Unconventional metal-insulator transition in two dimensions

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We show, by using a correlated Jastrow wave function and a mapping onto a classical model, that the two-dimensional Mott transition in a simple half-filled one-band model can be unconventional and very similar to the binding-unbinding Kosterlitz-Thouless transition of vortices and antivortices, here identified by empty and doubly occupied sites. Within this framework, electrons strongly interact with collective plasmon excitations that induce anomalous critical properties on both sides of the transition. In particular, the insulating phase is characterized by a singular power-law behavior in the photoemission spectrum, which can be continuously connected to the fully projected insulating state relevant to strongly correlated low-energy models.

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I. INTRODUCTION

The metal-insulator transition (MIT) driven by electron interaction, the so-called Mott transition,[1] is one of the most challenging issues in modern solid state physics, especially because of its possible connections with other phenomena, like high-temperature superconductivity. The prototypical model to study the MIT is the one-band Hubbard model, where the transition shows up if the ratio between the bandwidth W and the on-site Coulomb repulsion U is varied.[2] In a pioneering work, Brinkman and Rice[3] argued that the MIT could be continuous; however, their approach led to a Mott insulator where charge fluctuations are completely frozen. Recent developments, based on dynamical mean-field theory calculations,[4] are able to give a more realistic description of the MIT where, at zero temperature, a wide gap in the excitation spectrum opens immediately in the insulator. However, within this approach, the role of the dimensionality is not taken into account, whereas its relevance comes out from recent experiments on Si metal-oxide-semiconductor field-effect transistors[5] and organic materials.[6] Moreover, the situation can be radically different whenever the Hamiltonian contains a true long-range Coulomb interaction, as pointed out in the original Mott argument.[1]

In this work, we focus our attention on a correlated wave function (WF), which is expected to closely describe the MIT in two-dimensional (2D) systems with long-range Coulomb interactions. The important fact is that, in the strong-coupling regime, we can adiabatically connect our WF with the fully projected one, usually considered to describe systems in the limit of infinite Coulomb repulsion, e.g., the so-called resonating-valence-bond state.[7–10] Moreover, the metallic phase has no quasiparticles defined, showing low-energy properties similar to the one-dimensional Luttinger liquid.

The paper is organized as follows. In Sec. II we show the mapping between the quantum wave function and a classical model at finite temperature and in Sec. III we show our numerical results and draw the conclusions.

II. CLASSICAL MAPPING

Let us discuss how to construct a WF for correlated insulators. In general, starting from the ground state $|\Psi_0\rangle$ of a system with N electrons, with energy E_0, it is possible to construct simple variational states for the lowest-energy excitations. For instance, in analogy with the Feynman construction for liquid helium,[11] the plasmon excitation with momentum q is given by

$$|\Psi_q\rangle = n_q|\Psi_0\rangle, \tag{1}$$

where n_q is the Fourier transform of the local electron density. Its variational energy is

$$E_q = E_0 + \frac{\langle -k\rangle q^2}{2N_q}, \tag{2}$$

where $\langle k\rangle$ is the ground-state kinetic energy per particle and

$$N_q = \frac{\langle\Psi_0|n_q n_{-q}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \tag{3}$$

is its static charge structure factor. When applied to an insulator, with gapped charge excitations, this implies that, for small momenta, $N_q \sim q^2$. This argument has very general consequences for the form of $|\Psi_0\rangle$ that do not depend on the particular microscopic model. To this purpose, let us denote an electronic configuration by the positions $\{x\}$ of the particles. For all the operators θ that depend only on such positions, e.g., the structure factor itself, the quantum average

$$\langle\theta\rangle = \frac{\langle\Psi_0|\theta|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \tag{4}$$

can be written in terms of the *classical* distribution $|\Psi_0(x)|^2 = |\langle x|\Psi_0\rangle|^2/\Sigma_{x'}|\langle x'|\Psi_0\rangle|^2$ as

$$\langle\theta\rangle = \sum_x \langle x|\theta|x\rangle|\Psi_0(x)|^2. \tag{5}$$

