Absence of a quantum limit to charge diffusion in bad metals

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Abstract

Good metals are characterised by diffusive transport of coherent quasi-particle states and the resistivity is much less than the Mott-Ioffe-Regel (MIR) limit, $\frac{h a^2}{e^2}$, where $a$ is the lattice constant. In bad metals, such as many strongly correlated electron materials, the resistivity exceeds the Mott-Ioffe-Regel limit and the transport is incoherent in nature. Hartnoll, loosely motivated by holographic duality (AdS/CFT correspondence) in string theory, recently proposed a lower bound to the charge diffusion constant, $D \gtrsim \frac{h v_F^2}{(k_B T)}$, in the incoherent regime of transport. Using dynamical mean field theory (DMFT) we calculate the charge diffusion constant in a single band Hubbard model. We show that Hartnoll’s bound is violated by several orders of magnitude in the incoherent regime of transport. The bound is only satisfied for the weakly correlated regime of coherent transport. Our calculated charge diffusion constant, in the incoherent regime of transport, also strongly violates the quantum limit of spin diffusion, $D_s \sim 1.3 h/m$, experimentally observed and theoretically calculated in a cold degenerate Fermi gas in the unitary limit of scattering.
I. INTRODUCTION

Good metals like copper and gold are characterised by high optical reflectivity, electrical and thermal conductivity. The transport in these systems can be characterised by diffusive transport of coherent quasi-particle states, where the mean-free path is much larger than the lattice constant. The low temperature resistivity in good metals is well within the Mott-Ioffe-Regel (MIR) limit, \( \frac{e^2}{2a} \sim 250 \text{ } \mu\Omega \text{-cm} \), where \( a \) is the lattice constant. However, in a large class of strongly correlated systems like 3d-transition metal oxide compounds and most notably in the strange metal regime of doped cuprates (high \( T_c \) superconductors) at optimal doping the resistivity far exceeds the MIR limit \(^{[1]}\) and hence can not be characterised by diffusive transport of coherent quasi-particle states in the limit of weak scattering. Other signatures of a bad metal include a thermopower of order \( k_B/e \), the absence of a Drude peak in the optical conductivity, and a non-monotonic temperature dependence of the Hall constant and thermopower. \(^{[2-4]}\)

There have been a range of theoretical attempts to understand the incoherent regime of transport, especially for the strange metal phase of doped cuprates (high \( T_c \) superconductors) at optimal doping. Recently, there is a string theory based approach to understand transport in the incoherent regime \(^{[5,6]}\). String theory, originally proposed as a possible theory for quantum gravity, is mathematically consistent but yet has no experimental verification. In the following paragraph we briefly describe how a string theory based approach has been proposed to describe transport in condensed matter systems in the following paragraph.

Maldacena conjectured \(^{[7]}\) that the large \( N \) limit of certain supersymmetric conformal field theory (CFT) has correspondence to super gravity in anti-de Sitter spaces in higher dimension. This is known as the \textit{AdS/CFT correspondence} or \textit{gauge/gravity duality}. The most famous example of AdS/CFT correspondence states that IIB string theory in the product space \( AdS_5 \times S^5 \) is dual to large \( N \) limit of \( \mathcal{N} = 4 \) supersymmetric \( SU(N_c) \) Yang-Mills theory on the four dimensional boundary. Further AdS/CFT correspondences relate fluid dynamics to event horizon dynamics of a black hole in anti-de Sitter space. In the hydrodynamic regime (long wavelength limit) of the correspondence, Einstein’s equations of general relativity reduce to the Navier-Stokes equation for fluid mechanics. Classical fluids are characterised by transport coefficients such as shear viscosity and diffusion constant. Using the AdS/CFT correspondence Kovtun \textit{et al}. \(^{[8]}\) calculated the ratio, \( \eta/s \), of the shear
viscosity ($\eta$) and the entropy density ($s$) and proposed a lower bound $\frac{\eta}{s} \geq \frac{\hbar}{4\pi k_B}$. Such a bound is well respected in classical fluids like water, the quark-gluon plasma (QGP) created in the relativistic heavy ion collider (RHIC) [9], and in experiments on cold degenerate Fermi gases in the unitary limit [10]. Inspired by this result and using the AdS/CFT correspondence Hartnoll recently proposed [11] a lower bound for the diffusion constant,

$$D \gtrsim D_H \equiv \frac{\hbar v_F^2}{k_B T},$$

in the incoherent regime of transport in strongly correlated electron systems. But, except near a quantum critical point, condensed matter systems are probably neither relativistic nor conformal in general [12]. So, this proposal needs to be tested against model based calculations.

The temperature dependent diffusion constant, $D(T)$, is related to the temperature dependent conductivity, $\sigma(T)$, through the Nernst-Einstein relation

$$\sigma(T) = e^2 \frac{\partial n}{\partial \mu} D(T),$$

where $\kappa_e(T) = \frac{\partial n}{\partial \mu}$ is the charge compressibility. For completeness we give a derivation of this relation in the Appendix. Because of the above relation any knowledge of the charge diffusion constant, $D(T)$, will help us to understand the electrical conductivity, $\sigma(T)$.

