franz Law \cite{53} $\kappa_{\parallel} \propto T$. Chakraborty et al.\cite{55} suggested that the thermopower changes sign abruptly near the optimal doping in most of the cuprate materials, signaling a state with particle-hole symmetry. Also in the marginal Fermi liquid, the tunneling conductance $g(V) \sim g_0 + g_1 |V|$, where $g_0$ and $g_1$ weakly depend on $T$ and $V$.

A recent study\cite{58} reported the presence of a QCP in the two-dimensional Hubbard model at a filling of $n_c = 0.85$, where the quasiparticle spectral weight becomes zero. This QCP separates the non-Fermi liquid pseudogap from the Fermi liquid region. At finite temperatures, the two phases are separated by the marginal Fermi liquid. Interestingly, at the QCP, the density of states (DOS) is found to be nearly particle-hole symmetric at low frequencies with a sharp peak at $\omega = 0$. This filling is tantalizingly close to the optimal doping where the superconducting transition temperature $T_c$ attains its maximum. The proximity of the superconducting dome to the QCP was recently investigated by Yang et al.\cite{59}. Unlike the BCS case, they found that the bare d-wave pairing susceptibility $\chi''_{dd}(\omega = 0)$ decays algebraically as $\frac{1}{\sqrt{T}}$ at the QCP, thus leading to a strongly enhanced $T_c$. Using the Kramers-Kronig relation between the real part and the imaginary part of the susceptibility, $\chi'_{dd}(T) \approx \frac{1}{\pi} \int \frac{\chi''_{dd}(\omega)}{\omega} d\omega$, the algebraic divergence of $\chi''_{dd}(T)$ was found to come from a scaling behavior of the imaginary part $\chi''_{dd}(\omega)$. When $T^{3/2} \chi''_{dd}(\omega)/\omega$ is plotted against $\omega/T$, the different temperature curves fall on top of each other determining a scaling function $H(x)$ such that $T^{3/2} \chi''_{dd}(\omega)/\omega = H(\omega/T) \approx (\omega/T)^{-3/2}$ (see Fig. 1). The contribution from $H$ to $\chi(T) = -\frac{T^{-3/2}}{\pi} \int H(\omega/T) d\omega \propto T^{-1/2}$ which will dominate at low $T$. As shown in the inset, $\chi''_{dd}(\omega)/\omega|_{\omega=0}$ rises linearly with $1/T$ as expected for a Fermi liquid, when $n = 0.75$. For lower doping, $\chi''_{dd}(\omega)/\omega|_{\omega=0}$ rises more slowly, so that at the quantum critical doping, $H(0) = 0$, indicating that there is no contribution to $H$ coming from particles at the Fermi energy.

This discussion naturally raises the question about the role played by the van Hove singularity in the quantum criticality and its possible connection to the large superconducting $T_c$. In this manuscript, we use the Dynamical Cluster Quantum Monte Carlo method to explore the relationship between the QCP and the van Hove singularity for high-temperature superconductivity in the Hubbard model. We successfully obtain high quality estimates of the real-frequency single-particle self energy $\Sigma(K, \omega)$ by direct analytic continuation of the Matsubara self energy $\Sigma(K, i\omega_n)$ using the Maximum Entropy Method\cite{60,61}. This direct method avoid the artifacts on the self energy that come about by inverting the coarse-grained Dyson’s equation. In the model without next-nearest-neighbor hopping ($t' = 0$), we find that, as we dope the system across the quantum critical filling, an extended flat region in the dispersion crosses the Fermi level, accompanied by a sharp nearly symmetric peak in the DOS which also passes quickly through the Fermi level. We find that the resistivity follows a linear-$T$ dependence over a wide range of temperatures yet a narrow range of doping (see Fig. 4). We use these high quality estimates of the self energy to calculate the bare pairing polarization, we again find the collapse of the data found in Fig. 4. To understand the role played by the van Hove singularity in determining this critical behavior, we have calculated the pairing susceptibility in the $d$-channel for two models at half filling - the standard quadratic dispersion and a hypothetical quartic dispersion. While these forms can yield the observed algebraic divergence of $\chi'_{dd}(\omega = 0)$, they do not yield the collapse of the data found in Fig. 4 suggesting that a van Hove singularity alone does not capture this phenomena. For negative $t'$, the resistivity in Fig. 4 follows a linear-$T$ behavior over a wider range of doping, and the sharp peak
in the DOS and the flat region of the dispersion liner near the Fermi level for the same range of doping. These results suggest that the doping region affected by quantum criticality at low temperature becomes larger when \( t' < 0 \). We also show that the zero-frequency imaginary part of the self energy \( Im \Sigma(T, \omega = 0) \), the dominant contribution to the resistivity, has a wider range of linear-\( T \) behavior for \( t' < 0 \) than \( t' = 0 \). All this motivate us to speculate a phase diagram near the QCP in the Discussion section.