Since $|\Psi_0(x)|^2$ is a positive quantity, we can define an appropriate correspondence between the WF and an effective potential $V(x)$:

$$|\Psi_0(x)|^2 = e^{-V(x)}. \tag{6}$$

The size consistency of the WF implies that the potential $V(x)$ is extensive, namely, of order N for typical configurations. In the limit of strong Coulomb interactions, there are

small charge fluctuations and, therefore, we can safely assume that only the two-body term is relevant and all multiparticle interactions are negligible. This leads to the quadratic potential

$$V(x) = \sum_{q\neq 0} v_q^{eff} n_q(x) n_{-q}(x), \tag{7}$$

$n_q(x)$ being the Fourier transform of the local density of the configuration $|x\rangle$. To obtain the expected behavior

$$N_q = \sum_x n_q(x) n_{-q}(x) e^{-V(x)} \sim q^2, \tag{8}$$

the effective potential must diverge as

$$v_q^{eff} = \frac{\pi}{T^{eff} q^2} + (\text{less singular terms}). \tag{9}$$

Here T^{eff} can be considered as the effective temperature of classical charges interacting through a potential π/q^2. Within this choice of v_q^{eff}, $N_q \sim q^2$ is generally valid and can be understood by considering n_q as a complex continuous variable, so that the classical average of $n_q n_{-q}$ turns into a standard Gaussian integral, yielding

$$N_q \sim \frac{1}{v_q^{eff}} = \frac{T^{eff} q^2}{\pi}. \tag{10}$$

It should be noted that the fully projected wave function with no charge fluctuations, and therefore $N_q = 0$ for $|q| \neq 0$, is recovered when $T^{eff} \to 0$.

III. RESULTS

Let us now consider a general one-band fermionic system in 2D, in which every site of a square lattice can be either empty, singly occupied, the electron having spin either up or down, or doubly occupied. A true Mott insulator that does not break any lattice symmetry cannot be represented by a simple WF containing a single determinant, and, at this stage, it is useful to define a state that is simple enough and yet is compatible with the predicted form of v_q^{eff} in the insulating phase. A straightforward way to modify the effective potential determined by an uncorrelated determinant $|\mathcal{D}\rangle$ is obtained by taking into account an appropriate Jastrow factor $\mathcal{J}$:

$$|\Psi\rangle = \mathcal{J}|\mathcal{D}\rangle; \tag{11}$$

here $|\mathcal{D}\rangle$ is an electronic determinant that will be specified in the following and $\mathcal{J}$ is a Jastrow term that depends upon the electronic density:

$$\mathcal{J} = \exp\left(-\frac{1}{2}\sum_{q\neq 0} v_q n_q n_{-q}\right), \tag{12}$$

where v_q is the Jastrow potential, whose small-q behavior is given by

$$v_q = \frac{\pi\beta}{2[2 - (\cos q_x + \cos q_y)]} \sim \frac{\pi\beta}{q^2}, \tag{13}$$

β fixing its strength.

At half filling, in one-dimensional electronic systems, we found[12,13] that the singular Jastrow potential $v_q \sim \pi\beta/q^2$ always leads to an insulator, for any positive β. In 2D the situation is different and a much more interesting scenario is obtained, with a phase transition as a function of the correlation strength β. Indeed, given the behavior of the Jastrow potential $v_q \sim \pi\beta/q^2$, the potential $V(x)$ of Eq. (7) turns out to be the one of the classical Coulomb gas model (CGM). In this approach, particles with charge q_i, corresponding to empty ($q_i = 1$) and doubly ($q_i = -1$) occupied sites, interact through a Coulomb potential in a neutral background, represented by singly occupied sites ($q_i = 0$). In the half-filled case, there is an equal number of empty and doubly occupied sites, implying the charge neutrality of the CGM. The fugacity z of the CGM, which sets the average value of the charges, can be identified with the on-site Gutzwiller term in the Jastrow potential, i.e., $z = \exp(-g)$, where g is the Gutzwiller parameter.

