The Mott-Hubbard Transition on the $D = \infty$ Bethe Lattice

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Abstract. – In view of a recent controversy we investigated the Mott-Hubbard transition in $D = \infty$ with a novel cluster approach. i) We show that any truncated Bethe lattice of order $n$ can be mapped exactly to a finite Hubbard-like cluster. ii) We evaluate the self-energy numerically for $n = 0, 1, 2$ and compare with a series of self-consistent equation-of-motion solutions. iii) We find the gap to open continuously at the critical $U_c \sim 2.5t^*(t \equiv t^*/\sqrt{4d})$. iv) A low-energy theory for the Mott-Hubbard transition is developed and relations between critical exponents are presented.

Introduction. – The Mott-Hubbard (MH) transition, as the metal-insulator transition in translationally invariant systems of interacting electrons is called, is little understood at present. The nature of the order parameter remains unresolved and a number of phenomenological scenarios have been proposed to describe the underlying physics. In the Brinkmann-Rice [1] scenario the number of charge carriers drives the MH transition, another view [2] suggests a binding/unbinding transition of doubly-occupied and empty sites as the appropriate model. In this second picture the MH transition coincides with the convergence radius of a large-interaction expansion [3].

The study of interacting electrons in the limit of high dimensions [4, 5] has proven very useful, as both analytical and numerical methods simplify in the limit of infinite dimensions. For instance, Monte Carlo studies [6, 7] are not limited by finite-cluster effects, only by the imaginary-time resolution in infinite dimensions. Here we focus on the zero-temperature half-filled Hubbard model on the infinite-dimensional Bethe lattice in the paramagnetic state(1). A Mott-Hubbard transition is known [7, 8] to occur as a function of interaction strength and has been examined by Quantum Monte Carlo [7], by the iterative perturbation theory [7–10], by self-consistent diagonalization studies [11], by a non-crossing approximation [12] and a modified-equation-of-motion approach [13]. In a recently predicted [10, 11] scenario for the Mott-Hubbard transition the Fermi-liquid effective mass would diverge on the metallic side of the transition, while no precursor of the transition would be seen on the insulating side for any observable, e.g. that the gap would close discontinuously from a finite value to zero at the transition point. Here we want to examine this unusual scenario with a novel approach.

(1)Note that the Mott-Hubbard transition occurs at zero temperature only in the paramagnetic sector, while the true ground state is antiferromagnetically ordered at half-filling.

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Fig. 1 – Illustration of the Hubbard star, S(1), and of the star of the stars, S(2). The lines connect sites connected by hopping matrix elements.

Up to date it has not been clear how to formulate a systematic exact-diagonalization approach in infinite dimensions, as clusters of physical interest contain an infinite number of sites. The smallest cluster (see fig. 1) has been shown by van Dongen et al. [14], using an equation-of-motion approach, to be equivalent to a 3-site Hubbard cluster. Here we show, for the first time, that any truncated Bethe lattice may be mapped to an effective Hubbard-like cluster. The exact diagonalization of these clusters allows to calculate the local Green’s function. We then estimate the coefficients of the Laurent expansion of the self-energy and show that a simple phenomenological low-energy theory for the Mott-Hubbard transition can be formulated in terms of a truncated Laurent expansion of the self-energy.

*Star of the stars.*– Any truncated Bethe lattice in infinite dimensions can be mapped exactly to a Hubbard-like cluster with a finite number of sites. The ground state of this cluster can be used to obtain the desired Green’s function of the truncated lattice. By “S(n)” we denote a truncated Bethe lattice, which contains all sites which are separated by at most “n” steps from the central site. S(0) denotes the isolated atom, S(1) an atom connected to 2D n.n. sites and S(2) an atom with 2D n.n. and 2D(2D − 1) n.n.n. sites (see fig. 1 for an illustration). For the Hubbard-model there is an on-site repulsion $U$ on every site and a hopping $[1] t = t^*/\sqrt{4D}$ matrix element between n.n. sites.

We now consider the zero-temperature, retarded Green’s functions $G_0^{(n)}(\omega)$ and $G_1^{(n)}(\omega)$ of the central site of S(n) and a n.n. site respectively. In the limit $D \to \infty$ all diagrams contributing to $G_1^{(n)}(\omega)$ which contain the central site are suppressed as $t^2 \sim 1/D \to 0$. Therefore
that \( G_1^{(n)}(\omega) \equiv G_0^{(n-1)}(\omega) \) and the quantity of interest, \( G_0^{(n)}(\omega) \) can be calculated recursively.