Experiments on cold degenerate Fermi gas in the unitary limit show a quantum limit to the spin diffusion constant [13, 14], $D_s \approx 1.3\hbar/m$. This bound is also supported by theoretical calculations by Enss et al. [15]. However, experiments on a two-dimensional Fermi gas found a value of $D_s$ that was more than two orders of magnitude smaller than the proposed bound [16]. But spin diffusion in charge neutral systems such as cold atomic gases has no obvious relation to charge diffusion in charged quantum fluids such as strongly correlated electron systems. In the present article we do a model based calculation of the charge diffusion constant in a single band Hubbard model, and explore the possible existence of a quantum bound to charge diffusion constant and its possible relation to spin diffusion in atomic gases.

The organization of the paper is as follows. In Sec. II we introduce the single band Hubbard model and its solution under single site dynamical mean field theory (DMFT). We also briefly describe DMFT self-consistency using iterated perturbation theory (IPT) as a solver for the impurity problem arising under the single site DMFT. In Sec. III we briefly
introduce calculation of transport and thermodynamic quantities under single site DMFT approximation. Then in Sec. IV we show our results for a single band Hubbard model on the Bethe lattice at half-filling. We find clear violation of Hartnoll’s bound. Finally, in Sec. V we conclude and briefly consider how relaxing some of our assumptions may modify the results.

II. MODEL BASED CALCULATIONS

We consider the single band Hubbard model with nearest neighbor hopping, described by the Hamiltonian

\[ H = -t \sum_{\langle i,j \rangle, \sigma} (c_i^{\dagger} c_j + H.c.) - \mu \sum_{i, \sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (3) \]

where \( n_{i\sigma} = c_i^{\dagger} c_{i\sigma} \), \( t \) is the hopping amplitude \( \mu \) is the chemical potential and \( U \) is Coulomb repulsion for a doubly occupied site. This is probably the simplest model which incorporates nontrivial strong correlation effects. But this model has an exact solution only in one dimension and study of this model in higher dimension involves various approximations. Static mean field descriptions like the Hartree-Fock decomposition of the quartic term \( U n_{i\uparrow} n_{i\downarrow} \simeq U \langle n_{i\uparrow} \rangle n_{i\downarrow} + U n_{i\uparrow} \langle n_{i\downarrow} \rangle \) only shifts the local chemical potential. Because of the complete neglect of the quantum fluctuations this approximation does not generate any new energy scale (e.g. the Fermi liquid coherence scale) which can become relevant at low temperature regions. However, as in the case of classical mean field theory for the Ising model, in the limit of of large dimension, \( d \to \infty \), (or large connectivity \( z \)) the model reduces to an effective single impurity model provided the scaling \( t \to t^*/\sqrt{2d} \) is made on a \( d \)-dimensional hyper-cubic lattice [17]. Under this approximation we neglect all spatial fluctuations yet fully retain quantum dynamics for the single site. The self-energy \( \Sigma(\omega) \) only depends on frequency and not wave vector. This is known as the dynamical mean field theory [18] (DMFT). It has been found DMFT gives a good description of the Mott metal-insulator transition with increasing correlation strength, \( U \), and the crossover from a Fermi liquid to bad metal with increasing temperature [2]. Furthermore, DMFT has been found to give a quantitative description of the temperature dependence of the resistivity [19] and the frequency dependent optical conductivity [20] for organic charge transfer salts that are described by a two dimensional Hubbard model at half-filling [21]. Combining DMFT with
electronic structure calculations based on density functional theory has given an excellent
description of properties of a diverse range of transition metal and rare earth compounds [22].

A. Dynamical mean field theory

As a consequence of the scaling, \( t \rightarrow t^*/\sqrt{2d} \), all the self energy diagrams, arising under
skeletal graph expansion of the irreducible self energy and involving non local Green’s func-
tions vanishes in the limit \( d \rightarrow \infty \). Then the self energy becomes local and involves only
the local Green’s function. The lattice problem for the Hubbard model then can be mapped
onto an effective single impurity Anderson model [18] :

\[
H_{imp} = \sum_{l,\sigma} (\tilde{\epsilon}_l - \mu) c_{l\sigma}^{\dagger} c_{l\sigma} + \sum_{l,\sigma} (V_l c_{l\sigma}^{\dagger} d_{0\sigma} + H.c.) - \mu \sum_{\sigma} n_{d0\sigma} + U n_{d0\uparrow} n_{d0\downarrow},
\]

(4)

where \( n_{d0\sigma} = d_{0\sigma}^{\dagger} d_{0\sigma} \). The operators \( d_{0\sigma}^{\dagger} \) and \( d_{0\sigma} \) characterise a given site \( i = 0 \) and \( \{ c_{l\sigma}^{\dagger}, c_{l\sigma} \} \)
characterise the effective bath arising from electrons at all other sites. \( \tilde{\epsilon}_l \) and \( V_l \) are effective
parameters characterising the dispersion of the bath and its coupling to the local site. \( \tilde{\epsilon}_l \)
and \( V_l \) or equivalently the bath Green’s function, \( G_0(\omega) \), given by

\[
G_0^{-1}(\omega) = \omega + \mu - \int_{-\infty}^{+\infty} \Delta(\epsilon) \frac{d\epsilon}{\omega + \mu - \epsilon}
\]

\[
\Delta(\epsilon) = \sum_{l\sigma} V_l^2 \delta(\epsilon - \tilde{\epsilon}_l)
\]

