Equation of motion approach to the Hubbard model in infinite dimensions

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We consider the Hubbard model on the infinite-dimensional Bethe lattice and construct a systematic series of self-consistent approximations to the one-particle Green’s function, $G^{(n)}(\omega)$, $n = 2, 3, \ldots$. The first $n-1$ equations of motion are exactly fulfilled by $G^{(n)}(\omega)$ and the $n$'th equation of motion is decoupled following a simple set of decoupling rules. $G^{(2)}(\omega)$ corresponds to the Hubbard-III approximation. We present analytic and numerical results for the Mott-Hubbard transition at half filling for $n = 2, 3, 4$.

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INTRODUCTION

The Hubbard-model on the infinite-dimensional, half-filled Bethe lattice in the paramagnetic state has been considered in the last years more and more as the standard model for the Mott-Hubbard transition. One of the reasons for this interest is that the study of interacting Fermions in the limit of infinite spatial dimensions leads to considerable technical advantages, as the self-energy becomes strictly local. The Mott-Hubbard transition has been studied recently by Monte-Carlo, a self-consistent weak-coupling theory, rigorous and self-consistent exact diagonalization studies, with considerable different results, see [4].

Alternatively, Hubbard has considered an equation of motion approach to the Hubbard model. Unfortunatly his approach can not be systematically improved in any finite dimensions, since the resulting self-consistency equations would be numerically intracable, due to the involved summations over momenta. Here we point out that, uniquely to the infinite-dimensional Bethe lattice, the equation of motion approach may be systematically carried on. We develop a simple decoupling scheme applicable to equations of motion in any orders and resulting in a self-consistency equation for the one-particle Green’s function. We present results for the Green’s function is second, third and fourth order, with the second order corresponding to the Hubbard-III solution.

DEFINITIONS

At half filling, $n = 1$, the chemical potential $\mu \equiv U/2$. For general fillings we set $\mu = U/2 + \Delta \mu$ and find for the grand-canonical Hubbard Hamiltonian, $\hat{K} = \hat{H} - \mu \hat{N}$,

$$\hat{K} = t \sum_{<i,j>,\sigma} \hat{t}_{j,i,\sigma} + U/2 \sum_i (\hat{n}_i - 1) - \Delta \mu \sum_i \hat{n}_i,$$

where the symbol $<i,j>$ denotes pairs of nearest neighbour sites on a Bethe-lattice with coordination number $z$. The scaling $t = \tilde{t}/\sqrt{z}$ yields a non-trivial limiting behaviour in the limit $z \to \infty$. In Eq. (1) we have made use of $\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i,\sigma}$, $\hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}$ in Eq. (1) and of some of the following operator definitions:

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\[ \hat{\ell}_{j,i,\sigma} = \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} + \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \]
\[ \hat{j}_{j,i,\sigma} = \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} - \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \]
\[ \hat{u}_i = \hat{c}_{i,\uparrow}^\dagger \hat{c}_{i,\uparrow} + \hat{c}_{i,\downarrow}^\dagger \hat{c}_{i,\downarrow} \]
\[ \hat{d}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} - \hat{c}_{i,\sigma} \hat{c}_{i,\sigma}^\dagger = 2 \hat{n}_{i,\sigma} - 1, \]

where the \( \hat{c}_{i,\sigma}^\dagger \) and the \( \hat{c}_{i,\sigma} \) are creation/annihilation operators for electrons with spin \( \sigma = \uparrow, \downarrow \) on lattice sites \( i \). The following operator identities hold:
\[ \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} = (\hat{\ell}_{j,i,\sigma} + \hat{j}_{j,i,\sigma}) / 2 \]
\[ \hat{d}_{i,\sigma} \hat{d}_{i,\sigma} \equiv \hat{1}. \]

For the equation of motion we will make use of following operator commutation relations:
\[ [\hat{f}_{j,i,\sigma}, \hat{c}_{i,\sigma}] = -\hat{\ell}_{j,i,\sigma} \]
\[ [\hat{u}_i, \hat{c}_{i,\sigma}] = -\hat{d}_{i,-\sigma} \hat{c}_{i,\sigma} \]
\[ [\hat{t}_{j,i,-\sigma}, \hat{d}_{i,-\sigma}] = 2 \hat{j}_{j,i,-\sigma} \]
\[ [\hat{u}_j, \hat{j}_{j,i,-\sigma}] = \hat{d}_{j,i,-\sigma} \hat{j}_{j,i,-\sigma} \]
\[ [\hat{\ell}_{j,i,-\sigma}, \hat{j}_{j,i,-\sigma}] = 2 (\hat{n}_{i,-\sigma} - \hat{n}_{j,-\sigma}) \]
\[ [\hat{u}_j, \hat{j}_{j,i,-\sigma}, \hat{c}_{i,-\sigma}] = 0 = [\hat{u}_i, \hat{j}_{j,i,-\sigma}, \hat{c}_{i,-\sigma}] \]

