Critical scaling of the renormalized single-particle wave function near the Mott-Hubbard transition

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We present a quantum critical behavior of the renormalized single-particle Wannier function, calculated in the Gutzwiller correlated state near the insulator-metal transition (IMT) for cubic lattices. The wave function size and its maximum, as well as the system energy scale with increasing lattice parameter $R$ as $R^n$. Such scaling is interpreted as the evidence of a dominant role of the Coulomb repulsion. Relation of the insulator-metal transition lattice-parameter value $R = R_C$ to the original Mott criterion is obtained. The method is tested by comparing our results with the exact approach for the Hubbard chain.

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Insulator-metal transition (IMT) of the Mott-Hubbard type represents one of the central problems in quantum physics, since it exemplifies a transition from well defined atomic states to delocalized (Bloch- or Fermi-liquid-type) states in a solid$^3$ and in other systems$^2$. The model system is a lattice of spin-1/2 fermions with one particle per atomic site. Mott expressed this localized-delocalized transformation in terms of critical density $n_c$ of fermions (or equivalently, in terms of critical interparticle distance $R_C = n_c^{-1/D}$, where $D$ is the system dimensionality) and the effective Bohr- radius $a_B$ of the atomic states formed at the transition, in the form $n_c^{-1/D} a_B \simeq 0.25$. On the other hand, Hubbard$^2$ and others formulated the criterion in the form that at the transition the Coulomb repulsive energy among the particles (of magnitude $U$) is equal to their kinetic (band) energy characterized by the bare bandwidth $W$, $U \approx W$. These two criteria are regarded as equivalent.

The insulator-metal transition is also well defined as a phase transformation in thermodynamic sense$^2$. As close to IMT the band energy (negative) is almost compensated by the repulsive Coulomb interaction, the much smaller thermal or energy can drive the metallic system towards the state with localized spins. The resultant phase diagrams contain first-order pressure-temperature transition line with a terminal critical point at temperature $T_{cr} > 0$. The existence of the critical point was confirmed experimentally quite recently$^5$ and shown to represent properties of the Van der Waals liquid-gas point in the $D = 3$ case of $V_2O_3:Cr$, (see Limelette et al.$^5$). The basic question remains under what conditions a quantum critical point (QCP) appears at $T_{cr} = 0$ between metallic and insulating phases, as its existence marks explicitly the fundamental boundary between the atomic and the condensed (delocalized) quantum states. The appearance of such QCP is usually observed in real systems by the presence of antiferromagnetism on (at least) one side of the transition$^2$. Nonetheless, the answer to the above question even without inclusion of magnetic ordering would delineate the basic characteristics of the (quantum) critical point (at $T = 0$), which is of non-Landau character.$^2$

As IMT involves a drastic change of the nature of states individual carriers, the natural and not addressed so far question is how their wave-function changes when approaching the transition from either side. The parameterized-model approaches leave the Wannier functions determining the parameters as fixed. On the other hand, the original Mott approach introduces intuitively the concept of an emergent atomic state at the instability of the metallic state. Thus the missing question is: how the correlations and the single-particle aspects are interrelated microscopically?

We provide the explicit description of electronic states close to IMT in which both the interelectronic correlations and the single-particle Wannier wave functions $\{w_i(r)\}$ are treated on the same footing. As the result, we introduce a singular behavior of the single-particle (Wannier) wave function renormalized by the correlations. This nonanalytic behavior (and associated with it unique scaling laws) are only possible when the wave function is calculated a posteriori, i.e. in the correlated state, not before the correlations are taken into account. Such an approach is indispensable in the situation when the single-particle and interaction energies are comparable or the interaction is even dominant. In this sense, our analysis complements that performed within either LDA+DMFT$^{10}$ or LDA+U$^{11}$ methods, which contain parameters characterizing electronic correlations introduced after the LDA calculations have been carried out. We should also underline, that our method was applied earlier to both correlated nano-$^{14}$ and macro-$^{25}$ systems and is free from the double counting of the repulsive Coulomb interaction. Furthermore, the microscopic parameters are calculated explicitly within the mutually consistent procedure. Therefore, even though the presented below results concern model results, they should be regarded as an essential ingredient to be implemented in modeling real systems near IMT.
We start from extended Hubbard model with inclusion of intersite Coulomb interaction and ion-ion interaction as represented by the Hamiltonian:\$^1\$\$\$\$^2\$\$\$\$^3\$\$\$\$^2$

