Finite-Temperature Mott Transition in the Two-Dimensional Hubbard Model

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Mott transitions are studied in the two-dimensional Hubbard model by a non-perturbative theory of correlator projection that systematically includes spatial correlations into the dynamical mean-field theory. A nonzero second-neighbor transfer yields a first-order Mott transition at finite temperatures ending at a critical point.

Keywords: Mott transition; Hubbard model

The Mott transition has been one of the fundamental issues in strongly correlated electrons [1]. In spite of substantial progress [12], its full understanding in low dimensions remains open.

Here, we propose a non-perturbative theoretical framework of correlator projection method (CPM) [3]. The CPM combines the operator projection method [4] with the dynamical mean-field approximation (DMFA) by restoring spatial correlations along the coarse-graining concept in the energy-momentum space with increasing the order of projection. It does not suffer from a cluster-size problem. Then, we obtain the Mott transition phase diagram of the two-dimensional (2D) Hubbard model in the parameter space of the Coulomb repulsion $U$, the second-neighbor transfer $t'$, the temperature $T$ (scaled by the nearest-neighbor transfer $t$) and the filling $\langle n \rangle$. A first-order Mott transition surface with a critical end curve appears at half filling. Doping into the Mott insulator yields a diverging compressibility and/or a tendency to phase separation.

We consider the 2D Hubbard model. The formalism of CPM [3] is as follows: The operator projection leads to series of Dyson equations,

$$ G_{n-1}(\omega, \mathbf{k}) = 1/[\omega - \varepsilon_{k}^{(n,n)} - \Sigma_{n}(\omega, \mathbf{k})] $$

with $n = 1, 2, \cdots$. $G_{0} = \Sigma_{0}$ is the electron Green's function and $\Sigma_{1}$ is the self-energy part with $\varepsilon_{k}^{(1,0)} = 1$. Other coefficients up to the second order $n = 2$ are given by the Hartree-Fock dispersion $\varepsilon_{k}^{(1,1)} = -t_{k} - \mu - U \langle n \rangle / 2$, a source of Hubbard band splitting $\varepsilon_{k}^{(2,1)} = U^{2} M$ with $M = \langle n \rangle(2 - \langle n \rangle)/4$, and $\varepsilon_{k}^{(2,2)} = -\mu - U(1 - \langle n \rangle)/2 - \varepsilon_{\text{cor}} / M$. Here, $\mu$ is the chemical potential determined from the filling $\langle n \rangle$. $\varepsilon_{\text{cor}} = -\Sigma_{x,s}(k_{x}x')\{(1/2 - n_{x,s})c^{\dagger}_{x,s}c_{x,s} + h.c.\}/2$ is a local energy shift due to a correlated hopping process with $n_{x,s} = c_{x,s}^{\dagger}c_{x,s}$, $c_{x,s}$ and $c_{x,s}^{\dagger}$ are the electron creation and annihilation operators at a site $x$ with a spin $s$, respectively. $t_{k}$ and $i_{k}$ are the Fourier transforms of the transfer $t_{x,x'}$ and $i_{x,x'} = t_{x,x'}(\langle n_{x}n_{x'} \rangle / 4 + \langle S_{x}^{z} \cdot S_{x'}^{z} \rangle - \langle \Delta_{x}^{z} \Delta_{x'}^{z} \rangle) / M$, respectively, where $n_{x,s}$,$S_{x}^{z}$ and $\Delta_{x}^{z}$ represent the charge, spin and local-pair operators, respectively. $i_{k}$ introduces $k$ dependences of $\Sigma_{1}(\omega, \mathbf{k})$ mainly through the superexchange process and produces antiferromagnetic precursors. Here, we determine it from Ref. [3].