This paper has been organized as follows. Section II briefly outlines the model and methods used in this study. Results are presented in section III. Single particle properties are discussed in section III A; the susceptibility calculation in III B; and transport results in III C. The paper is concluded with the discussion in section IV.

II. FORMALISM

In this work, we look for direct evidence of the van Hove singularity and the marginal Fermi liquid behavior in the spectra, electronic dispersion, and transport properties of the two-dimensional Hubbard model

\[
H = \sum_{k\sigma} e_{k\sigma}^0 c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( c_{k\sigma}^\dagger (c_{k\sigma}) \) is the creation (annihilation) operator for electrons with wavevector \( k \) and spin \( \sigma \), \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) is the number operator, and the bare dispersion is given by

\[
e_{k\sigma}^0 = -2t (\cos k_x + \cos k_y) - 4t' (\cos k_x \cos k_y - 1)
\]

with \( t \) and \( t' \) being the hopping amplitude between the nearest-neighbor and the next-nearest-neighbor sites, respectively, and \( U \) is the on-site Coulomb repulsion.

We employ the Dynamical Cluster Approximation (DCA)\(^{62,63} \) with a Quantum Monte Carlo (QMC) algorithm as the cluster solver. The DCA is a mean-field theory that maps the original lattice onto a periodic cluster of size \( N_c = L_c^2 \) embedded in a self-consistently determined host. This many-to-one map is accomplished by dividing the lattice Brillouin zone into cells centered at momenta \( \mathbf{K} \), and coarse graining the lattice Green’s functions by summing over the momenta labeled with \( \mathbf{k} \) within each cell

\[
\tilde{G}(\mathbf{K}, \omega) = \frac{N_c}{N} \sum_{\mathbf{k}} G(\mathbf{K} + \mathbf{k}, \omega),
\]

where \( \tilde{G} \) and \( G \) are the coarse-grained and the lattice single-particle propagators, respectively. The coarse-grained Green’s function defines the cluster problem. Spatial correlations up to a range \( L_c \) within the cluster are treated explicitly, while those at longer length scales are described at the mean-field level. However the correlations in time, essential for quantum criticality, are treated explicitly for all cluster sizes. To solve the cluster problem, we use Continuous-Time QMC\(^{64} \), which has no Trotter error\(^{65,66} \) and the Hirsch-Fye QMC method\(^{66,67} \) for the charge susceptibility in Fig. 2. We employ the Maximum Entropy Method\(^{68} \) to calculate the real-frequency spectra.

A. Calculation of Single-Particle Spectra

In previous calculations of the single-particle spectra, we analytically continue the QMC \( \tilde{G}(\mathbf{K}, \omega) \) to obtain \( \tilde{G}(\mathbf{K}, \omega) \), and then invert the coarse-graining Eq. (3) to obtain the self energy \( \Sigma(\mathbf{K}, \omega) \). This last step can introduce spurious features in \( \Sigma(\mathbf{K}, \omega) \). As observed previously\(^{69} \), it is better to analytically continue the self energy directly. However, the self energy spectra does not share the normalization of \( \int d\omega \tilde{A}(\mathbf{K}, \omega) = 1 \), where \( \tilde{A}(\mathbf{K}, \omega) = -\frac{1}{\pi} \text{Im} \tilde{G}(\mathbf{K}, \omega) \). This normalization is a desirable feature since it allows us to treat the spectrum as a normalized probability distribution. Since the Hubbard \( \Sigma(\mathbf{K}, \omega_n) = \Sigma_H + U^2 \chi_{\alpha,\alpha}/i\omega_n + \cdots \), where \( \chi_{\alpha,\alpha} = \langle n_{\alpha\sigma} n_{\alpha\sigma} \rangle - \langle n_{\alpha\sigma} \rangle^2 = n_{\alpha}(1 - n_{\alpha}) \) is the local polarizability of a single spin species \( \sigma \), and \( \Sigma(\mathbf{K}, \omega_n) - \Sigma_H = \int d\omega \frac{1}{\pi} \tilde{G}(\mathbf{K}, \omega) \). It is easy to see that the integral of \( \Sigma(\mathbf{K}, \omega_n) - \Sigma_H \) is \( U^2 \chi_{\alpha,\alpha} \). Therefore we will analytically continue

\[
\frac{\Sigma(\mathbf{K}, \omega_n) - \Sigma_H}{U^2 \chi_{\alpha,\alpha}} = \int d\omega \frac{\sigma(\mathbf{K}, \omega)}{i\omega_n - \omega},
\]

where \( \sigma(\mathbf{K}, \omega) = -\frac{1}{\pi} \int \Sigma(\mathbf{K}, \omega)/U^2 \chi_{\alpha,\alpha} \), \( \int d\omega \sigma(\mathbf{K}, \omega) = 1 \), using \( \chi_{\alpha,\alpha} \) calculated in the QMC process. After that we obtain the lattice self energy \( \Sigma(\mathbf{K}, \omega) \) by interpolating the cluster self energy \( \Sigma(\mathbf{K}, \omega) \) to get the single-particle spectral function \( A(\mathbf{K}, \omega) \).