Denoting by \( N_n \) the number of poles of \( G_0^{(n)}(\omega) \) we may write \( G_0^{(n-1)}(\omega) = \sum_{j} f_j/ (\omega + \mu - \varepsilon_j) \), with \( f_j \geq 0 \) and \( \sum f_j = 1 \). \( G_0^{(n-1)}(\omega) \) enters the equation of motion for \( G_0^{(n)}(\omega) \) always as \( t^2 G_0^{(n-1)}(\omega) \). Therefore \( S(n) \) is equivalent to an effective system where every one of the 2D n.n. sites is replaced by \( N_{n-1} \) interacting orbitals which are coupled by hopping matrix elements \( t_j = t\sqrt{f_j} \) to the central site. The central site Green’s function couples only to the respective symmetric combination of these \( N_{n-1} \) orbitals, as they are mutually non-interacting. \( G_0^{(n)}(\omega) \) is, therefore, determined by solving an effective Hubbard cluster where one central site (with finite \( U \)) is connected to \( N_{n-1} \) other sites (with on-site energies \( \varepsilon_j \) and zero \( U \)) by hopping matrix elements \( t_j^{\text{eff}} = \sqrt{2D t_j} = t^*\sqrt{f_j}/2 \). For \( N_0 = 2 \) we find \( G_0^{(0)}(\omega) = 1/2[1/(\omega - U/2) + 1/(\omega + U/2)] \) at half-filling and, therefore, \( S(1) \) is equivalent to an effective 3-site Hubbard-cluster [14]. The 22 poles of the Hubbard-star Green’s function, \( G_0^{(1)}(\omega) \), are reduced by symmetries to an effective \( N_1 = 14 \). Using standard techniques [16], we have been able to obtain \( G_0^{(2)}(\omega) \) at half-filling from the ground-state of the 15-site Hubbard-like cluster in the parametric sector, which was obtained by a direct-diagonalization technique.

**Self-energy.** – The Laurent series of the self-energy has the following functional form:

\[
\Sigma(\omega) = \frac{\alpha}{\omega} + \mu + (1 - 1/z^*) \omega \frac{1 - \omega G_{\text{inc}}(\omega)}{1 - (1 - 1/z^*) \omega G_{\text{inc}}(\omega)},
\]

where \( \alpha \) and \( z^* \) are parameters depending on \( U \). \( G_{\text{inc}}(\omega) \) is an “incoherent” Green’s function yet to be determined. Equation (1) turns out to be useful in the discussion of the low-energy properties of the self-energy. The Fermi-liquid state corresponds to \( \alpha = 0 \), the MH insulating state to \( \alpha > 0 \) [8, 17].

The first two terms of the r.h.s. of eq. (1) arise from the definition of self-energy

\[
\Sigma^{(n)}(\omega) \equiv \omega + \mu - \frac{(t^*)^2}{2} G_0^{(n-1)}(\omega) - \frac{1}{G_0^{(n)}(\omega)},
\]

on clusters \( S(n) \) [18] and particle-hole symmetry at half-filling which demands \( \alpha = \sum_{j} 2 f_j \omega / (\omega^2 - \varepsilon_j^2) \) and, therefore, \( \alpha = \sum_{j} \varepsilon_j^2/(2 f_j) \geq 0 \).

The third term of the r.h.s. of eq. (1) is a consequence of the fact that in infinite dimensions the self-energy is site diagonal. In the metallic state (\( \alpha = 0 \)) we write the Green’s function at the Fermi level as [19]

\[
\frac{Z}{\omega} + (1 - Z) G_{\text{inc}}(\omega) \approx \frac{1}{\omega + \mu - \omega(\omega)},
\]

Solving eq. (3) for \( \sum(\omega) \) as a function of \( G_{\text{inc}}(\omega) \) and \( Z \), we obtain eq. (1) with \( \alpha = 0 \) and \( z^* \equiv Z \). \( G_{\text{inc}}(\omega) \) is defined through eq. (1) for the case \( \alpha > 0 \). Our numerical results indicate that this \( G_{\text{inc}}(\omega) \) has indeed all the properties of a Green’s function, in particular that \( \Im G(\omega) < 0 \) and \( - \int d\omega \Im G(\omega)/\pi = 1 \).
Fig. 2 – Results from exact diagonalization of the atom ($S(0)$, triangles), the star ($S(1)$, open circles) and the star of the stars ($S(2)$, filled circles) as a function of $U$ in units of $t^*$. a) The smallest pole of $G_0^{(n)}(\omega)$, which corresponds to half the gap. Denoted by ‘rec’ is the prediction for the thermodynamic limit by the recursion method analysis. b), c) The coefficients $\alpha$ of the Laurent-series of the self-energy: $\Sigma(\omega) = \alpha/\omega + U/2 + (1 - 1/z^*)\omega + ...$ as given by eq. (1). Only for $\alpha = 0$ is $z^* \equiv Z = m/m^*$. The $\alpha^{(n)}$ and $Z^{(n)}$ ($n = 2, 3, 4$) are the predictions of the equation-of-motion solutions. $\triangle S(1), \circ S(2), \bullet S(3)$. The dotted lines are guides to the eye.