To reproduce a Mott insulator in particle-hole asymmetric cases, the local dynamics of $\Sigma_{2}(\omega, \mathbf{k})$ must be obtained in a sufficiently correct manner. Then, instead of decoupling approximations [4,6], we adopt the following gen-
eralized DMFA: (i) We calculate a local normalized self-energy part \( G_{1,\text{loc}}(\omega) = \frac{1}{N} \sum_k G_1(\omega, k) \) from an arbitrary \( \Sigma_{2,\text{loc}}(\omega) \) by replacing \( \Sigma_2(\omega, k) \) with \( \Sigma_{2,\text{loc}}(\omega) \) in Eq. (2), (ii) calculate the Weiss self-energy part \( S_1(\omega) = \epsilon^{(2)} / [G_{1,\text{loc}}^{-1}(\omega) + \Sigma_{2,\text{loc}}(\omega)] \), and (iii) obtain the Weiss Green's function \( G_0(\omega, k) = 1 / [\omega - \epsilon^{(1)}(\omega) - S_1(\omega)] \). (iv) Within the iterative perturbation scheme, we calculate a new \( \Sigma_{2,\text{loc}}(\tau) = \frac{1}{N} \sum_{k,k',q} \Gamma_{k,k',q} G_0(\tau, k+q) G_0(\tau, k'-q) \) where \( \Gamma_{k,k',q} = 4 |t_k|^2 - t_{k'-q}^2 - t_{k+q}^2 + 4 \epsilon_{\text{cor}} / (\langle n \rangle (2 - \langle n \rangle))^2 / (\langle n \rangle (2 - \langle n \rangle)) \). This loop continues to (i) until convergence is reached.

This second-order CPM reproduces a Mott insulator at low \( T \)'s for \( t' = 0 \) at half filling and its single-particle spectra and momentum distributions show a remarkable similarity to numerical results \[8]. As we introduce \( t' \neq 0 \) with \( U \) and \( \langle n \rangle = 1 \) being fixed, the system undergoes a first-order Mott metal-insulator transition (MIT) at a low \( T \) accompanied by a discontinuity in the double occupancy \( \langle n_\uparrow n_\downarrow \rangle \). In the space of \( (U, t', T) \), this first-order MIT boundary forms a surface \[9\]. Within the surface with \( U \) being fixed, the jump in \( \langle n_\uparrow n_\downarrow \rangle \) decreases with increasing \( T \) and disappears above a critical temperature \( T_{\text{cr}} \); the first-order surface ends at a critical curve at \( T > 0 \). Then, without any spontaneous symmetry breaking as in two dimensions at \( T > 0 \), the Mott transition shows a similarity to a liquid-gas phase transition, as in Refs. \[8,2\]. The MIT boundary at \( T \to 0 \) agrees with numerical results \[9\].

Doping carriers into Mott insulators yields a metallic state characterized by an enhanced charge compressibility \( \kappa = \partial \langle n \rangle / \partial \mu \). The present results of \( \mu - \delta \) curves near half filling are shown in Fig. 1 with \( \delta = 1 - \langle n \rangle \). The slope \( \partial \mu / \partial \langle n \rangle \) represents \( 1 / \kappa \). Then, from high \( T \)'s, \( \kappa \) increases with decreasing \( T \) and shows a divergence towards the filling-controll MIT at low \( T \)'s. Even an instability to a phase separation appears as emergence of \( \kappa < 0 \) at lower \( T \)'s. However, the issue if the phase separation is an artifact of the present approximation requires a further intensive study.

In summary, using the CPM that systematically includes spatial correlations into the DMFA, the MIT phase diagram of the 2D Hubbard model has been clarified in the \((U, |t'|, T)\) space with a first-order MIT surface with a \( T > 0 \) critical end curve for \( t' \neq 0 \) at half filling as well as a diverging charge compressibility and/or a tendency to a phase separation.

![Figure 1. \( \mu-\delta \) curves obtained with \( U/t = 4 \). The bold circles lie in the Mott-insulating side of the MIT surface at half filling.](attachment:image.png)

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