(5)
can be calculated self consistently by solving the impurity problem iteratively. The solution
of the impurity problem is the toughest part and usually involves various numerical
methods like quantum Monte Carlo (QMC), exact diagonalization (ED), or the numerical
renormalization group (NRG). We use iterated perturbation theory (IPT) [23, 24] as it is
easy to implement, computationally cheap and captures the essential physics in the param-
eter regime we are interested in, \( U < 0.8U_c \) where \( U_c \) is the critical value of \( U \) at which the
Mott metal-insulator transition occurs. For example Bulla [25] showed that for the Bethe
lattice at half-filling the results of IPT and NRG are similar except extremely close to the
Mott transition. Indeed in the proximity of the Mott transition, Terletska et al. [26] found
that the temperature dependent resistivity calculated from IPT was in agreement with that
found by continuous time QMC (CT-QMC). Also, recently Arsenault et al. [27] showed that
for lattices with a van Hove singularity in density of states (DOS), even in the proximity
of the Mott transition, IPT with a modified self-consistency condition matches with results from CT-QMC. So, for single band Hubbard model results from IPT are generic in nature. In the next section we review DMFT self-consistency using IPT.

B. Iterated Perturbation Theory

The iterated perturbation theory (IPT) is a semi-analytical method. The irreducible self-energy in IPT is approximated using second order polarization bubble involving bath Green’s function, $G_0(\omega)$. The self-energy under this approximation can be shown (using moment expansion) to smoothly interpolates between the atomic limit $t = 0$ and the weak coupling limit $U \to 0$. In the following paragraph we elaborate DMFT self-consistency method using IPT as impurity solver. We work with real, not imaginary, frequencies and so no analytic continuation is necessary.

(i) For a given lattice density of states $N_0(\epsilon)$ and self energy $\Sigma(\omega)$ the local Green’s function is given by

$$G(\omega) = \int_{-\infty}^{+\infty} \frac{N_0(\epsilon)d\epsilon}{\omega^+ + \mu - \Sigma(\omega^+) - \epsilon},$$

where $\mu$ is the local chemical potential.

(ii) From knowledge of the local Green’s function $G_{loc}(\omega)$ we can calculate the bath hybridization function, $\Delta(\omega)$ by using-

$$\Delta(\omega) = \omega^+ + \mu - \Sigma(\omega) - G^{-1}(\omega).$$

(iii) Subsequently using bath hybridization we can calculate the bath Green’s function as

$$G_0(\omega) = \frac{1}{\omega + \tilde{\mu}_0 - \Delta(\omega)}.$$ 

The parameter $\tilde{\mu}_0 = \mu - Un$ is the bath chemical potential and it vanishes at half filling for the particle-hole symmetric case, which we consider in the present study.

(iv) The fully interacting Green’s function can be calculated using the Dyson’s equation

$$G(\omega) = \frac{1}{G^{-1}_0(\omega) - \tilde{\mu}_0 + \mu - \Sigma(\omega)}.$$ 

(v) The new self-energy can be calculated following the IPT ansatz [24] as

$$\Sigma(\omega) = Un + \frac{A\Sigma^{(2)}(\omega)}{1 - B\Sigma^{(2)}(\omega)}.$$
where,

\[ A = \frac{n(1 - n)}{n_0(1 - n_0)} ; \quad B = \frac{U(1 - n) - \mu + \mu_0}{n_0(1 - n_0)U^2} \]  

(11)

and

\[ n = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega n_F(\omega) \text{Im}[G(\omega^+)], \]  

(12)

\[ n_0 = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega n_F(\omega) \text{Im}[G_0(\omega^+)] \]  

(13)

are the local and bath particle numbers, respectively. \( \Sigma(\omega) \) is the self energy from second order perturbation theory and is given by

\[ \Sigma^{(2)}(\omega) = U^2 \int_{-\infty}^{+\infty} \prod_{i=1}^{3} (d\epsilon_i \rho_0(\epsilon_i)) \left[ \frac{n_F(-\epsilon_1) n_F(-\epsilon_2) n_F(-\epsilon_3) + n_F(\epsilon_1) n_F(-\epsilon_2) + n_F(\epsilon_3)}{\omega + i\eta - \epsilon_1 + \epsilon_2 - \epsilon_3} \right] \]  

(14)

where \( \rho_0(\omega) = -\frac{1}{\pi} \text{Im}[G_0(\omega^+)] \) and \( \eta \to 0^+ \). We iterate (i) - (v) until the desired self-consistency in self-energy and other physical quantities are achieved. Hence, we focus solely on the case of half-filling \( (n = 1) \). Due to particle-hole symmetry \( \mu = \frac{U}{2} \) for all \( U \) and \( T \). This speeds up computation significantly, as it is not necessary to self-consistently determine \( \mu \) from Eq. (12)