Results. – We have exactly diagonalized the half-filled Hubbard-like Hamiltonian on $S(n)$ for $n = 0, 1$ (for $S(2)$ we have $8 - \uparrow$ and $7 - \downarrow$ particles corresponding to $\sim 4 \cdot 10^7$ different configurations) and determined the one-particle Green’s function, $G_0^{(n)}(\omega)$, in the paramagnetic (see footnote (1)) superposition of the degenerate spin doublets via a continued-fraction expansion [16].
In fig. 2a) we have plotted the position of the lowest pole in \( G_0^{(n)}(\omega) \) (as a function of \( U \)), corresponding to half of the optical gap, \( \Delta \). In order to estimate the influence of the finite system size on \( \Delta \) we have subjected the Green’s function for \( S(2) \) to a continued-fraction analysis which has been successfully used \[20\] to eliminate finite-size effects in numerical calculations of dynamical correlation functions from small systems. The first few coefficients of the continued-fraction representation of the Green’s function allow for reliable estimates of its low-energy behavior in the thermodynamic limit. We find that the gap vanishes identically for \( U \leq 2 \) in the thermodynamic limit and that it is nicely linear for \( U \geq 3 \), with the same slope as the cluster data for \( S(2) \). These results, see fig. 2a), indicate that our estimates of the self-energy parameters from \( S(2) \) are well controlled and that we may reliably estimate \( U_c \sim 2.5 t^* \).

In fig. 2b) we present the results for \( \alpha \), as defined by eq. (1). \( \alpha(U) \) increases between \( U = 2 \) and \( U = 3 \) by a factor of twelve for \( S(2) \), indicative of a gap opening in the thermodynamic limit, \( S(n \to \infty) \).

In fig. 2c) we show the results for \( z^* \), as defined by eq. (1). Note that \( z^* \) corresponds to the quasi-particle renormalization factor \( Z \equiv m/m^* \) in the thermodynamic limit whenever \( \alpha \equiv 0 \). We find for both \( S(1) \) and \( S(2) \) the minimum of \( z^* \) occurs at approximately the same \( U_{\text{min}} \sim 2.5 t^* \) and that \( z^* \) is a continuous function of \( U \).

In fig. 2 we have included the results of a recently proposed systematic series of self-consistent equation-of-motion solutions \[21\], \( \alpha^{(n)} \) and \( Z^{(n)} \) (with \( n = 2, 3, 4 \)). The \( n \)-th-order equation-of-motion solution satisfies the first \( n - 1 \) equations of motion exactly, while the \( n \)-th-order equation of motion is decoupled self-consistently \[21\]. \( n = 2 \) corresponds to the Hubbard-III solution \[22\]. The critical \( U_c^{(2)} = U_c^{(3)} = \sqrt{6} t^* \sim 2.45 t^* \) and \( U_c^{(4)} = \sqrt{40} t^* \sim 2.52 t^* \) found by the equation-of-motion solutions \[21\] agree very well with the \( U_c \sim 2.5 t^* \) estimated from the \( S(2) \) cluster with the recursion method, see fig. 2a) and b), and agrees also well with the location of the minimum in \( z^*(U) \), as obtained for both \( S(1) \) and \( S(2) \), see fig. 2c). The crowding of lines in fig. 2b) for \( U > 3 \) puts into evidence the remarkable consistency between the cluster results and the equation-of-motion results for \( \alpha \).

In fig. 3 we plot the results for \( -\text{Im} G_0(\omega + i\delta) \) and \(+\text{Im} G_{\text{inc}}(\omega + i\delta)\) as obtained for the star of the stars for \( \delta = 0.05 t^* \) and \( U = 2 \). \( G_0(\omega) \) has, as expected, poles at very small frequencies, an indication of a gapless density of states in the thermodynamic limit. \( G_{\text{inc}}(\omega) \), on the other hand, has no poles at small frequencies, the structure in \( G_{\text{inc}}(\omega) \) seems to start at about \( U/2 \). In the metallic state the quasi-particle damping if given by \( \sim \omega^2 \text{Im} G_{\text{inc}}(0) \) and \( \text{Im} G_{\text{inc}}(0) \) is finite in the thermodynamic limit. In the insulating state for both \( G_0(\omega) \) and \( G_{\text{inc}}(\omega) \) a gap \( \Delta \) opens and \( \text{Im} G_{\text{inc}}(0) = 0 \).