\[ H = \epsilon_a \sum_i n_i + \sum_{i \neq j} t_{ij} a_i^\dagger a_j + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ + \frac{1}{2} \sum_{i \neq j} K_{ij} \delta n_i \delta n_j + V_{\text{ion-ion}}, \]

where the first term describes the effective atomic energy with

\[ \epsilon_a^\text{eff} = \epsilon_a + \frac{1}{2N} \sum_{i \neq j} (K_{ij} + 2/R_{ij}), \]

the second represents the hopping between the nearest-neighbor sites, the third the Hubbard (intraatomic) and the fourth is a part of intersite Coulomb interaction, with \( \delta n_i \equiv 1 - n_i \) being the deviation from the integer electron occupancy \( n_i = 1 \), and \( K_{ij} \) - the intersite Coulomb interaction. The term \( (2/R_{ij}) \) in (2) expresses the classical Coulomb repulsion (in atomic units) for two ions separated by the distance \( R_{ij} \).

In the Mott-Hubbard insulating state the hole-hole correlations are absent i.e. \( \langle (1 - n_i)(1 - n_j) \rangle \approx 0 \). The role of these correlations is indeed negligible if the fundamental correlation function \( d^2 \equiv \langle n_i n_{i\pm} \rangle \) vanishes for \( U \sim W \).

The microscopic parameters of this model are expressed via the Wannier functions \( \{ w_i(r) \} \equiv \{ w_r - R_i \} \) as follows: \( \epsilon_a \equiv \langle w_i | H_1 | w_i \rangle \), \( t_{ij} \equiv \langle w_i | H_1 | w_j \rangle \), \( U \equiv \langle w_i w_j V_{12} w_i w_j \rangle \), and \( K_{ij} \equiv \langle w_i w_j V_{12} w_i w_j \rangle \), where \( H_1 \) is the Hamiltonian for a single particle in the system, and \( V_{12} \) represents interparticle (Coulomb) repulsion. The Wannier functions are expressed in terms of adjustable Slater functions, i.e. \( w_i(r) = \beta \Psi_i(r) - \gamma \sum_j \Psi_j(r) \) where \( z \) is the number of nearest neighbors, \( \beta \) and \( \gamma \) are mixing coefficients, and \( \Psi_i(r) \equiv (\alpha^3/\pi)^{1/2} \exp(-\alpha |r - R_i|) \) is the 1s Slater function centered on the site \( i \equiv R_i \). In the concrete calculations, they are represented by adjustable Gaussians (e.g. STO-7G basis in dimensions \( D = 1, 2, \) and 3) and where discussed before \$^4\$\$\$\$^5\$\$\$\$^6\$\$\$\$^1\$\$\$\$^2\$\$\$\$^3\$\$\$\$^4\$\$\$\$^5\$\$\$\$^6\$\$\$\$^1\$\$\$\$^2\$\$\$\$^3\$\$\$\$^4\$\$\$\$^5\$\$\$\$^6\$.

As said above, the fundamental principle behind our approach is that the wave functions \( \{ w_i(r) \} \) are treated on the same footing as the diagonalization of \( H \) in the Fock space. Such diagonalization is possible in an exact manner for nanoscopic and infinite Hubbard chain (\( D = 1 \)) systems.\$^7\$ However, also the Gutzwiller wave-function (GWF) and the Gutzwiller-ansatz (GA) approximations lead to close results in the latter case (see below) provided the wave functions \( \{ w_i(r) \} \) are properly readjusted variationally in the correlated state to achieve the ground-state energy as a global minimum for a given lattice parameter \( R \). In other words, the energy of the correlated state is readjusted iteratively multiple times by adjusting the wave function size \( \alpha^{-1} \) and in effect, also the microscopic parameters. As a result of such iterative approach, we obtain the renormalized wave function and the microscopic parameters, as well as the ground-state energy, and most importantly, scaling of the physical properties, all as a function of \( R \). Below we analyze first the results obtained for GA for three-dimensional cubic lattices, before testing their validity for \( D = 1 \) and 2 situations. The main emphasis is lead on the novel singular scaling properties near the Mott-Hubbard critical spacing \( R = R_C \).