B. \( d \)-wave Pairing Susceptibility

We calculate the susceptibility in the \( d \)-wave channel to the pair field \( \mathcal{V} = -f_d b_d^\dagger \) h.c, for various models with a van Hove singularity at the Fermi level. Here \( b_d^\dagger = \frac{1}{2} \sum_{i} \left( b_{i+\alpha}^\dagger - b_{i+\alpha}^\dagger \right) \) is the singlet creation operator, where \( b_{i+\alpha}^\dagger \) creates a singlet at bond \( i-(i+\alpha) \), \( \alpha = x, y \), and \( f_d \) is a complex constant. The non-interacting \( d \)-wave pairing susceptibility \( \chi_{\text{sd}} \) can be computed by calculating the polarization bubble

\[
\chi_{\text{sd}}(T) = T \sum_{\mathbf{k}, \omega_n} g_{d}(\mathbf{k}) G(\mathbf{K}, \omega_n) G(\mathbf{K}, -\omega_n),
\]

where \( T \) is the temperature, \( \omega_n = (2n + 1)\pi T \) the fermionic Matsubara frequency, and \( g_d(\mathbf{k}) \) is the \( d \)-wave
form factor given by \( g_d(k) = \cos k_x - \cos k_y \). \( G^0(k, i\omega_n) \) is the non-interacting Green function given by

\[
G^0(k, i\omega_n) = \frac{1}{i\omega_n - \epsilon^0_k}.
\]

with \( \epsilon^0(k) \) the bare band dispersion in Eq. (2). \( \chi_{ad} \) can be evaluated using standard Matsubara summation which gives

\[
\chi_{ad}(T) = \sum_k g_d^2(k) \left( \frac{1 - 2f_k}{2\omega_0 - 2\epsilon^0_k} \right),
\]

where \( f_k \) is the Fermi function.

C. Transport Coefficients

To explain the anomalous transport properties of the marginal Fermi liquid, Varma et al.\textsuperscript{14} postulate that for a wide range of wavevectors \( q \), excitations make a contribution to the absorptive spin and charge susceptibility reflected by

\[
\chi''(q, \omega) \propto \min ([|\omega/T|, 1] \text{sign}(\omega)).
\]

Electrons scattering from these excitations acquire a self energy

\[
\Sigma(k, \omega) \propto \omega \ln (x/\omega_c) - i\pi x/2,
\]

where \( x = \max(|\omega|, T) \), and \( \omega_c \) is a cutoff. The marginal Fermi liquid ansatz has several consequences on experimentally relevant quantities, including transport anomalies, such as the linear-\( T \) electrical resistivity, the tunneling conductance \( g(V) \sim g_0 + g_1|V| \), the photoemission, the nuclear relaxation rate \( T_1^{-1} \sim aT + b \), the optical conductivity \( \sigma(\omega) \), the Raman scattering, and the superconductive pairing. For the specific heat \( C_v(T) \) and thermal conductivity \( \kappa(T) \), Varma argued that the normal state’s electronic contribution is hard to extract from the experimental data due to the large phonon contribution. The electronic thermal conductivity for the marginal Fermi liquid approximates to a constant because the Wiedemann-Franz law roughly holds.

To calculate the various Onsager transport coefficients we use the Kubo formula\textsuperscript{19}

\[
L^{ij}_{\alpha\beta} = \pi \int d\omega \left( \frac{df}{d\omega} \right) \omega^{i+j-2} D_{\alpha\beta}(\omega),
\]

where \( f \) is the Fermi function and

\[
D_{\alpha\beta}(\omega) = \frac{1}{N} \sum_k v^\alpha(k)v^\beta(k)A(k, \omega)^2,
\]

where \( v^\alpha(k) \) is the \( \alpha \)-component of the electron group velocity and \( A(k, \omega) \) is the single-particle spectral function.

\[
\begin{array}{c}
\text{FIG. 2: (Color online) The local } r = 0 \text{ imaginary part of the dynamic charge susceptibility divided by the initial slope at } \\
\omega = 0, \text{ for } n = 0.85, U = 6t, 4t = 1, t' = 0 \text{ and } N_c = 16. \\
\text{It satisfies the marginal Fermi liquid form given by Eq. (3).} \\
\text{Inset: the zero frequency slope of } \chi''(r = 0, \omega) \text{ is roughly linear in inverse temperature, as expected.} \\
\end{array}
\]

The different transport coefficients are given by combinations of \( L^{ij} \). For example, in units where \( e = 1 \) and the chemical potential \( \mu = 0 \), the resistivity \( \rho(T) = 1/L^{11} \), the thermopower \( S = -L^{12}/TL^{11} \), the thermal conductivity \( \kappa = 1/T(L^{22} - (L^{12})^2/L^{11}) \), and the Peltier coefficient \( \Pi = L^{21}/L^{11} \).