The classical CGM in 2D is particularly interesting because it shows a Kosterlitz-Thouless (KT) transition at a finite temperature T_c^{CGM}.[14] This transition is transparent from the classical dielectric function:

$$\frac{1}{\epsilon} = \lim_{q\to 0}\left(1 - \frac{2\pi}{T^{eff} q^2} N_q\right), \tag{14}$$

where T^{eff} is the temperature of the classical model. The charge structure factor is quadratic at small momenta, i.e., $N_q \sim \alpha q^2$, for all temperatures, but the coefficient α changes discontinuously at T_c^{CGM}. Above T_c^{CGM}, the CGM is in the plasma phase, i.e., a metallic phase with infinite dielectric function, perfect screening, and exponential correlation functions. On the other hand, below T_c^{CGM}, the CGM is in the confined phase, with a finite dielectric constant. In this phase the charges are bound together, forming dipoles, that, because of their residual interaction, induce power-law correlations. At the transition, the inverse of the dielectric function has a finite jump, changing from zero, in the plasma phase, to a finite value, in the confined phase.

A similar mapping between a quantum state and a classical model has been emphasized also in the context of the fractional quantum Hall effect: the Laughlin WF can be related to a classical system with particles interacting through a logarithmic potential.[15] However, in this case, all the particles have the same charge, forming a one-component plasma, and by varying the strength of the potential, there is a first-order transition between an incompressible fluid and a Wigner crystal.[16] The peculiarity of our approach is that, due to the mapping onto the two-component CGM, it is possible to connect continuously the plasma phase to the insulating one.

In the following, we show that, in analogy with the classical CGM, also in the case of fermionic systems at zero temperature, a KT-like transition is found by varying the correlation strength that can be tuned by the Jastrow strength β. However, the existence of the fermionic part induces nontrivial properties for the two phases involved that are not present in the classical problem. For example the uncorrelated part of the WF may contribute to the expression of the

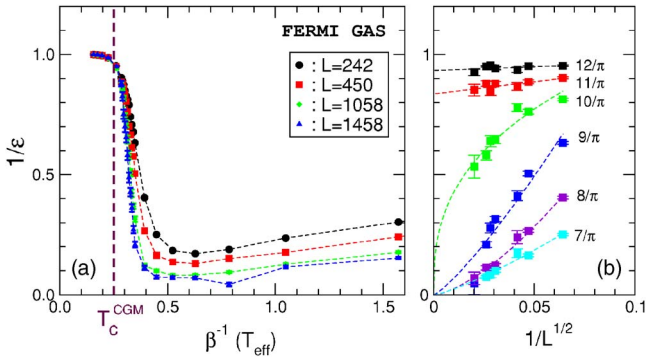

FIG. 1. (Color online) Inverse of the dielectric function $1/\epsilon$ [see Eq. (14)] for the free-electron determinant. Left panel: $1/\epsilon$ as a function of the effective temperature $1/\beta$ and for different sizes L of the cluster. The critical temperature of the classical Coulomb gas model T_c^{CGM} is marked with a dashed line for a comparison. Right panel: Size scaling of $1/\epsilon$ for various β.

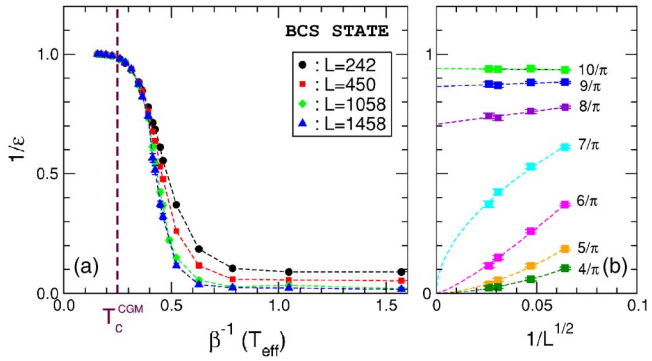

FIG. 2. (Color online) The same as in Fig. 1 but for a gapless BCS state with $\Delta/t=1.1$ and $d_{x^2-y^2}$ symmetry.

effective temperature T^{eff}, as shown below. Whenever the square of the WF describes the plasma phase of the corresponding classical model, we can safely assume that the Gaussian fluctuations are exact for small q's and the classical temperature can be determined by imposing $1/\epsilon=0$ in Eq. (14), namely, $T^{eff}=2\pi \lim_{q\to 0} N_q/q^2$. In the language of quantum states, the Gaussian approximation leads to the well-known expression

$$N_q = \frac{N_q^0}{1+2v_q N_q^0}, \tag{15}$$

where N_q^0 is the charge structure factor of the uncorrelated determinant $|\mathcal{D}\rangle$.[17,18] The previous form of N_q allows us to identify the effective temperature as:

$$\frac{1}{T^{eff}} = \beta + \frac{\alpha_0}{2\pi} \tag{16}$$

where $\alpha_0=\lim_{q\to 0} q^2/N_q^0$.

