Characterizing Featureless Mott Insulating State by Quasiparticle Interferences - A DMFT Prospect

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The quasiparticle interferences (QPIs) of a Mott insulator are investigated using the $T$-matrix formalism implemented with the dynamical mean-field theory (T-DMFT). In Mott insulating state, because DMFT predicts a singularity in the real part of the electron self energy $\text{Re}\Sigma(\omega) \sim \eta/\omega$ at low frequency, where $\eta$ can be considered as the 'order parameter' for Mott insulating state, QPIs are completely washed out at the small bias voltage. However, a further analysis shows that $\text{Re}\Sigma(\omega)$ in fact serves as an energy-dependent chemical potential shift. As a result, the effective bias voltage seen by the system is $eV + \text{Re}\Sigma(eV)$. Due to the singular behavior of $\text{Re}\Sigma(\omega)$, a critical bias voltage $eV_c = \sqrt{\eta}$ satisfying $eV' = 0$ exists if and only if in Mott insulating state. Consequently, the same QPI patterns produced by the non-interacting Fermi surfaces appears at this critical bias voltage $eV_c$ in Mott insulating state. We propose that this reentry of non-interacting QPI patterns at $eV_c$ could serve as an experimental signature of Mott insulating state, and the 'order parameter' can be experimentally measured as $\eta = (eV_c)^2$.

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Introduction – Mottness, the physics of understanding how insulating state arises from partially-filled conduction band due to strong local interaction, has been one of the most challenging subjects in the condensed matter physics, for it may hold the key to understand the mechanism of high-temperature superconductivity observed in materials with narrow bandwidth. The essential physics of Mottness can emerge from Hubbard model,

$$H_{\text{Hubbard}} = H_t + H_U$$

$$H_t = -t \sum_{<i,j>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c.,$$

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(1)

where $t$ is the hopping parameter between nearest neighbor sites $<i,j>$, and $U$ the Hubbard on-site interaction. While Hubbard model has been successful in conceptually demonstrating the metallic state in limit of $U/t << 1$ and insulating state in the limit of $U/t >> 1$, the nature of Mott transition, the transition from metallic to insulating states as a function of $U/t$, remains a challenging and unsolved problem. One particular difficulty lies in the fact that Mott transition does not seem to involve breaking of symmetry for which Landau-Ginzburg theory can be employed. Consequently, an 'order parameter' that is theoretically well-defined and experimentally observable is lacking. DC resistivity exhibiting a change from metallic to insulating behavior as a function of temperature is often used as an indication of Mott transition, but it also depends on many other details of the materials, e.g., impurity and disorder. As a result, DC resistivity can not be a conclusive experimental signature for Mott transition.

Among the various theoretical approaches proposed to solve Hubbard model, the dynamical mean-field theory (DMFT) has been shown to be a great tool to understand Mott insulating state. DMFT maps the problem of solving Hubbard model to the problem of solving Anderson impurity model that is relatively much better understood, and such a mapping is shown to be 'exact' in the limit of spatial dimension $d$ going to infinity. The price paid for this, however, is that momentum-dependence of the electron self energy is completely neglected, but the resulting electron self energy $\Sigma(\omega)$ includes all the local quantum fluctuations. Since Mott insulating state concerns mostly the local physics, $\Sigma(\omega)$ from DMFT contains a lot of information that can not be accessed by other approaches easily regardless of its lacking of momentum dependence.