We note that a simpler estimate exists for the thermopower \( S \). Here, we perform a Sommerfeld expansion of \( L^{12} \) at the Fermi level and get an alternative form:

\[
S = -\frac{2}{3T} \frac{\partial \log [D_{\alpha\beta}(\omega)]}{\partial \omega} |_{\omega = 0}.
\]

If the electron group velocity is a constant, and the square of the single-particle spectra is approximated by \( \delta(\omega - \epsilon_k)A(k) \), where \( \tau_k \) is the relaxation time, also assumed constant, the thermopower over temperature becomes just the derivative of the logarithm of the DOS at the Fermi level\textsuperscript{10}.

III. RESULTS

A. Single Particle Properties for \( t' = 0 \)

We first explore the charge polarizability in the marginal Fermi liquid region at \( n = 0.85 \). The imaginary component of the local charge polarizability \( \chi''(r = 0, \omega) \) is plotted in Fig. 2. The main plot shows \( \chi''(r = 0, \omega) \) divided by its initial slope at zero frequency, so that the curves coincide for low \( \omega \). At higher frequencies, the curves break from this linear rise at a frequency roughly proportional to the temperature. The inset shows that the zero frequency slope, \( \chi''(r = 0, \omega)/|\omega|_{\omega = 0} \), is roughly linear in inverse temperature up to \( T \approx 0.2 \) or roughly \( 2J = 8t^2/U \), as expected for the form of the marginal
Fermi liquid susceptibility in Eq. (8). The spin polarization (not shown) does not display such an extended region of marginal Fermi liquid character.

Fig. 3 shows the frequency dependence of the imaginary part of the self energy at the Fermi momenta, $\Sigma''(k_F, \omega)$, along $\Gamma M$ and $X\Gamma$ for $U = 6t$, $4t = 1$, $t' = 0$, $N_e = 16$ and $\beta = 58$. Right panels show a zoom of the low frequency region. Dashed lines fit the data linearly for $n = 0.85$ and quadratically for $n = 0.75$.

FIG. 3: (Color online) Frequency dependence of the imaginary part of the self energy at the Fermi momenta, $\Sigma''(k_F, \omega)$, along $\Gamma M$ and $X\Gamma$ for $U = 6t$, $4t = 1$, $t' = 0$, $N_e = 16$ and $\beta = 58$. Right panels show a zoom of the low frequency region. Dashed lines fit the data linearly for $n = 0.85$ and quadratically for $n = 0.75$.

FIG. 4: (Color online) Temperature dependence of the imaginary part of the self energy at the Fermi energy, $\Sigma''(k_F, \omega = 0)$ at the Fermi energy and momenta, $U = 6t$, $4t = 1$, $t' = 0$ and $N_e = 16$. The linear dashed lines fit the self energies for $n = 0.85$ and 0.86 below $T = 0.031$.

The marginal Fermi liquid self energy is a form given by Eq. (9), which states that the imaginary self energy is proportional to negative temperature for small frequency and to negative $\omega$ when temperature is small. The marginal Fermi liquid self energy in Fig. 3 (upper right panel) shows a linear behavior, but interestingly with different slopes for positive and negative $\omega$. This is not consistent with Eqn. (9). This effect can be due to the presence of some short range order. Markiewicz et al. calculated the self-energy associated with the random-phase approximation (RPA) magnetic susceptibility for the single band Hubbard model. The bare dispersion was obtained by a fitting to the tight binding local-density approximation (LDA). They found that the self-energy has linear forms but with different slopes on positive and negative $\omega$ when the van Hove singularity is at the Fermi level and quadratic otherwise. Fig. 4 shows the temperature dependence of the self energy when $\omega = 0$ and $t' = 0$. Again we get a result consistent with Eqn. (9). $\Sigma''(k_F, \omega \to 0) \propto -T$, around the marginal Fermi liquid filling for $n = 0.85$ and 0.86. The dashed lines are linear fits. The error bars are estimated by changing the random seeds in the QMC data.

The density of states (DOS) for several fillings is shown in Fig. 5. Since we have highly enhanced the quality of the self energy by direct analytic continuation of $\Sigma(K, i\omega_n)$, the DOS in Fig. 5 shows sharper features as compared to the results of Vidhyadhiraja et al. As the doping decreases from the Fermi liquid to the pseudogap region, the peak of the DOS moves from positive to negative energy while its intensity is reduced. For $n = 0.95$, a pseudogap begins to open and a peak to form at positive frequencies. The half-filled case ($n = 1$, not shown) shows upper and lower Hubbard bands located at positive and negative frequencies, respectively. The DOS for filling 0.88 shows a low-energy particle-hole symmetry at the filling of $n = 0.88$.