**Discussion.**— Our cluster results for \( \Delta, \alpha \) and \( z^* \) (see fig. 2), the analysis of the cluster Green’s function with the recursion method \[20\] and the series of self-consistent equation-of-motion solutions \[21\] are all consistent with i) a \( U_c \sim 2.5 t^* \), ii) the gap \( \Delta \) opening continuously at \( U_c \) and iii) the parameter \( z^* \) of the self-energy representation equation (1) being a continuous function of \( U \) at the Mott-Hubbard transition. These three results do not agree with other studies \[8\]- \[11\], based on the iterative perturbation theory and self-consistent diagonalization studies, which find a) a \( U_c - 4.2 t^* - 4.7 t^* \), b) the gap \( \Delta \) to open discontinuously at \( U_c \) and c) the parameter \( z^* \) to be discontinuous at \( U_c \).

**Effective theory.**— The results for the \( G_{\text{inc}}(\omega) \) presented in fig. 3 indicate that \( G_{\text{inc}}(\omega) \) is a smooth function, for small frequencies, in the thermodynamic limit. The first few terms of
Fig. 3 – $-\text{Im} G_0(\omega + i\delta)$ and $+\text{Im} G_{\text{inc}}(\omega + i\delta)$, as defined by eq. (1), as a function of frequency in units of $t^*$, for $U = 2$ and $\delta = 0.05 t^*$. Note the absence of low-energy poles in the incoherent Green’s function.

a small-frequency expansion for the self-energy (compare Eq. (1))

$$\sum(\omega) = \frac{\alpha}{\omega} + \frac{U}{2} + \left(1 - \frac{1}{z^*}\right) \omega + i \left(1 - \frac{1}{z^*}\right) \frac{\gamma}{z^*} w^2,$$

where $\gamma = G_{\text{inc}}(0)$, are then sufficient to describe the asymptotic, small-frequency behavior near the Mott-Hubbard transition. The three parameters $x \equiv \alpha, z^*, \gamma$ entering eq. (4) are expected to scale like $|U - U_c|^{\lambda_x}$ in the critical region $|U - U_c| \ll U_c$ of the Mott-Hubbard transition. The exact values of the critical exponents, $\lambda_x$, are not yet known. The equation-of-motion solutions [21] predict, for the Bethe lattice $\lambda_x = 1$ and $\lambda_{z^*} = 2$, the iterative perturbation theory and self-consistent diagonalization studies [8]-[11] $\lambda_{z^*} = 2$.

From the small-frequency expansion of the self-energy, eq. (4), one can determine the low-frequency behavior of the one-particle Green’s function $[\omega - (\varepsilon_\beta - \mu) - \sum(\omega)]^{-1}$, where the $\varepsilon_\beta$ are the one-particle eigenenergies of the Bethe lattice. For the position of the quasi-particle poles one finds $z^* \varepsilon_\beta / 2[1 \pm \sqrt{1 + 4\alpha/(z^* \varepsilon_\beta^2)}]$. For $\alpha > 0$ a Mott-Hubbard gap opens, which scales for $\lambda_{z^*} > \lambda_\alpha$ as $\sim \sqrt{\alpha z^*} \sim |U - U_c|/(\lambda_x + \lambda_{z^*})/2$. Defining the scaling exponent of the gap, $\Delta$, via $\Delta \sim |U - U_c|^{2\Delta} \Theta(U - U_c)2$ we then arrive at the prediction

$$2\lambda_\Delta = \lambda_x + \lambda_{z^*}.$$

We then find for the equation-of-motion solutions $\lambda_\Delta = 3/2$ while the iterative perturbation
theory and self-consistent diagonalization studies [8]- [11] predict $\lambda_\Delta = 0$.

Conclusions.– We have shown that the properties of the Hubbard star of the stars can be obtained by exact diagonalization of certain 15-site Hubbard clusters. We have presented estimates for the optical gap $\Delta$, and the quasi-particle spectral weight $z^*$. We find our estimate of $U_c \sim 2.5t^*$ to be in good agreement with the predictions of a recently proposed series of self-consistent equation-of-motion solutions [21].

We used the results obtained from the cluster calculations to estimate qualitatively the low-energy behavior of the self-energy, which in turn led us to propose a simple, phenomenological theory for the small-frequency behavior of the Mott-Hubbard transition, in terms of a truncated Laurent expansion of the self-energy.

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