Following the framework of DMFT, the real part of electron self energy has the following singular behavior at low frequency

$$\text{Re}\Sigma(\omega) = \frac{\eta}{\omega} + O(\omega),$$

(2)

where the constant term $-U/2$ has been absorbed into the chemical potential, and

$$\eta = \left[ -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \sum_{\vec{k}} \text{Im} G_b(\vec{k}, \omega + i0^+) \right]^{-1}$$

(3)

can be considered as the 'order parameter' of Mott insulating state because $\eta = 0$ in metallic phase while $\eta \neq 0$ in Mott insulating phase. $G_b(\vec{k}, \omega)$ is the full Green function obtained from DMFT with the following form,

$$G_b(\vec{k}, \omega) = \left[ \omega - E(\vec{k}) - \Sigma(\omega) \right]^{-1}.$$  

(4)

This $1/\omega$ singularity in $\text{Re}\Sigma(\omega)$ inherits from the self energy in the atomic limit of Hubbard model ($t = 0$), and
DMFT captures it pretty well even with non-zero $t$. However, $\eta$ remains a purely theoretically-defined ‘order parameter’ because no any experimental probe has actually been applied to measure it with enough resolution.

In this paper, we propose that the quasiparticle interferences (QPIs) measured from the spectroscopic imaging scanning tunnelling microscopy (SI-STM) could be a feasible tool to directly measure $\eta$. QPIs have been widely used to extract the spectroscopic information of the electronic structure in materials including, but not limited to, cuprates [9–11], iron-based superconductors [12–14], topological insulators [15–18], Sr$_3$Ru$_2$O$_7$ [19–21], and heavy fermion systems [22, 23]. On the theoretical side, the $T$-matrix formalism [24, 25] developed in the non-interacting Fermi surface appear at a non-zero energy. We develop the $T$-matrix formalism implemented with DMFT (T-DMFT) to analyze the QPI patterns in Mott insulating state. At small bias voltage, no meaningful QPI images are found due to the singular behavior of the electron self energy given in Eq. 2, as expected. However, by a closer look into the T-DMFT formalism, we find that the QPI patterns resembling the one produced by the non-interacting Fermi surface appear at a non-zero critical bias voltage $V_c$, and this critical bias voltage is directly related to the ‘order parameter’ of Mott insulating state given in Eq. 2. We propose that this novel reentry of non-interacting QPI at high bias voltage could serve as an experimental signature of Mott transition, and the order parameter can be measured by $\eta = (eV_c)^2$ accordingly.

Formalism – We start from the following model Hamiltonian of

$$H = H_{\text{Hubbard}} + H_{\text{imp}},$$
$$H_{\text{imp}} = \sum_{\vec{k}, \vec{k}' \sigma} V_{\vec{k}, \vec{k}'} c_{\vec{k} \sigma}^\dagger c_{\vec{k}' \sigma},$$

where $H_{\text{Hubbard}}$ is Hubbard model described in Eq. 1 and $V_{\vec{k}, \vec{k}'}$ is the impurity scattering matrix element which is assumed to be spin-independent. To specifically compute the QPI image, we employ a $T$-matrix approach [25] with DMFT using Hirsch-Fye quantum Monte Carlo algorithm as the impurity solver. The imaginary time interval $[0, \beta]$ is divided into $L = 128$ slices, and the maximum Matsubara frequency used is $n_{\text{max}} = 8192$. After the self-consistent calculation is converged, we obtain the time-ordered electron self energy $\Sigma(i\omega_n)$ directly. We then adopt the continuous-pole-expansion method [26] recently developed by Staar, et. al. to numerically perform the analytic continuation on $\Sigma(i\omega_n)$. This method is shown to be an efficient approach to find an accurate and unambiguous result of analytic continuation within a finite range of frequency, which is necessary for the current study. The electron Green function with DMFT given in Eq. 3 can finally be obtained.