C. Bethe lattice

We choose a Bethe lattice (Cayley tree) because it makes computation even faster because of particle-hole symmetry and the local Green’s function, \( G(\omega) \), has an exact analytical form. It produces qualitatively similar results to the hyper-cubic lattice [18] and lower dimensional tight binding models. In the limit of infinite coordination number \( (z \to \infty) \), the density of states has semi-circular form [28] :

\[ N_0(\epsilon) = \frac{2}{\pi W^2} \sqrt{W^2 - \epsilon^2} \Theta(W - |\epsilon|) \]  

(15)

where \( \Theta(x) \) is the familiar unit step function, \( W = 2t^* \) is the half-band width and the hopping amplitude in this case is scaled as \( t \to t^*/\sqrt{z} \). Most importantly the local Green’s function has the exact analytical form

\[ G(\omega) = \frac{2}{W^2} \left[ \zeta - \sqrt{\zeta^2 - W^2} \right], \]  

(16)

\[ \zeta \equiv \omega + i\eta + \mu - \Sigma(\omega). \]  

(17)
It can be easily verified that in this case the bath hybridization function, \( \Delta(\omega) = \frac{W^2}{4} G(\omega) \equiv t^a G(\omega) \), is proportional to the local Green's function.

### III. TRANSPORT PROPERTIES

Using the self-consistent self energy we can calculate various quantities like \( dc \) conductivity, charge compressibility, and diffusivity.

#### A. \( dc \) Conductivity

In the limit of \( d \to \infty \) all vertex corrections to two-body correlation functions drop out \([29]\) and the temperature dependent \( dc \) conductivity, \( \sigma(T) \), can be calculated using the simple polarization bubble as \([18, 30]\)

\[
\sigma(T) = \frac{\pi e^2}{\hbar} \frac{1}{\nu} \int_{-\infty}^{+\infty} d\epsilon \Phi_{xx}(\epsilon) \int_{-\infty}^{+\infty} d\omega \left( -\frac{\partial n_F(\omega)}{\partial \omega} \right) A^2(\omega, \epsilon)
\]

where \( \nu = a^d \) is the volume of the unit cell of a \( d \)-dimensional hyper-cubic lattice with lattice constant \( a \),

\[
A(\omega, \epsilon) = -\frac{1}{\pi} \text{Im} \left[ \frac{1}{\omega + \mu - \Sigma(\omega) - \epsilon} \right],
\]

\[
n_F(\omega) = \frac{1}{e^{\beta \omega} + 1}
\]

are the spectral density and Fermi function, respectively and

\[
\Phi_{xx}(\epsilon) = \frac{1}{N} \sum_k \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 \delta(\epsilon - \epsilon_k)
\]

is the transport density of states. \( N \) is the number of lattice sites.

Because of its tree like structure the Bethe lattice has no loop and no energy dispersion relation in \( k \). But, by invoking f-sum rule it can be shown that \([31, 33]\)

\[
\Phi_{xx}(\epsilon) = \frac{1}{3d} (W^2 - \epsilon^2) N_0(\epsilon),
\]

is the correct transport density of states in the limit of \( d \to \infty \). It is interesting to mention that for a Bethe lattice with coordination number \( z \) the connectivity \( K = z - 1 \) while that for the hyper-cubic lattice is \( 2d \). So, in the limit of large coordination number we can take the connectivity to be equal to \( 2d \) and we can always do the mapping \( z \leftrightarrow 2d \).
B. Charge Compressibility

In a general many-body system the local particle number is given by

$$n = \frac{1}{\nu} \int_{-\infty}^{+\infty} d\omega n_F(\omega) \sum_k A(k, \omega),$$  \hspace{1cm} (23)

where, the spectral function is

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} \left[ \frac{1}{\omega + \mu - \epsilon_k - \Sigma_k(\omega)} \right].$$  \hspace{1cm} (24)

The self-energy, $$\Sigma_k(\omega)$$, in the limit of $$d \to \infty$$ is independent of wave vector $$k$$ and is given by $$\Sigma(\omega)$$. Hence, differentiating with respect to $$\mu$$, the charge compressibility, $$\kappa_e(T) = \frac{\partial n}{\partial \mu}$$, under the DMFT approximation is given by

$$\kappa_e(T) = \frac{1}{\nu} \int_{-\infty}^{+\infty} d\omega n_F(\omega) \int_{-\infty}^{+\infty} d\epsilon \frac{N_0(\epsilon)}{1} \frac{1}{\pi} \text{Im} \left[ \frac{1}{\omega + \mu - \Sigma(\omega) - \epsilon} \right]^2. \hspace{1cm} (25)$$

In the case of Bethe lattice this reduces to

$$\kappa_e(T) = -\frac{2}{\pi} \int_{-\infty}^{+\infty} d\omega n_F(\omega) \frac{1}{W^2} \text{Im} \left[ \frac{\zeta}{\sqrt{\zeta^2 - W^2}} \right], \hspace{1cm} (26)$$

where $$\zeta$$ is given by Eq. (17). The inverse of the charge compressibility can be interpreted as the energy cost to add or remove a particle from a system. For the non-interacting system ($$U = 0$$) at zero temperature ($$T = 0$$), $$\kappa_e = N_0(E_F)$$, where $$N_0(E_F)$$ is the density of states at the Fermi level.