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FIG. 6: (color online) Energy dispersion obtained from the peaks of the spectral function \( A(k, \omega) \) for various fillings around the Fermi vector \( k_F \) along the anti-nodal direction for \( t' = 0, U = 6t, 4t = 1, N_c = 16 \) and \( \beta = 58 \). By fixing \( k_y = 0 \) we explore the dispersion along the horizontal direction, and for \( k_x = k_F \) the dispersion along the vertical direction is plotted.

of the spectral function \( A(k, \omega) \) for four fillings: \( n = 0.85, n = 0.87, n = 0.88 \) and \( n = 0.95 \), along the anti-nodal direction and around the Fermi vector \( k_F \). For a particular filling, the left panel shows the dispersion along the \( k_x \) direction \( (k_y = 0) \), while the right panel shows the dispersion along \( k_y \) \( (k_x = k_F) \). A common identifiable feature for all fillings is the presence of an extended flat region in the dispersion. This flat region is responsible for the van Hove singularity in the density of states. Interestingly, the van Hove singularity passes through the Fermi level at a filling of \( n \approx 0.88 \), which is near the quantum critical filling where the quasi-particle weight \( Z \) goes to zero along the anti-nodal direction.  

It is also interesting to note that the dispersion around the singularity is not quadratic, as it is the case for the bare dispersion, but flatter. The dispersion around \( (\pi, 0) \) is so flat that it looks extended in nature, and it is not possible to fit it using a simple quadratic or quartic form. This broad flat region can be clearly seen in the dispersion along the anti-nodal direction for various fillings, as displayed in Fig. 7. This have implications for the critical behavior of the particle-particle susceptibility as discussed in the next section.

FIG. 7: (color online) Single particle dispersion around the Fermi energy taken along the anti-nodal direction \( (k_y = 0) \). The data is from Fig. 6.
correlation effects which strongly modify the dispersion scaling behavior as seen in Fig. 1. As shown in the inset, the imaginary part does not show scaling found by Yang et al. Thus, the simple non-interacting picture of the van Hove singularity at the Fermi level does not completely describe the true temperature and frequency dependence of the susceptibility.

C. Effect of negative $t'$

The single-band Hamiltonian used to model the hole-doped cuprates generally includes a negative next-neighbor hopping $t'$. For $t' = -0.1t$, the temperature dependence of the self energy at the Fermi momenta and energy is shown in Fig. 11. We find that $\Sigma''(k_F, \omega = 0)$ follows a linear behavior over a wider range of fillings, from $n = 0.83$ to 0.87. This finding is consistent with the phase diagram obtained by Khatami et al. They found that the inclusion of a negative $t'$ moves the system away from the QCP, but at the same time the effect of the QCP is observed over a larger range of doping (also see Fig. 14 in this manuscript).

Fig. 14 shows how the inclusion of a negative $t'$ also results in the pinning of the van Hove singularity to the Fermi level for a larger range of fillings: 0.83 to 0.86. Thus both measurements, the temperature dependence of the self energy and the pinning of the van Hove singularity to the Fermi level, are consistent. If we take the viewpoint that the QCP and the pinning of the van Hove singularity to the Fermi level are concomitant, then negative $t'$ leads to a large range of fillings to be quantum critical. We will also see the signature of this behavior in the real part of the bare susceptibility is found to be algebraic for this quartic dispersion, the inset reveals that the imaginary pairing susceptibility does not exhibit the expected logarithmic behavior. This is confirmed by explicit calculation of the sum in Eq. (7) as illustrated in Fig. 8. As shown in the inset, the imaginary part does not show scaling behavior as seen in Fig. 1.

Clearly this simplistic model does not incorporate the correlation effects which strongly modify the dispersion near $(\pi, 0)$. Motivated by the flatter nature of the dispersion around the Fermi vector in Fig. 6 and Fig. 7, we consider the next higher order model allowed by the symmetry of the square lattice, a hypothetical model with a quartic dispersion

$$\epsilon_k = -\frac{4}{\pi^4} (|k_x| - \pi)^4 - k_y^4). \quad (13)$$

Such an extended form has been observed in experiments and also confirmed by theoretical studies. The low energy density of states for the quartic dispersion becomes $N(\epsilon) \sim \sqrt{|\epsilon|}$. Following a similar logic as we used for the tight binding dispersion, for a quartic dispersion, we get $\chi'_{0d} \sim \frac{1}{\sqrt{T}}$.

Results for the explicit calculation (Eq. 7) are shown in Fig. 9 and are consistent with the analytical arguments above. Though the temperature dependence of the imaginary part of the particle-particle susceptibility is consistent with the analytical arguments for the tight binding dispersion, for a quartic dispersion, we consider the next higher order model allowed by the symmetry of the square lattice, a hypothetical model with a quartic dispersion.

B. Pairing Susceptibility for $t' = 0$

Here we calculate the pairing susceptibility in the $d$-wave channel for two simple models having a van Hove singularity at the Fermi level. We begin with the tight binding model given by Eq. (2) at half filling and $t' = 0$. The associated DOS has a logarithmic singularity at $\epsilon = 0$, $N(\epsilon) = \log |\epsilon|$. The temperature dependence of $\chi'_{0d}$ can be obtained by converting Eq. (7) to an integral over energy with a temperature $T$ cutoff. It results in a $-(\log T)^2$ behavior. This is confirmed by explicit calculation of the sum as illustrated in Fig. 8. As shown in the inset, the imaginary part does not show scaling behavior as seen in Fig. 1.