Once the Hubbard model is solved by DMFT, we treat impurity scatterings necessary for the QPI images as a perturbation around the DMFT solution. If the impurity scatterings are weak, $T$-matrix formalism [25] allows us to sum over all the vertex corrections due to the impurity scatterings with $G_{\text{b}}(\vec{k}, \omega)$ as the ‘bare’ Green function. The resulting Green function with impurity scatterings can be written as

$$G(\vec{k}, \vec{k}', \omega) = G_{\text{b}}(\vec{k}, \omega) \delta_{\vec{k}, \vec{k}'} + G_{\text{b}}(\vec{k}, \omega) T_{\vec{k}, \vec{k}'}(\omega) G_{\text{b}}(\vec{k}', \omega)$$

where the $T$-matrix satisfies

$$T_{\vec{k}, \vec{k}'}(\omega) = V_{\vec{k}, \vec{k}'} + \int d^2p V_{\vec{k}, \vec{p}} G_{\text{b}}(\vec{p}, \omega) T_{\vec{p}, \vec{k}'}(\omega),$$

For the case of single impurity, $V_{\vec{k}, \vec{k}'} = V_0$ and consequently $T_{\vec{k}, \vec{k}'}(\omega)$ can be further reduced to $T(\omega)$. As a result, $T(\omega)$ can be evaluated from $G_{\text{b}}(\vec{k}, \omega)$ by

$$\left\{ \left. \frac{1}{\rho(\omega)} = \frac{1}{V_0} - \int d^2p G_{\text{b}}(\vec{p}, \omega) \right| \right.$$
QPI pattern is not expected to deviate from the one obtained in the non-interacting case. The situation, however, changes dramatically as $U$ is large enough for the occurrence of Mott insulating state ($2 < U_c < 3$ in the current calculation). In Mott insulating state, $\text{Im} \Sigma(\omega)$ has a delta-function-like peak at $\omega = 0$, while $\text{Re} \Sigma(\omega)$ exhibits a $1/\omega$ behavior at small frequency. This behavior of self energy makes $G_0(\vec{k}, \omega)$ very small at small frequency, which washes away any meaningful features in the QPI images at small bias voltage.

Intriguing features appear at high bias voltage. The singular behavior of $\text{Re} \Sigma(\omega)$ described in Eq. (2) guarantees the existence of a critical bias voltage $eV_c = \sqrt{\eta}$ satisfying

$$eV'_c = eV_c - \frac{n}{eV_c} = 0.$$  

In other words, in Mott insulating state, there is always a non-zero critical bias voltage $V_c$ at which the QPI pattern is exactly the same as the non-interacting one except extra broadening, and the ‘order parameter’ of Mott insulating state can be mapped out by $\eta = (eV_c)^2$.

To confirm this, we consider the one-band Hubbard model with the nearest neighbor hopping at half-filling. The non-interacting QPI exhibits a strong peak at $\vec{q} = (\pi, \pi)$ at zero bias and the peak shifts to a smaller momentum as the bias voltage increases. Fig. 2 plots the QPI along the nodal direction at the critical bias voltage $V_c$ for different $U$, and all of them exhibit exactly the same peak at $\vec{q} = (\pi, \pi)$, resembling the non-interacting QPI at zero bias. For $U/t = 1, 2$, the system is not in Mott insulating state and $V_c = 0$. For $U/t \geq 3$, this QPI pattern appears at $eV_c = 0.44t, 0.88t, 1.37t$. Longer range hopping parameters can be added in order to capture more details about the Fermi surface, but these additions do not change the conclusion at all except the critical bias voltage might be slightly modified.

**Discussions and summary** – The current result is primarily based on the feature that the electron self energy is momentum-independent in DMFT. This feature is correct in the atomic limit of Hubbard model[4], but generally speaking the electron self energy should depend on momentum as well whenever $t/U$ is non-zero. Nevertheless, since we are mainly interested in Mott insulating state in which $t/U$ is a small parameter, the momentum-dependence of the electron self energy should be weak in the region that we are interested in, which has been explicitly shown in previous study[27–29]. As a result, the predicted reentry of the non-interacting QPIs at a critical bias voltage should be robust even as the momentum dependence of the self energy is considered.