and similar one’s. Given operators \( \hat{A} \) and \( \hat{B} \), the Matsubara Green’s function \( \langle \langle \hat{A}; \hat{B} \rangle \rangle \) is defined as
\[ \langle \langle \hat{A}; \hat{B} \rangle \rangle = \int_0^\beta d\tau (-1) < T^\tau \hat{A}(\tau) \hat{B}(0) > e^{i\omega_n \tau}, \]
with \( \tau \) being the imaginary time and the brackets \( < \ldots > \) denoting the thermodynamic expectation value. The retarded Green’s function is obtained via the analytic continuation \( i\omega_n \to \omega + i\delta \). Here we are interested in constructing systematic approximations to the onsite one-particle Green’s function \( G(i\omega_n) = \langle \langle \hat{c}_{0,\sigma}^\dagger; \hat{c}_{0,\sigma} \rangle \rangle \). In the following we will define sites 1, 1’, 1’’, . . . to be different n.n. sites of the central site, 0, and 2, 2’, 2’’, . . . to be different n.n.n. sites of the central site.

**EQUATIONS OF MOTION**

For any imaginary-time-dependent operator, \( \hat{A}(\tau) \) in the Heisenberg picture, the equation of motion is given by
\[ \frac{d}{d\tau} \hat{A}(\tau) = [\hat{K}, \hat{A}], \]
where, in the grand-canonical formulation, \( \hat{K} = \hat{H} - \mu \hat{N} \) is given by Eq. (1). Note that we have set \( \mu = U/2 + \Delta \mu \). Some examples of specific equation of motion in \( \tau \)-space are
\[
\frac{d}{dt} \hat{c}_{i,\sigma}^\dagger (\tau) = -\Delta \mu \hat{c}_{i,\sigma}^\dagger (\tau) + t \sum_j \hat{c}_{j,\sigma}^\dagger (\tau) + \frac{U}{2} \hat{d}_{i,-\sigma} \hat{c}_{i,\sigma}^\dagger (\tau)
\]
\[
\frac{d}{dt} \hat{c}_{i,\sigma} (\tau) = \Delta \mu \hat{c}_{i,\sigma} (\tau) - t \sum_j \hat{c}_{j,\sigma} (\tau) - \frac{U}{2} \hat{d}_{i,-\sigma} \hat{c}_{i,\sigma} (\tau)
\]
\[
\frac{d}{dt} \hat{d}_{i,-\sigma} \hat{c}_{i,\sigma} (\tau) = \Delta \mu \hat{d}_{i,-\sigma} \hat{c}_{i,\sigma} (\tau) + t \sum_j \left[ 2 \hat{J}_{j,i,-\sigma} \hat{c}_{i,\sigma} (\tau) - \hat{d}_{i,-\sigma} \hat{c}_{j,\sigma} (\tau) \right] - \frac{U}{2} \hat{d}_{i,\sigma} (\tau)
\]
where \( j \) is a n.n. site of \( i \) and where we have used definitions Eq. (2) and the operator identity Eq. (4). In Fourier-space the first equation of motion is
\[
(i \omega_n + \Delta \mu) \langle \langle \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle = 1 + z t \langle \langle \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle + U/2 \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle,
\]
where the site 1 is any of the \( z \) equivalent n.n. site of the central site 0. In the limit \( z \to \infty \) the decoupling
\[
\langle \langle \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle \to t \langle \langle \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle \langle \langle \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]
is exact since all diagrams contributing to the propagation of the particle from site 1 to site 1 have only a vanishing probability \( 1/z \to 0 \) to visit the central site. Using that \( \langle \langle \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle = \langle \langle \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle \equiv G(\omega_n) \) in the paramagnetic state and that \( z t^2 = \hat{\sigma}^2 \) we rewrite the equation of motion of first and second order as
\[
[i \omega_n + \Delta \mu - \hat{\sigma}^2 G(\omega_n)] G(\omega_n) = 1 + U/2 \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]
\[
(i \omega_n + \Delta \mu) \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle = 2 \Delta n_{0,-\sigma} + U/2 G(\omega_n)
\]
\[
- 2 z t \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle + z t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle,
\]
where \( \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle = 2 n_{0,-\sigma} - 1 = 2 \Delta n_{0,-\sigma} \) and where we have measured \( n_{0,-\sigma} \equiv 1/2 + \Delta n_{0,-\sigma} \) with respect to half-filling. The second-order equation of motion, Eq. (15), generates two new Green’s function. In third order we have the equation of motion for \( \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle \),
\[
(i \omega_n + \Delta \mu) \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle = \langle \langle \hat{c}_{1,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle + z t \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle
\]
\[
- z t \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle + z t \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle + 2 t \langle \langle \hat{n}_{1,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle - 2 t \langle \langle \hat{n}_{1,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]
\[
- U/2 \langle \langle \hat{d}_{1,\sigma} \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle,
\]
where we have used various commutator-relations, in particular Eq. (4). We can simplify Eq. (17) in infinite-dimensions where the decoupling
\[
\langle \langle \hat{n}_{1,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle \to < \hat{n}_{1,-\sigma} > \langle \langle \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]
becomes exact. Again \( < \hat{n}_{1,-\sigma} > = 1/2 + \Delta n_{1,-\sigma} \) and using Eq. (4), \( 2 \hat{n}_{0,-\sigma} - 1 = \hat{d}_{0,-\sigma} \), we can rewrite
\[
2 t \langle \langle \hat{n}_{1,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle - 2 t \langle \langle \hat{n}_{1,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle = 2 t \Delta n_{1,-\sigma} \langle \langle \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle - t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]
in Eq. (16). In third order we have with the equation of motion for \( \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle \) a second equation of motion,
\[
(i \omega_n + \Delta \mu) \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle = z t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{2,\sigma}; \hat{c}_{2,\sigma}^\dagger \rangle \rangle - 2 z t \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle
\]
\[
+ t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}; \hat{c}_{0,\sigma}^\dagger \rangle \rangle + U/2 \langle \langle \hat{d}_{0,-\sigma} \hat{d}_{1,-\sigma} \hat{c}_{1,\sigma}; \hat{c}_{1,\sigma}^\dagger \rangle \rangle.
\]
A total of six new Green’s functions are generated in third order by Eq. (16) and Eq. (19): \( \langle \langle \hat{d}_{0,-\sigma} \hat{d}_{1,-\sigma} \hat{c}_{1,\sigma} \hat{c}_{0,\sigma} \rangle \rangle \) and \( \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{2,\sigma} \hat{c}_{0,\sigma} \rangle \rangle \), by Eq. (19) alone, \( \langle \langle \hat{d}_{1,\sigma} \hat{c}_{0,\sigma} \rangle \rangle \), \( \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle \), \( \langle \langle \hat{t}_{1,1,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle \) by Eq. (16) alone, and \( \langle \langle \hat{U}_{1,0,-\sigma} \hat{c}_{1,\sigma} \hat{c}_{0,\sigma} \rangle \rangle \) by both Eq. (16) and Eq. (19). We present the equation of motion for these six Green’s functions in Appendix A. Now we specialize on half-filling, where \( \Delta \mu = 0 \). For an overview we rewrite here the first two equation of motion, Eq. (14) and Eq. (15): 