In Fig. 1 we plot the exemplary Wannier function centered at \( R_i = 0 \) for simple cubic (SC) lattice for \( R < R_C \) (dot-dashed line) \( R = R_C \) (solid line), and \( R \gg R_C \) (dashed line). One observes immediately that the wave function for \( R > R_C \) is more extended than that for \( R = R_C \) and with increasing \( R \) gradually reaches its atomic value \( a_0 \). To study this nontrivial effect in detail, we have plotted in Fig. 2 the relative inverse size \( \delta \alpha / \alpha \equiv \alpha(R) - \alpha(R_C) / \alpha(R_C) \) as a function of relative lattice spacing \( \delta R / R \equiv (R - R_C) / R_C \) in the regime \( R > R_C \). A clear \( \delta \alpha / dR \) discontinuity (cf. inset) is observed at \( R = R_C \) for all cubic lattices, a rather unique and unexpected feature, which is completely absent for the case with bare (unrenormalized) wave functions. Note that the wave function is the narrowest at the Mott-Hubbard transition at which \( \delta^2 \approx 0 \) (\( \delta^2 > 0 \) in the metallic phase). To determine the universality of the behavior we have replotted in Fig. 3 the result of Fig. 2 for \( R > R_C \) in a doubly logarithmic scale. One observes a clear power law scaling \( \delta \alpha / \alpha \sim [(R - R_C)/R_C]^s \), with \( s = 0.96 \pm 0.1 \) for not too large \( R \). The results for \( R < R_C \) exhibit also a similar scaling property for \( R \lesssim R_C \), with the exponent \( s \) slightly lower (\( s \approx 0.93 \)) and weakly dependent on the type of cubic lattice selected. This means that the results in the metallic phase show a lesser degree of universality. Note that this power-law scaling describes the singular behavior of the wave-function size \( a_B = 1/\alpha \).

Lattice dependence of the scaling with \( \delta R / R \) is also observed for the ground state energy, as shown in Fig. 4. The approximate dependence \( \sim R^1 \) of \( E_C \) when approaching the atomic limit can be attributed to the dominant role of the Coulomb repulsion between the electrons localized on neighboring ions.

Both the Figs. 2 and 4 demonstrate the appearance of a simple scaling properties of \( R^{\pm 1} \) type. This dependence could be seen in the pressure dependence of the orbital size when close to the critical value \( R = R_C \). However, the
FIG. 1: (Color online) Exemplary shapes of the Wannier function centered at the site $\mathbf{R}_i = 0$ for simple cubic (SC) lattice and for three lattice spacings marked: $R < R_C$ (dot-dashed line), $R = R_C$ (solid line), and $R > R_C$ (dashed line). $a_0$ is the 1s Bohr radius.

FIG. 2: (Color online) Relative inverse wave function size $\delta \alpha/\alpha$ as a function of relative lattice parameter $\delta R/R$ for simple cubic (SC), body centered cubic (BCC), and face centered cubic (FCC) lattices. The Mott-Hubbard transition is marked by the vertical dashed line. Inset: derivative $d\alpha/dR$ vs. $\delta R/R$ with a singularity at $\delta R \equiv R - R_C = 0$.