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FIG. 10: (Color online) Temperature dependence of the imaginary part of the self energy $\Sigma''(k_F, \omega = 0)$ at the Fermi energy and momenta, $U = 6t$, $N_c = 16$, $4t = 1$, and $t' / t = -0.1$. The self energy for filling between $n = 0.83$ and 0.87 shows a linear-$T$ behavior.

various transport properties discussed in Section III.D.

Fig. 12 shows the density of states for $t'/t = -0.1$ and various fillings as a function of $\omega$. For a given filling, the inset of Fig. 12 shows that the peak in the density of states is slightly shifted to smaller frequencies if compared with the peak in the DOS for $t' = 0$. The peak displaying particle-hole symmetry is roughly at $n = 0.84$, not $n = 0.88$ as for $t' = 0$. Moreover, if we use $\Delta \omega_p / \Delta n$, where $\omega_p$ is the location of peak in the DOS and $n$ is the filling, to estimate the rate at which the peak crosses the Fermi level, we find that the peak of the DOS for $t' = 0$ crosses the Fermi level more quickly than the peak for negative $t'$. This can be seen in the inset of Fig. 12 where the filling dependence of the peak location has a steeper slope for $t' = 0$ than that for $t'/t = -0.1$ at the Fermi level. This confirms that negative $t'$ leads to a wider range of fillings with quantum critical properties.

Another interesting point to be noted here is that, when compared to the $t' = 0$ result, the quasi-particle peaks become more incoherent for negative $t'$. This can be seen in the Matsubara quasiparticle weight along the antinodal momentum direction, $Z_{AN}$, displayed in Fig. 13 as a function of temperature for different fillings. The quasiparticle fraction is consistently smaller for $t'/t = -0.1$ than for $t' = 0$ for all fillings. This can also be seen through the increase of the blue color in the dispersion curves in Fig. 11 when compared with Fig. 6.

D. Transport Properties

It is difficult to detect the presence of the van Hove singularity in the dispersion by direct probes like the Angle Resolved Photoemission Spectroscopy (ARPES). So we revert to study transport properties that provide an indirect method of validating the van Hove singularity picture.

Using the Kubo formula under the relaxation time approximation in Eqs. (10) and (11), we obtain the resistivity, thermal conductivity, and thermopower in the Fermi liquid, marginal Fermi liquid, and pseudo-gap regions. Linear resistivity reveals evidence of the marginal Fermi liquid because the electronic cross section is proportional to $-\Sigma''(k_F, \omega = 0)$ at low $T$, as seen in Fig. 13 and Fig. 16. Fig. 14 shows the resistivity as a function of temperature for $t' = 0$, left panel, and $t'/t = -0.1$, right panel. Again, for $t' = 0$ a narrow range of fillings, from $n = 0.85$ to 0.86, displays a linear-$T$ resistivity at low $T$, while for $t'/t = -0.1$ a larger range of filling, $n = 0.83$ to 0.87, exhibits a linear temperature dependence. The linear resistivity in the marginal Fermi liquid region is consistent with experiments. For $n = 0.75$, both $t' = 0$ and $t'/t = -0.1$ show Fermi liquid character, with a resistivity which goes to zero quadratically when $T$ approaches zero. We will further discuss the phase diagram near the QCP in Section IV.

According to the the Wiedemann-Franz Law, $\kappa / (\sigma T) = \pi^2 / 3 (k_B = e = 1)$, the thermal conductivity of a Fermi liquid is inversely proportional to $T^2$. Fig. 15 shows that $\kappa / (\sigma T)$ approaches a constant which is less than $\pi^2 / 3$ when $T \leq 0.08$. Daln et al. investigated the two-dimensional Hubbard model for $n \approx 0.9$ and also found a smaller Wiedemann-Franz ratio. However, we find that the Wiedemann-Franz ratio is larger than $\pi^2 / 3$ for the marginal Fermi liquid ($n = 0.85$) and pseudo-gap ($n = 0.95$) regions. We also see that the thermal conductivity becomes very small as $T \rightarrow 0$ for $n = 0.95$ and saturates to a constant for $n = 0.85$. So, when studying $\kappa$, the marginal Fermi liquid seems to separate the Fermi liquid from the pseudo-gap region. The dashed curves in Fig. 15 for $t'/t = -0.1$ data are always below the solid curves for $t' = 0$ when plotting $\kappa$. However, the $t'/t = -0.1$ data is above the $t' = 0$ results when we focus on the ratio $\kappa / \sigma T$. This implies that negative $t'$ reduces the electrical conductivity more than the thermal conductivity.