C. Diffusivity

As mentioned earlier the diffusivity, $$D(T)$$ can be calculated using the Nernst-Einstein relation in Eq. (2). To compare to the limit of diffusion constant, proposed by Hartnoll, we need to find the Fermi velocity under single site DMFT approximation, in the limit of infinite dimensionality, $$d \to \infty$$. Since, $$v_k^2 = \left( \frac{\partial \omega}{\partial k} \right)^2$$ appears in the expression for transport density of states in Eq. (21) we define

$$\hbar v_F^2 = \frac{1}{\hbar} \frac{\Phi_x(\epsilon = 0)}{N_0(\epsilon = 0)}$$  \hspace{1cm} (27)

in the limit of $$d \to \infty$$. This definition of $$\hbar v_F^2$$ gives the correct Fermi velocity [30] for the hyper-cubic lattice in the limit of $$d \to \infty$$. Also, by pure dimensional analysis for any
lattice structure $\hbar v_F = \lambda W a$ ($\lambda$ being a numerical constant of order one for a given lattice). Hartnoll’s proposed quantum bound for diffusion constant on the Bethe lattice is then given by

$$D_H = \frac{W^2 a^2}{3dhk_B T}. \quad (28)$$

The dimensionless scaled diffusivity is then given by

$$\frac{D(T)}{D_H} = \pi \left( \frac{k_B T}{W} \right) \frac{1}{\tilde{\kappa}_e(T)} \int_{-W}^{+W} d\epsilon \int_{-\infty}^{+\infty} d\omega (W^2 - \epsilon^2) N(\epsilon) A^2(\epsilon, \omega) \left( -\frac{\partial f(\omega)}{\partial \omega} \right), \quad (29)$$

where $\tilde{\kappa}_e(T) = \frac{\partial n}{\partial \mu}$ is the dimensionless charge compressibility and $\mu = \tilde{\mu} W$, $\tilde{n} = n\nu$. The advantage of calculating scaled diffusivity is that it does not depend on universal constants such as $\hbar$ or material dependent constants such as the lattice constant, $a$, and the unit cell volume, $\nu$, and the temperature appears only as a dimensionless scaled quantity.

We now turn to comparison with bound for the spin diffusion constant. In a similar spirit we use $\frac{1}{m} = \frac{1}{m^*} \frac{\partial^2 \epsilon}{\partial k^2}$ as a generalized definition for inverse mass. Then for the hyper-cubic lattice we get $\frac{W^2}{d\mu^2}$ as an effective inverse mass averaged over the Fermi surface at half-filling. If we take this to be same in the Bethe lattice as well then we will have

$$D_A = \frac{\alpha W a^2}{d\hbar} \quad (30)$$

with $\alpha = 1.3$ a dimensionless constant. However in an interacting system the bare mass $m$ gets renormalized to an effective mass $m^* = m/Z$ due to interactions. So the corresponding limit $D_A$ will get renormalized to

$$D_A^* = \alpha \frac{\hbar}{m^*} = ZD_A \quad (31)$$

where $Z = \frac{m}{m^*}$ is the quasi-particle renormalization factor which can be easily calculated from the self energy, $\Sigma(\omega) = \Sigma_R(\omega) + i\Sigma_I(\omega)$:

$$Z = \left( 1 - \frac{\partial \Sigma_R(\omega)}{\partial \omega} \bigg|_{\omega \rightarrow 0} \right)^{-1}. \quad (32)$$

The scaled diffusivity in this case is then given by

$$\frac{D(T)}{D_A^*} = \pi \frac{1}{3\alpha Z \tilde{\kappa}_e(T)} \int_{-W}^{+W} d\epsilon \int_{-\infty}^{+\infty} d\omega (W^2 - \epsilon^2) N(\epsilon) A^2(\epsilon, \omega) \left( -\frac{\partial f(\omega)}{\partial \omega} \right). \quad (33)$$
IV. RESULTS

We consider the case of half filling, \( n = 1 \), i.e. each site on the average is occupied by one electron. We study spectral and transport properties as a function of correlation strength \( U \) and temperature, \( T \) (enters as \( k_B T \) with dimension of energy). Henceforth, unless stated otherwise, all the energy scales will be measured in units of half-bandwidth, \( W \).

A. Spectral function

In Fig. 1 we show the evolution of the spectral function,

\[
A_d(\omega) = -\frac{1}{\pi} \text{Im} \left[ G(\omega^+) \right],
\]

as a function of \( U \) and \( T \). Similar results has been obtained previously by other authors \cite{23}. For completeness we show these results here because they illustrate the essential physics (the destruction of quasi-particles) that is essential to violation of the MIR limit and Hartnoll’s bound. In panel (a) of Fig. 1 we show the spectral function for a weakly correlated system \( U = 0.5 \). The spectral function is dominated by a broad central peak and a very small smearing of the non-interacting (\( U = 0 \)) band edges at \( \omega = \pm 1 \). The integrated spectral weight is dominated by the contribution from the central peak and \( A_d(0) \simeq 2/\pi \), as in the non-interacting case. At finite temperature, due to particle-hole excitations across the Fermi surface, the spectral weight at the Fermi energy \( \omega = 0 \) gets transferred to finite frequency but the central peak still remains intact.