Relative changes of $\alpha$ (cf. Fig. 2) are rather subtle and the question is if they can be observable in the present day e.g. scanning tunneling observations of atomic orbitals. For that purpose we have plotted in Fig. 5 the maximal value $w_0(0)$ of the Wannier function relative to that at $R = R_C$. The occupancy depletion reaches up to 20% of the peak value upon change of 20−25% of the lattice constant. Also, one observes the behavior of the same type, as that for $\alpha$ in Fig. 2. However, a clear scaling takes place only for $R > R_C$ (see inset), where it assumes the shape $\sim (R/R_C)^u$, with $u = 0.92 \pm 0.01$, not much different from that displayed in Fig. 3. On the basis of the results one can say that our approach provides evidence for long-range effects in the single-particle wave function which are pronounced already in the Mott-Hubbard insulating state. In other words, the Hubbard split subband picture of the Mott insulator is concomitant with a strong renormalization of the wave function characteristics near the transition point.
Finally, we have also examined the role of lattice dimensionality on the singular behavior of the wave function. For that purpose we plot in Fig. 6 the inverse wave-function size vs. $R/a_0$ for the linear chain within the modified exact Lieb-Wu (LW) and Gutzwiller-wave-function (GWF) and Gutzwiller-ansatz (GA) solutions. None of the methods provides in $D = 1$ case (and GA for $D = 2$) the type of singular behavior observed in Figs. 2 and 4 for $D = 3$ case. What is more important, all three methods provide quite similar results for $D = 1$. This circumstance gives us with some confidence, that the modified above GA method for $D = 3$ cubic lattice bears physical relevance to the problem considered as it removes, among others, a spurious IMT transition for $D = 1$ lattice. Therefore, it appears that only correlation effect treated in GA combined with the singular behavior of the wave function provide a correct IMT characterization. Furthermore, in the inset to Fig. 6 we plot the Wannier function maximum vs. $R/a_0$ for linear chain (CH), square (SQ), and triangular lattices (TR), respectively. The results for $D = 2$ are obtained for GA solution. Again, no critical behavior is observed. On the basis of these results we draw the conclusion that within
FIG. 5: (Color online) Same as in Fig. 2, but for the maximum $w_0(0,0,0)$ of the Wannier function. Inset: Detailed scaling of the Wannier function maximum (of same type as in Fig. 3). Fitted straight line represents the function $\sim (R/R_C)^{0.92}$.

FIG. 6: (Color online) Inverse size of the renormalized wave function for linear chain (CH) vs. $R/a_0$ within the exact Lieb-Wu (LW), the Gutzwiller-wave-function (GWF), and the Gutzwiller-ansatz (GA) solutions. No singular behavior is observed at any $R$. Inset: Wannier-function maximum $w_0(0)$ vs. $R/a_0$ for linear chain (CH), square (SQ), and triangular lattices (TR), with no discontinuity detected in either of the cases.

our approach the critical behavior appears only for $D = 3$. The striking coincidence of these results to the critical dimensionality ($D > 2$) for the onset of Landau-Fermi liquid stability should therefore be mentioned.\footnote{One additional basic feature of our approach should be mentioned. Namely, in Table I we list microscopic characteristic of the Mott-Hubbard transition. These results intercorrelate nicely with the Mott criterion in the following manner. The carrier concentration is $n_C = 1/R_C^3$ for SC, $2/R_C^3$ for BCC, and $4/R_C^3$ for FCC. Thus $n_C = n/R_C^3$, with $n = 1, 2, \text{ and } 4$, respectively. Therefore, the Mott criterion takes the form: $n_C^{1/3} \cdot a_B = n^{1/3}/(R_C a_C) = 0.20, 0.26, \text{ and } 0.33$, for SC, BCC, and FCC lattices, very close values to that obtained originally by Mott.\footnote{This connection provides additional argument of our approach.}
TABLE I: Microscopic parameters at the critical point for GA solutions for the lattices specified.

| Struct. | $\alpha/a_0$ | $R_C/a_0$ | $(U/W)_C$ |
|---------|--------------|-----------|-----------|
| SC      | 1.099        | 4.236     | 1.337     |
| BCC     | 1.109        | 4.334     | 1.080     |
| FCC     | 1.128        | 4.351     | 0.880     |

In summary, we have extended the standard treatment of the Mott-Hubbard transition by incorporating into the consistent scheme the wave function renormalization and demonstrating its singular behavior. On the basis of our results one can expect also important effect of temperature and magnetic ordering onto this behavior. The long-range effects on the wave function shape develop already in the insulating phase and become the strongest at the transition by narrowing the atomic wave-function down by about 10%. The wave-function characteristic length $\alpha^{-1}$ plays the role of a coherence length for a single fermion in the sea of all other particles. Such an approach can also be extended to orbitally degenerate 3d along the lines proposed earlier.\textsuperscript{18,19}

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