Chakraborty et al. argue that the thermopower changes sign near the QCP, and that this is related with the development of a state with particle-hole symmetry. Fig. 16 shows the thermopower $S$ as a function of filling. For $t' = 0$ and $\beta = 58$, the filling at which $S$ changes sign is roughly 0.84. We expect that the zero-crossing of the thermopower will approach the critical filling of 0.85 for decreasing $T$. However, this is different for the filling at which the DOS displays particle-hole symmetry. In the Fermi liquid theory, if we assume constant relaxation time and group velocity, the thermopower is proportional to the derivative of the logarithm of the DOS at the Fermi level. However, in this approach $A(k, \omega)^2$ in Eq. (11) is approximated by $\delta(\omega - c_k \tau)$, where $\tau = \tau_k$ is a $k$-independent relaxation time. In addition, the elec-
FIG. 11: (color online) Energy dispersion obtained from the peaks of the spectral function $A(k, \omega)$ for various fillings around the Fermi vector $k_F$ along the anti-nodal direction for $t'/t = -0.1$, $U = 6t$, $4t = 1$, $N_c = 16$ and $\beta = 48$.

FIG. 12: (Color online) Single-particle density of states for $t'/t = -0.1$ when $U = 6t$, $N_c = 16$, $4t = 1$, and $\beta = 48$. Inset: Comparison of the filling dependence of the position of the peak of the DOS ($\omega_p$) for $t' = 0$ and $t'/t = -0.1$. As the filling changes, $\omega_p$ for $t' = 0$ crosses the Fermi level more quickly than for $t'/t = -0.1$.

FIG. 13: (Color online) Temperature dependence of the Matsubara fraction along the anti-nodal direction, $Z_{AN}$, for various fillings for $t' = 0$ and $t'/t = -0.1$. At the same filling and the same temperature, the Matsubara fraction decreases when $t' < 0$.

electron group velocity we use in our calculation also has a
FIG. 14: (Color online) Resistivity versus temperature for $t' = 0$ (left) and $t'/t = -0.1$ (right) with $U = 6t$, $N_c = 16$, and $4t = 1$. The dashed lines in the insets are linear fits. For $t' = 0$, the resistivity shows linear-$T$ behavior for $n = 0.85$ and $n = 0.86$. For $t'/t = -0.1$, the resistivity shows linear-$T$ behavior from $n = 0.83$ to $n = 0.87$.

FIG. 15: (Color online) Thermal conductivity versus temperature for $U = 6t$, $N_c = 16$, and $4t = 1$. Inset: Wiedemann Franz ratio for the same physical parameters. The horizontal solid line labels the constant $\pi^2/3$.

$k$-dependence:

$$v^x(k) = \frac{\partial^2 E_0}{\partial k_x} = 2t \sin k_x + 4t' \sin k_x \cos k_y. \quad (14)$$

If we compare the quantity $D_{xx}(\omega)$ (the inset of Fig 10 and the DOS (Fig. 5) for different fillings and the same $t' = 0$, we find that the effect of $v^x(k)^2$ is to pull the peak of the DOS to the left, because the $\sin k_x$ term suppresses the contribution of the van Hove singularity at $X(\pi, 0)$ and enhances the contribution from the states below the Fermi level. As a result, the filling where the thermopower changes sign and the quantity $D(\omega)$ has a zero slope at the Fermi level, around $n = 0.85$, is different from the one where the DOS displays particle-hole symmetry, $n = 0.88$ for $t' = 0$.

IV. DISCUSSION

In this work, we focus on the role of the van Hove singularity near the quantum critical point (QCP) in the Hubbard model. Near the QCP, we find that the van Hove singularity is pinned to the Fermi level (Fig. 6 and 7) and the low energy DOS exhibits particle-hole symmetry (Fig. 3). It is a well-known fact that within DMFT if the van Hove singularity is pinned to the Fermi level for the non-interacting case, it remains pinned even for
linear in $n$ in agreement with the marginal Fermi liquid theory.

is quadratic in $T$ in Fig. 3, we find that the imaginary part of the self energy

the single particle self energy at low $T$ measurements become crucially important. We explore

ment effects. The standard quadratic dispersion gives a

singularity in photoemission experiments due to matrix ele-

$11–13$

pinning also occurs away from half filling.

In a recent work, the bare d-wave pairing susceptibility $\chi_{\delta d}$ was found to decay algebraically as $1/\sqrt{T}$ at the QCP, instead of logarithmically, giving rise to a higher $T_c$. We explore the role of the van Hove singularity in this algebraic quantum critical behavior and we found that a simple non-interacting picture with a van Hove singularity at the Fermi level does not explain the observed phenomena. The standard quadratic dispersion gives a logarithmic decay of $\chi_{\delta d}$ for the half filled model. As the dispersion is flatter than quadratic near $(\pi, 0)$ (Figs.3, 7), a hypothetical quartic dispersion is considered. It shows the observed algebraic decay for $\chi_{\delta d}$ but does not give the correct scaling for the imaginary part of the bare susceptibility found in Yang et al. This can be explained by the vanishing of the spectral weight near the QCP. It means that the singularity in the DOS near the QCP is composed mainly of the incoherent part of the spectral function. Thus the non-interacting picture of the van Hove singularity can not completely describe the critical temperature dependence of the bare susceptibility.