As we increase the correlation strength (\( U = 1 \)) side bands develop on either side of the central peak as shown in the panel (b) of Fig. 1. The side bands eventually develop into high energy Hubbard bands at \( \omega = \pm \frac{U}{2} \) as shown in panel (c) of Fig. 1 for \( U = 2 \). The Hubbard bands are well separated from the central peak which arises due to Kondo resonance effects in the effective single impurity Anderson model \cite{18}. The width and height of the Kondo resonance is controlled by the effective Kondo temperature \( T_K \). Since, \( T_K \sim W \exp(-\Gamma_{\text{eff}}/U) \), where \( \Gamma_{\text{eff}} \) is an effective hybridization strength, the width of the Kondo resonance decreases while its height increases with increasing \( U \) as shown in panel (d) for \( U = 2.5 \). For very large \( U > U_c \) the Kondo resonance gets completely killed and we enter into the Mott insulating state characterised by fully gapped spectral function at the Fermi
energy. The numerical value of $U_c$ depends on the numerical technique that one uses and $U_c \simeq 3.3 - 3.4$ for the IPT based impurity solver \cite{23, 25}.

At finite temperature in the moderately correlated regime like $U = 1.0$ the central peak, despite getting broadened, remains intact even for temperatures as high as $T \sim W$. The side bands thermally broaden out. For the strongly correlated regime of $U = 2$ and $U = 2.5$ the central peak (quasi-particle peak) as well as the integrated spectral weight under it decreases with increasing temperature and eventually the central peak gets completely destroyed for temperatures $T \gg T_K$. This corresponds to the finite temperature crossover from the strong coupling regime into the local moment regime of the effective Anderson impurity model. The crossover region becomes increasingly sharp as evident in panel (d), which corresponds to the fragile nature of the quasi-particle state in the strongly correlated regime. In the Hubbard model this cross-over is between a Fermi liquid and a bad metal \cite{2, 34}.

B. Quasi-particle weight

In Fig. 3 we show the continuous decrease of the quasi-particle renormalization factor, $Z$, with increasing $U$. This also tracks the continuous destruction of coherent quasi-particle states. Comparison of $Z$ against results from numerical renormalization group (NRG) based calculations by Bulla \cite{25} validates the qualitative correctness of IPT based approach though $Z$ begins to differs by 50% in the strong correlation regime ($U = 2.5$). We also note that for $U = 2.5$, $Z > 0.2$ and so in some sense for that regime the system is not extremely correlated. Yet we will see that even in this regime Hartnoll’s bound is violated. For comparison, in the doped Hubbard model on the square lattice (with $U = 16t = 3.5W$ at 15% doping $n = 0.85$) DMFT gives $Z \simeq 0.2$ \cite{4}.

C. Charge compressibility

In Fig. 2 we also show the evolution of the zero temperature charge compressibility, $\kappa_e$, as a function of correlation strength, $U$. The charge compressibility continuously goes to zero with increasing, $U$. As already mentioned earlier, $1/\kappa_e$ can be thought of as the energy required to add/remove an electron to/from the systems. Hence it gets increasingly
FIG. 1: (Color online) Energy dependent spectral function, $A_d(\omega)$, for various values of the interaction strength $U$ and temperature $T$. Panel (a): weakly correlated regime. (Green) dashed line is the density of states for the non-interacting case. Panel (b): moderately correlated regime. Panel (c) and (d): strongly correlated regime. With increasing $U$, the integrated spectral weight under central peak (Kondo resonance) gets transferred to high energy Hubbard bands which corresponds to destruction of quasi-particle states. In these cases, there is a temperature dependent crossover between strong coupling regime (Fermi liquid) and local moment regime (bad metals). All energies and temperatures are measured in units of $W$, the half-bandwidth.

harder to add or remove an electron into the system as we increase $U$, i.e., the system increasingly becomes incompressible and finally at $U = U_c$ the system becomes completely incompressible. Note that at $U = 0$, $\kappa_e = N_0(E_F) = 2/\pi$ as it should be. A similar decrease in charge compressibility with increasing $U$ was observed in exact diagonalization calculations for the Hubbard model on the triangular lattice at half-filling [34].
FIG. 2: (Color online) The zero-temperature quasi-particle renormalization factor $Z$ and charge compressibility $\kappa_e$ as a function of $U$. The system becomes increasingly incompressible with increasing $U$ and the coherent quasi-particle state gets continuously destroyed as evident from the continuous vanishing of $Z$. The transition to the Mott insulator occurs at $U_c \simeq 3.4$. $U$ is measured in units of $W$.

In Fig. 3 we show the temperature dependence of the charge compressibility for a range of $U$. In the non-interacting case ($U = 0$) for the Bethe lattice we can easily show that

$$\kappa_e(T) = \int_{-\infty}^{+\infty} \left(-\frac{\partial n_F(\omega)}{\partial \omega}\right) N_0(\omega)$$

This expression is similar to the expression for Pauli spin susceptibility, $\chi(T)$. Using standard integral expressions involving the Fermi function

$$\int_{-\infty}^{+\infty} H(\epsilon)n_F(\epsilon)d\epsilon = \int_{-\infty}^{\mu} H(\epsilon)d\epsilon + \frac{\pi^2}{6} (k_B T)^2 H'(\mu) + \cdots$$

the expression for charge compressibility in Eq. (35) reduces to

$$\kappa_e(T) = N_0(\mu) + \frac{\pi^2}{6} (k_B T)^2 \left| \frac{d^2 N_0(\omega)}{d\omega^2} \right|_{\omega=\mu} + \cdots.$$ 