In order to show the general validity of our approach, we consider the case of a free-electron determinant, obtained by occupying the lowest-energy states in the tight-binding model with dispersion $E_k=-2t(\cos k_x+\cos k_y)$, and a gapless BCS state with a superconducting order parameter $\Delta_k=\Delta(\cos k_x-\cos k_y)$. In these cases $\alpha_0=0$ and, therefore, the effective temperature in Eq. (16) is determined only by the Jastrow coefficient, namely, $T^{eff}=1/\beta$. In Fig. 1, we report the inverse of the dielectric function for the free-electron determinant and different sizes L of the system at half filling, i.e., $N=L$. In order to have closed-shell states for $|\mathcal{D}\rangle$, we used 2D square lattices tilted by 45° (i.e., with $L=2l_x^2$ and l_x odd) and periodic boundary conditions. By increasing L, the curves show a steeper and steeper shape in the vicinity of the critical temperature T_c. This result is further confirmed by the size scaling of $1/\epsilon$, which clearly supports the existence of a finite jump in the thermodynamic limit: $1/\epsilon\to 0$ for $T^{eff}>T_c$, whereas $1/\epsilon\to$const for $T^{eff}<T_c$. Interestingly, T_c depends slightly upon the choice of the uncorrelated determinant (see for comparison Fig. 2 for the gapless BCS state) and is quite close to the CGM critical temperature $T_c^{CGM}=1/4$. These results give an important and transparent insight into the strong-coupling limit described by the fully projected WF,[7] which can be connected to our WF by letting $\beta\to\infty$, i.e., $T^{eff}\to 0$. Indeed, in the confined phase for $T^{eff}<T_c$, the classical KT scaling equations of the CGM flow to fixed points with zero fugacity: this translates into the fact that the fully projected state represents the fixed point of the correlated WFs describing the 2D Mott insulating phase. Therefore, in the confined regime, the ground-state properties are universal and represented by those of the fully projected WF. In this respect, total projection is not an unrealistic assumption and can accurately reproduce the low-energy physical properties of a strongly correlated system. On the other hand, for $T^{eff}>T_c$ the classical KT scaling equations flow to strong coupling and are useful only close to the transition point.

In Fig. 3 we show that in the plasma phase the Gaussian approximation, given by Eq. (15), is very accurate, not only for small q's (where it is exact) but also for large momenta. In this case, the cusp singularity in N_q for $Q=(\pi,\pi)$, related to the Friedel oscillations, is not removed, even though $N_q\sim q^2$ at low momenta. Thus, for $T^{eff}>T_c$, the WF (11) describes a "Coulomb metal," with $N_q\sim q^2$ at small q's but with the sign of the Fermi surface at large momenta. As shown previously in the limit of infinite Coulomb repulsion[19] or in the low-density regime,[20] this WF has low-energy properties similar to those of one-dimensional Luttinger liquid conductors, where the absence of a jump in the momentum distribution is replaced by a weaker singularity, yielding to $2k_F$ and $4k_F$ power-law density correlations. It is important to emphasize that, in the quantum case, the power-law correlations come from the large momentum singularity, that are absent in the classical CGM.[14] Indeed, in the quantum state, the subleading corrections in the classical potential of Eq. (6) are very important and can actually turn the CGM exponential correlations to power laws in the plasma phase, and vice versa in the confined phase. On the other hand, in the confined phase the Gaussian approximation is not adequate both at small and large momenta (see Fig. 3). Indeed, at small q's, the coefficient of the quadratic term is not simply given by the Gaussian approximation and, more importantly, the strong Jastrow factor washes out completely the singularities of N_q^0, leading to a smooth charge-structure factor, a genuine fingerprint of an insulating phase.