Next we consider the effect of a negative next-nearest-neighbor hopping $t'$ on the single particle dispersion. We found that for $t'/t = -0.1$, the van Hove singularity remains in close proximity to the Fermi level for a large range of fillings: $0.83 \leq n \leq 0.87$. As the van Hove singularity pinning is believed to give rise to the marginal Fermi liquid behavior, we expect to observe this behavior for a larger range of fillings. This is confirmed by our calculation of the resistivity with a linear-$T$ dependence in the same range of doping.

It is hard to detect the presence of the van Hove singularity in photoemission experiments due to matrix element effects. Therefore indirect probes like transport measurements become crucially important. We explore the single particle self energy at low $T$ for $t' = 0$. In Fig. 4 we find that the imaginary part of the self energy is quadratic in $\omega$ for the Fermi liquid, e.g., $n = 0.75$ and linear in $\omega$ for the marginal Fermi liquid, e.g., $n = 0.85$, in agreement with the marginal Fermi liquid theory. Moreover, both resistivity and self energy show quadratic dependence on $T$ for the Fermi liquid and linear-$T$ behavior for the marginal Fermi liquid (Figs. 4, 13). The linear-$T$ resistivity and self energy are observed for the same fillings where the van Hove singularity is pinned to the Fermi level, thus providing an indirect evidence for the presence of the van Hove singularity.

In addition, the resistivity for various $t'$ gives information about the chemical potential-temperature, $\mu - T$, phase diagram shown in Fig. 17. When $t' > 0$, the critical point is a second order critical point at finite temperature. In analogy with the phase diagram of water, the phase above the first order transition line is an incompressible spin liquid and we call it Mott liquid (ML), and the phase below is a weakly compressible Fermi liquid named as Mott gas (MG). When $t' \rightarrow 0$, the critical point goes to zero temperature and thus becomes a QCP. This point separates the Fermi liquid and pseudo-gap phases. Above the QCP, the marginal Fermi liquid phase is found to exist in the V-shape quantum critical region. Inside this region, the only scale is the temperature (like Eq. (5) and (9)). $T^*$ is the temperature separating the marginal Fermi liquid from the pseudo-gap. $T^*$ does not separate the quantum critical region from a region of hidden order. Rather in our scenario, it is only the boundary of the quantum critical region. As we cross from the quantum critical region to the Mott liquid, the character of the Mott liquid becomes apparent including a pseudo-gap. For the QCP, both $T$ and negative $t'$ are relevant variables, which are roughly isotropic in their effect. Thus when $t' < 0$, the QCP may be viewed as moving to negative temperatures so that the quantum critical region broadens to allow the linear-$T$ resistivity and the pinning of the van Hove singularity to the Fermi level to exist in a wider range of fillings.

The thermal conductivity $κ$ in Fig. 13 shows $1/T$ behavior for the Fermi liquid, but weakly depends on $T$ for the marginal Fermi liquid and the pseudo-gap phase. The inset of Fig. 13 shows the Wiedemann Franz law approximately holds for the Fermi liquid and the marginal Fermi liquid, but is violated for the pseudo-gap. However, it’s difficult to see experimental evidence for this behavior because the phonon’s contribution always dominates the electronic contribution to $κ$ for the relevant temperatures. We also study the thermopower $S$ (Fig. 10) and its filling dependence at low temperature. We find that due to the $k$-dependence of the relaxation time and the electron group velocity, the filling at which the thermopower crosses zero does not occur at the filling where the DOS shows a particle-hole symmetry at low energies.

Thus, we conclude that the quantum critical point in the Hubbard model is accompanied by an extended van Hove singularity in the single particle dispersion pinned near the Fermi level. Both $T$ and negative $t'$ are relevant variables for the quantum critical behavior. Several transport properties and the motion of the van Hove singularity with filling suggest that $T$ and $t'$ are roughly isotropic in their effect. In particular, the extent of fil-

FIG. 17: Schematic chemical potential-temperature ($\mu - T$) phase diagram for three values of $t'$: (left) $t' > 0$, (center) $t' = 0$, and (right) $t' < 0$. CC (QC) means classical (quantum) criticality. ML (MG) means Mott liquid (gas).
nings displaying quantum criticality expands when $t'$ becomes negative. The proximity of the van Hove singularity to the QCP suggests that the singularity may be responsible for the enhancement of $\rho_c$, due to the observed algebraic decay of the bare d-wave pairing susceptibility. However, we find that a non-interacting van Hove singularity with even a quartic dispersion does not give the correct scaling for the imaginary part of the bare susceptibility found in Yang et al.\textsuperscript{12}.

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