In the interacting case we expect in the Fermi liquid state

$$\kappa_e(T) \simeq \kappa_e(0) \left[ 1 - \frac{\delta}{Z^2} \left( \frac{k_B T}{W} \right)^2 + \cdots \right],$$
with $\delta \sim 1$. So, because of the thermal broadening effects, just as in the case of the spin susceptibility, the charge compressibility in the Fermi liquid state will decrease quadratically in temperature $T^2$. This explains the rapid decrease of charge compressibility in the coherent Fermi liquid state because the temperature scale for the decrease is that of the coherence temperature. But as in the case of resistivity in the incoherent regime the decrease is very roughly linear in $T$.

![Graph showing temperature dependence of charge compressibility](image)

**FIG. 3:** (Color online) Temperature dependence of the charge compressibility, $\kappa_e$, for for various correlation strengths $U$. Both $T$ and $U$ are measured in units of $W$.

### D. Resistivity

In Fig. 4 we show the temperature dependence of the resistivity, $\rho(T)$, scaled by the Mott-Ioffe-Regel limit, $\rho_{MIR} = \frac{h\alpha}{e^2}$, for various correlation strengths, $U$. In the weakly correlated regime ($U = 0.5$) the resistivity is well within the Mott-Ioffe-Regel limit in the entire temperature range up to $W$. Hence, the transport can be characterised by weak scattering of coherent quasi-particle states. At very low temperatures ($T < T_K \ll W$) the resistivity is proportional to $T^2$ as expected in the coherent Fermi-liquid regime. The
$T^2$ behaviour is due to the fact that in the Fermi liquid regime the imaginary part of the self-energy, or equivalently the inverse of quasi-particle life time ($\tau_{qp}^{-1}$) is very roughly proportional to $T^2$ (or $\omega^2$ at $T = 0$). At high temperatures ($T \gg T_K$), the resistivity is proportional to $T$ and this corresponds to the incoherent (bad metal) regime of transport [3].

As we increase $U$, the resistivity smoothly crosses the Mott-Ioffe-Regel limit and in the strongly correlated regime ($U = 2.0$ and above) the resistivity far exceeds the MIR limit. This is due to the sharp cross-over from the strong coupling (Fermi liquid) regime to the local moment (bad metal) regime in the strong correlation regime and is consistent with the picture of fragile quasi-particles states in the strong correlation regime. It is important to mention that even though the derivative $d\rho(T)/dT$ changes sign there is no metal-insulator transition as evident from the finite temperature spectral function, $A_d(\omega)$ at $\omega = 0$ and the finite charge compressibility $\kappa_e$. Also, for the given choice of $U$ we are still far away from Mott transition at $U_c \approx 3.4$. This is also evident from relatively large quasi-particle weight $Z \sim 0.2$ even for $U = 2.5$ where the MIR limit is violated by a factor of 100. So, the transport in this bad metal phase is incoherent in nature.

![FIG. 4: (Color online) Resistivity shows violation of the Mott-Ioffe-Regel limit ($\rho_{MIR} = \hbar a/e^2$) with increasing $U$. This is consistent with the picture that transport becomes increasingly incoherent with increasing correlation effects. Both $T$ and $U$ are measured in units of $W$.](image-url)
E. Diffusivity

Finally, using the Nernst-Einstein relation we calculate the charge diffusivity. In Fig. 5 we show scaled diffusivity, $D(T)/D_H$, as a function of temperature ($T$) for various correlation strengths ($U$). In the weakly correlated regime ($U = 0.5$) the diffusivity is well above Hartnoll’s bound but as we increase $U$, the diffusivity starts to violate Hartnoll’s bound ($U = 1.0$ and $U = 1.5$). In the strongly correlated regime, $U = 2.0$ and above, the violation of Hartnoll’s bound is severe. For example for $U = 2.0$ the violation is by more than a factor of 200 and for $U = 2.5$ the violation is by more than 1000. Again we stress that the system is not extremely correlated with $Z \sim 0.2$ at low temperatures.

The behaviour of the scaled diffusivity is closely related to the scaled resistivity. In the weakly correlated regime ($U = 0.5$), transport is through diffusive scattering of coherent quasi-particle states and the resistivity, $\rho(T)$, is well within the MIR limit. So, Hartnoll’s bound characterizes the quasi-particle regime of transport and its violation in the moderately to strongly correlated regime nearly coincides with the violation of MIR limit of resistivity. So, in the incoherent regime of transport Hartnoll’s bound is strongly violated.