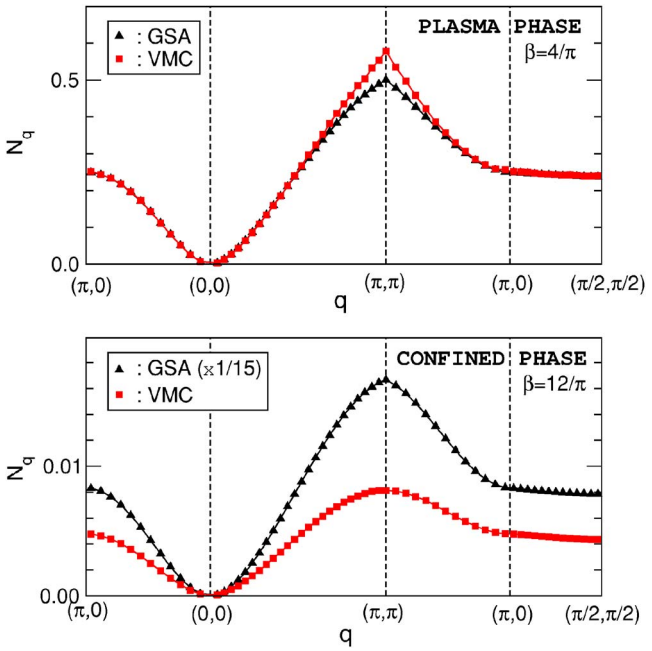

FIG. 3. (Color online) Equal-time density structure factor N_q for the correlated wave function of Eq. (11) (full squares), compared to the same quantity calculated within the Gaussian approximation [indicated as GSA and given by Eq. (15)] (full triangles) for $\beta=4/\pi$ (upper panel) and $\beta=12/\pi$ (lower panel; notice the different scale of the GSA data).

In order to further characterize the two phases, we consider the quasiparticle weight

$$Z_k = \frac{|\langle \Psi_{N-1}|c_{k,\sigma}|\Psi_N\rangle|^2}{\langle \Psi_N|\Psi_N\rangle\langle \Psi_{N-1}|\Psi_{N-1}\rangle}, \tag{17}$$

where $|\Psi_N\rangle$ and $|\Psi_{N-1}\rangle$ are the WFs with N and $(N-1)$ particles, and $c_{k,\sigma}$ is the destruction operator of a particle of momentum k and spin σ. In particular, the wave function with $N-1$ particles is constructed from $|\Psi_N\rangle$:

$$|\Psi_{N-1}\rangle = \mathcal{J}c_{k,\sigma}|\mathcal{D}\rangle. \tag{18}$$

In a previous work,[20] it was argued that the singular Jastrow factor can induce non-Fermi-liquid properties, and in particular a vanishing Z_k at the Fermi surface. In Fig. 4, we report Z_k for $k=(\pi/2,\pi/2)$ and for different Jastrow strengths β. We find that the quasiparticle weight vanishes with a power-law behavior

$$Z_k \sim L^{-\theta} \tag{19}$$

both in the confined and in the plasma phases, with an exponent θ that depends upon β and the type of the uncorrelated state. In the plasma phase, θ varies continuously with the Jastrow strength β and there is no appreciable dependence on the uncorrelated determinant. On the other hand, in the confined phase, the exponent is constant, i.e., $\theta \simeq 1/2$ for the BCS state and $\theta \simeq 3/4$ for the free-electron state, and equal to the value found for the fully projected WF, as shown in Fig. 5. It must be mentioned that, for the BCS state, θ does not depend upon the value of the superconducting order parameter Δ (see Fig. 4), indicating the universal properties of the confined phase.