It is worthy of being mentioned that the critical bias voltage is smaller than Mott gap as we can see in Fig. 2. The typical value of $t$ for cuprates is around 350 meV, which gives the critical bias voltage about 150 meV to 600 meV for $U/t = 3 – 5$. The fundamental limitation of the STM is the range of the energy within which the density of states of the STM tips remains flat. A typical STM tip has a flat density of states within $E_F \pm 500$ meV. As a result, although the critical voltage is a higher than the typical range where the spectroscopic STM are routinely performed, it is still feasible for experiments.

The existence of the critical bias voltage $eV_c$ is not...
limited to electron self energy obtained from DMFT. In fact, any theory having an electron self energy with diverging behavior at low frequency is likely to have a non-zero $eV_c$. From the Dyson’s equation, the self energy can be expressed as $\Sigma = G_0^{-1} - G_{-1}$, where $G_0$ and $G$ are the non-interacting and full Green functions. Since $G_0$ is non-zero always, $\Sigma$ could have a diverging behavior if and only if the full Green function has zeros at low frequency. The appearance of zeros in full Green function has been recently found in various theories of strongly correlated electrons\cite{29,30,31,32}, including AdS-CFT\cite{33,34}. As a result, it is expected that similar results will be obtained if these theories could be incorporated into $T$-matrix formalism.

In summary, we have employed the $T$-matrix formalism implemented with the dynamical mean-field theory (DMFT) to study the QPI patterns in a Mott insulator. While QPIs are completely washed out by the singular Fermi surface appear at a non-zero critical bias voltage. Because the existence of this non-zero critical bias voltage is a direct consequence of the singular behavior of $\text{Re} \Sigma(\omega) \sim \eta/\omega$ with $\eta$ as the ‘order parameter’ of Mott insulating state, this novel reentry of non-interacting QPI at high bias voltage could serve as an experimental signature of Mott transition, and the order parameter can be measured by $\eta = (eV_c)^2$ accordingly.