We now compare the charge diffusivity to the quantum limit of the spin diffusion constant, $D_s \simeq 1.3\hbar/m$, experimentally observed $^{13}$ and theoretically calculated $^{15}$ in the degenerate Fermi gas in the unitary limit. In Fig. 6 we show the scaled diffusivity, $D(T)/D_A^*$, as a function of temperature for various $U$. The scaled diffusivity also violates the quantum limit of spin diffusion constant, $D_s \simeq 1.3\hbar/m$. The violation is severe in the strongly correlated regime. All the temperature dependence is ultimately due to inherent temperature dependence of self energy, $\Sigma(\omega)$. It is important to mention that spin diffusion in charge neutral systems like the degenerate Fermi gas in the unitary limit has no clear relation to charge diffusion in electron liquids. For a degenerate non-interacting Fermi gas in three dimensions the charge diffusion constant is given by $D = \frac{1}{3} \frac{\hbar}{m} k_F \ell$, where $k_F$ is the Fermi wave vector and $\ell$ is the mean free path. In the weak scattering limit $k_F \ell \gg 1$ and $D \gg \frac{1}{3} \frac{\hbar}{m}$. So, just like the upper limit (MIR) of resistivity we can define lower limit for the charge diffusion...
FIG. 5: (Color online) Scaled diffusivity shows strong violation of Hartnoll’s bound in the incoherent regime of transport. Only in the weakly correlated quasi-particle regime of transport, Hartnoll’s bound is well respected. $D(T)/D_H$ for $U = 2.5$ is small but finite at the lowest point. Both $T$ and $U$ are measured in units of $W$.

constant $D_{lim} = \frac{1}{3} \hbar m$. In the weakly interacting quasi-particle regime of transport the limit will be renormalized to $D_{lim}^* = \frac{1}{3} \hbar m^*$. The quantum spin diffusion limit in degenerate Fermi gas will roughly correspond to $k_F \ell \sim 4$ for charge diffusion in a condensed matter system and the diffusion will correspond to transport through coherent quasi-particle states.

V. CONCLUSIONS

We have studied the conductivity, charge compressibility, and charge diffusivity in a single band Hubbard model using single site dynamical mean field theory. The calculated resistivity far exceeds the MIR limit in the strong correlation regime. The transport in the weakly correlated region can be characterized by diffusive scattering of coherent quasi-particle states but in the strongly correlated bad metal state the transport is incoherent. The charge compressibility decreases with increasing $U$ which corresponds to the fact that in the correlated regime, the energy cost to create a charge fluctuation increases with increasing $U$. 
Then using the Nernst-Einstein relation we calculated the charge diffusivity in the system. The charge diffusivity strongly violates Hartnoll’s proposed bound in the incoherent regime of transport. The bound is only well respected in the weakly correlated regime of transport where diffusive scattering of coherent quasi-particle states is the dominant mechanism for transport. We also compared the calculated charge diffusivity against the quantum limit of spin diffusion observed in the degenerate Fermi gas in the unitary limit. The calculated diffusivity in this case also strongly violates quantum limit of spin diffusion in the incoherent regime. So, within the single site DMFT approximation we do not observe any quantum limit to charge diffusion in the strongly correlated incoherent regime.

Hartnoll’s proposed bound is based on the AdS/CFT correspondence and various conservation laws in fluids. But within single site DMFT approximation there is energy conservation but there is no momentum conservation at a given site. Other approximations like the dynamical cluster approximation (DCA) in which momentum is conserved within
the cluster, bath as well as at the boundary of the cluster should be able to address this issue. One might also consider how vertex corrections could modify the results. A recent study of the role of vertex corrections in the doped two-dimensional Hubbard model found they altered the calculated resistivity by less than a factor of two [38].

APPENDIX: Derivation of the Nernst-Einstein equation

Fick’s law for diffusion is given by
\[ \mathbf{j}_m(\mathbf{r}) = -D(\mathbf{T}) \nabla n(\mathbf{r}) \tag{39} \]
where \( D(\mathbf{T}) \) is the diffusion constant, \( \mathbf{j}_m(\mathbf{r}) \) is the mass current and \( n(\mathbf{r}) \) is the local particle number. On the other hand Ohm’s law for electrical conductivity is given by
\[ \mathbf{j}_e(\mathbf{r}) = \sigma(\mathbf{T}) \mathbf{E}(\mathbf{r}) \tag{40} \]
where \( \sigma(\mathbf{T}) \) is the electrical conductivity, \( \mathbf{j}_e(\mathbf{r}) \) is the electric current and \( \mathbf{E}(\mathbf{r}) \) is the external electric field. We have
\[ \mathbf{j}_e(\mathbf{r}) = e\mathbf{j}_m(\mathbf{r}) = -eD(\mathbf{T}) \frac{\partial n}{\partial \mu} \nabla \mu(\mathbf{r}) \tag{41} \]
where \( \mu(\mathbf{r}) = \mu_0 + e\phi(\mathbf{r}) \) is the chemical potential in the presence of external field and \( \mu_0 \) is that in the absence of external field and \( \phi(\mathbf{r}) \) is the electric potential. Then
\[ \nabla \mu(\mathbf{r}) = e \nabla \phi(\mathbf{r}) = -e\mathbf{E}(\mathbf{r}). \tag{42} \]
Combining Eq. (41) and (42) gives
\[ \mathbf{j}_e(\mathbf{r}) = e^2 \frac{\partial n}{\partial \mu} D(\mathbf{T}) \mathbf{E}(\mathbf{r}). \tag{43} \]
Comparing this with Ohm’s law in Eq. (40) we finally get
\[ \sigma(\mathbf{T}) = e^2 \frac{\partial n}{\partial \mu} D(\mathbf{T}) \tag{44} \]

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