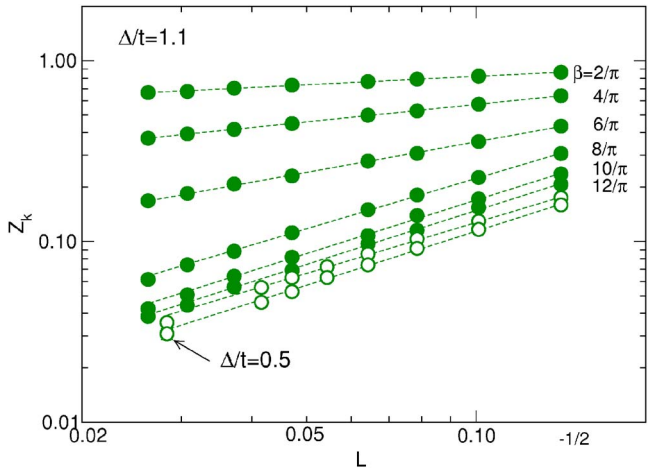

FIG. 4. (Color online) Quasiparticle weight Z_k at $k=(\pi/2,\pi/2)$ for the gapless BCS state with $\Delta/t=1.1$ and $d_{x^2-y^2}$ symmetry as a function of L and for different Jastrow strengths β (full circles). The case of the fully projected wave function (empty circles) is also reported for $\Delta/t=1.1$ and 0.5.

Our results show that it is possible to describe a continuous MIT in 2D electronic systems with a Jastrow correlated WF. We characterized both the metallic region, with a zero quasiparticle weight $Z_k=0$, and the insulator, which can be continuously connected to the totally projected Gutzwiller WF. Of course, other scenarios are possible for the MIT, e.g., the one proposed in the infinite-dimensional limit. Indeed, whenever the metallic phase has $N_q \sim c|q|+dq^2$ with $c>0$, the MIT is not described by the functional form (13) of the Jastrow potential: By approaching the transition from the metallic phase, we enter directly into the confined phase with a quadratic charge structure factor at small momenta, i.e., $c \to 0$ with a large finite d at the critical point. In this case, in the metallic region, a less singular Jastrow factor $v_q \sim 1/|q|$ is expected, leading to a finite quasiparticle weight.

Finally, we would like to comment on the possibility to stabilize the "Coulomb metal" phase in a microscopic model. For simplicity, let us consider the one-band Hubbard model on the square lattice with nearest-neighbor hopping:

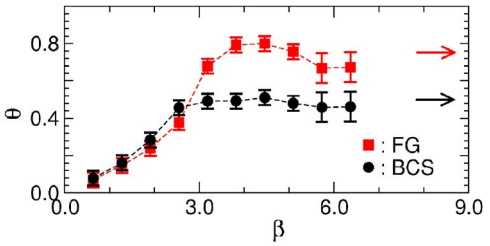

FIG. 5. (Color online) The behavior of θ [the exponent of the quasiparticle weight; see Eq. (19)] as a function of β for BCS state (full circles) and the Fermi gas (FG) determinant (full squares). The values of the fully projected states are also reported (arrows).

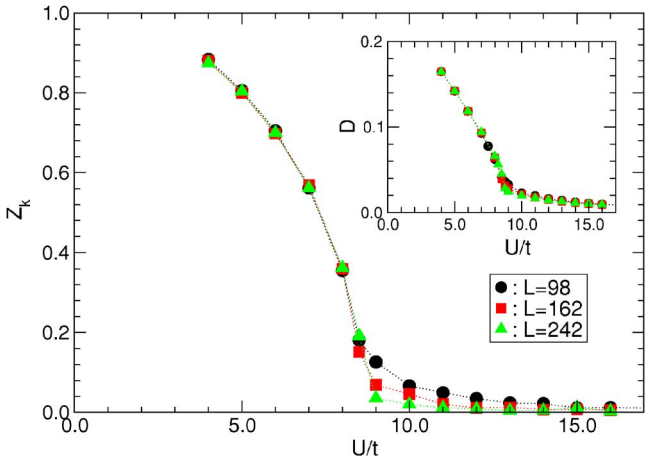

FIG. 6. (Color online) Quasiparticle weight Z_k at $k=(\pi/2,\pi/2)$ of the optimized *paramagnetic* wave function containing a Jastrow factor applied to the Fermi gas as a function of the interaction U/t in the Hubbard model, for three different sizes of the system. Inset: The number of double occupancies D as a function of U/t.