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\begin{thebibliography}{99}
\bibitem{1} M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. \textbf{70}, 1039 (1998).
\bibitem{2} P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. \textbf{78}, 17 (2006).
\bibitem{3} P. Phillips, Rev. Mod. Phys. \textbf{82}, 1719 (2010).
\bibitem{4} A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. \textbf{68}, 13 (1996).
\bibitem{5} G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev. Mod. Phys. \textbf{78}, 865 (2006).
\bibitem{6} G. Sordin, K. Haule, and A.-M. S. Tremblay, Phys. Rev. Lett. \textbf{104}, 226402 (2010).
\bibitem{7} A. Rüegg, H.-H. Hung, E. Gull, and G. A. Fiete, Phys. Rev. B \textbf{89}, 085122 (2014).
\bibitem{8} H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, Rev. Mod. Phys. \textbf{86}, 779 (2014).
\bibitem{9} A. R. Schmidt, K. Fujita, E.-A. Kim, M. J. Lawler, H. Eisaki, S. Uchida, D.-H. Lee, and J. C. Davis, New Journal of Physics \textbf{13}, 065014 (2011).
\bibitem{10} K. Fujita, M. H. Hamidian, S. D. Edkins, C. K. Kim, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, H. Eisaki, S.-i. Uchida, et al., Proceedings of the National Academy of Sciences \textbf{111}, E3026 (2014).
\bibitem{11} E. H. da Silva Neto, P. Aynajian, A. Frano, R. Comin, E. Schierle, E. Weschke, A. Gymen, J. Wen, J. Schneckloch, Z. Xu, et al., Science \textbf{343}, 393 (2014).
\bibitem{12} T.-M. Chuang, M. P. Allan, J. Lee, Y. Xie, N. Ni, S. L. Budko, G. S. Boebinger, P. C. Canfield, and J. C. Davis, Science \textbf{327}, 181 (2010).
\bibitem{13} M. P. Allan, A. W. Rost, A. P. Mackenzie, Y. Xie, J. C. Davis, K. Kihou, C. H. Lee, A. Iyo, H. Eisaki, and T.-M. Chuang, Science \textbf{336}, 563 (2012).
\bibitem{14} M. P. Allan, K. Lee, A. W. Rost, M. H. Fischer, F. Masseo, K. Kihou, C.-H. Lee, A. Iyo, H. Eisaki, T.-M. Chuang, et al., Nat. Phys. \textbf{11}, 177 (2015).
\bibitem{15} Z. Alpichshev, J. G. Analytis, J.-H. Chu, I. R. Fisher, Y. L. Chen, Z. X. Shen, A. Fang, and A. Kapitulnik, Phys. Rev. Lett. \textbf{104}, 016401 (2010).
\bibitem{16} T. Zhang, P. Cheng, X. Chen, J.-F. Jia, X. Ma, K. He, L. Wang, H. Zhang, X. Dai, Z. Fang, et al., Phys. Rev. Lett. \textbf{103}, 206603 (2009).
\bibitem{17} W.-C. Lee, C. Wu, D. P. Arovas, and S.-C. Zhang, Phys. Rev. B \textbf{80}, 245430 (2009).
\bibitem{18} X. Zhou, C. Fang, W.-F. Tsai, and J. Hu, Phys. Rev. B \textbf{80}, 245317 (2009).
\bibitem{19} M. P. Allan, A. Tamai, E. Rozbicki, M. H. Fischer, J. Voss, P. D. C. King, W. Meveasana, S. Thirupathaiah, E. Rienks, J. Fink, et al., New Journal of Physics \textbf{15}, 063029 (2013).
\bibitem{20} W.-C. Lee and C. Wu, Phys. Rev. Lett. \textbf{103}, 176101 (2009).
\bibitem{21} W.-C. Lee, D. P. Arovas, and C. Wu, Phys. Rev. B \textbf{81}, 184403 (2010).
\bibitem{22} P. Aynajian, E. da Silva Neto, A. Gymen, R. E. Baumbach, J. D. Thompson, Z. Fisk, E. D. Bauer, and A. Yazdani, Nature \textbf{486}, 201 (2012).
\bibitem{23} P. Aynajian, E. da Silva Neto, B. B. Zhou, S. Misra, R. E. Baumbach, Z. Fisk, J. Mydosh, J. D. Thompson, E. D. Bauer, and A. Yazdani, Journal of the Physical Society of Japan \textbf{83}, 061008 (2014).
\bibitem{24} Q.-H. Wang and D.-H. Lee, Phys. Rev. B \textbf{67}, 020511 (2003).
\bibitem{25} A. V. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. \textbf{78}, 373 (2006).
\bibitem{26} P. Staar, B. Ydens, A. Kozhevnikov, J.-P. Locquet, and T. Schulthess, Phys. Rev. B \textbf{89}, 245114 (2014).
\bibitem{27} P. Phillips, Rev. Mod. Phys. \textbf{82}, 1719 (2010).
\bibitem{28} W.-C. Lee and P. W. Phillips, Phys. Rev. B \textbf{84}, 115101 (2011).
\bibitem{29} K. B. Dave, P. W. Phillips, and C. L. Kane, Phys. Rev. Lett. \textbf{110}, 090403 (2013).
\bibitem{30} T. D. Stanescu, P. Phillips, and T.-P. Choy, Phys. Rev. B \textbf{75}, 104503 (2007).
\bibitem{31} S. Hong and P. Phillips, Phys. Rev. B \textbf{86}, 115118 (2012).
\bibitem{32} P. W. Phillips, B. W. Langley, and J. A. Hutasoit, Phys. Rev. B \textbf{88}, 115129 (2013).
\bibitem{33} G. Vanacore and P. W. Phillips, Phys. Rev. D \textbf{90}, 044022 (2014).
\bibitem{34} J. Alsup, E. Papantonopoulos, G. Siopsis, and K. Yeter, Phys. Rev. D \textbf{90}, 126013 (2014).
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