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} + \text{H.c.} + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}, \tag{20}$$

where $c^{\dagger}_{i,\sigma}$ creates an electron with spin σ at the site i, and $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$ is the density operator at the site i. In the following, we will consider a *paramagnetic* state, by taking a projected Fermi gas wave function, as described above, and by minimizing the variational energy for the determination of the Jastrow factor $\mathcal{J}$. In particular, by using the method described in Ref. 21, we are able to optimize all the independent Jastrow parameters in the real space $v_{i,j}$ (i.e., the Fourier transform of v_q). Within this approach, which neglects magnetic phases, we obtain a MIT for $U_c/t=8.5\pm0.5$. In the weak-coupling regime, for $U<U_c$, we obtain a Fermi liquid with a finite quasiparticle weight, whereas at strong couplings, i.e., for $U>U_c$, we have an insulating phase with a vanishing Z_k; see Fig. 6.[22] Moreover, the calculation of the double occupancy D clearly indicates that the transition is continuous and the insulating phase still possesses finite charge fluctuations (see inset of Fig. 6). As discussed above, in the metallic region, we find that $v_q \sim 1/|q|$ (see Fig. 7). Unfortunately, as soon as we enter the insulating phase, $\lim_{q\to 0} v_q|q|^2$ defines an effective β that is larger than the critical value for the KT transition, and, therefore, no evidence for the Coulomb metal is found.[23] Indeed, we expect that the optimized Jastrow factor v_q, containing subleading corrections with respect to Eq. (13), will define a critical β very close to the value of the classical CGM, i.e., β_c

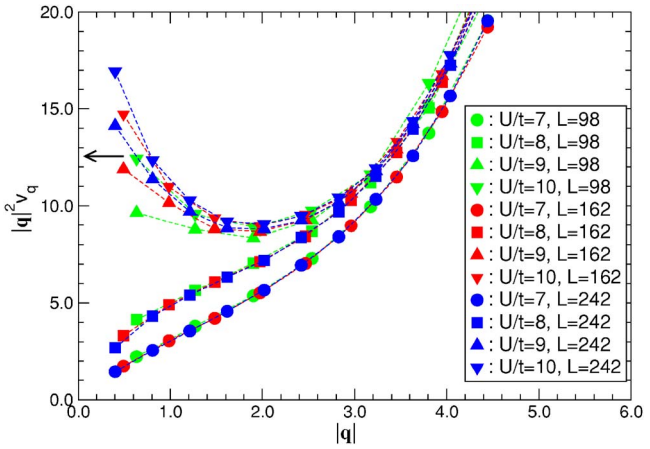

FIG. 7. (Color online) Optimized Jastrow potential v_q, multiplied by $|q|^2$, for the Hubbard model as a function of $|q|$ [in the (1,1) direction] for different sizes of the cluster and ratios U/t. The arrow indicates π/T_c^{CGM}, the expected value of $\lim_{q\to 0} v_q|q|^2$ at the classical transition point.

$=1/T_c^{CGM}=4$. Therefore, in light of the results of Fig. 7, the stabilization of the Coulomb metal seems to be very unlikely: Although there are large size effects around U_c, we have clear evidence that $\lim_{q\to 0} v_q|q|^2 \to 0$ for $U<U_c$ and $\lim_{q\to 0} v_q|q|^2 \gtrsim 4\pi$ for $U>U_c$ (see Fig. 7).

On the other hand, we can safely predict the occurrence of the KT-like scenario described above in 2D systems with long-range (logarithmic) interaction. In this case, the application of the Gaussian approximation for small interaction and our ansatz for the insulating phase imply the presence of a transition of the type considered here. It is remarkable that the proposed picture crucially depends on the long-range nature of the Coulomb interaction, recalling Mott's original idea. In this regard, it should be mentioned that the original Mott argument for a discontinuous metal-insulator transition, driven by the long-range Coulomb interaction, cannot be applied in 2D. In such case there always exists a bound state for two opposite charges interacting with the screened Coulomb potential, so that, according to this argument, no metallic phase with unbound charges is possible. However, this is clearly an artifact of the mean-field argument, since for small interaction the random-phase approximation leads to an anomalous metallic state (see Ref. 20).

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[22] In order to minimize the size effects on Z_k, we calculate the momentum distribution n_k and extract, by fitting around the known Fermi surface, the value of the jump.
[23] This outcome is expected to be the same for generic short-range Hamiltonians, and, therefore, the presence of a frustrating hopping term does not help to stabilize the Coulomb metal phase.