\[
[i\omega_n - t^2 G(i\omega_n)] G(i\omega_n) = 1 + U/2 \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle \\
i\omega_n \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle = U/2 G(i\omega_n) - 2zt \langle \langle \hat{U}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + zt \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle.
\]

(20)

(21)

Noting that there is no current flowing in equilibrium, \( \langle \langle \hat{c}_{1,\sigma} \hat{c}_{0,\sigma} - \hat{c}_{0,\sigma} \hat{c}_{1,\sigma} \rangle \rangle \leq 0 \) and using Eq. (18) with \( \Delta n_{1,-\sigma} = 0 \) the first third-order equation of motion, Eq. (14), takes the form

\[
i\omega_n \langle \langle \hat{U}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle = zt \langle \langle \hat{U}_{1,0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle - zt \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + zt \langle \langle \hat{t}_{1,1,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle - t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle - U/2 \langle \langle \hat{d}_{1,\sigma} \hat{c}_{1,\sigma} \rangle \rangle.
\]

(22)

For completeness, we rewrite also the second third-order equation of motion, Eq. (15), for the half-filled case,

\[
i\omega_n \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle = zt \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{2,\sigma} \rangle \rangle - 2zt \langle \langle \hat{U}_{1,0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle + t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + U/2 \langle \langle \hat{d}_{1,\sigma} \hat{d}_{1,\sigma} \rangle \rangle.
\]

(23)

Particle-hole symmetry at half-filling implies that the real part of \( G(\omega) \) is an odd function of frequency. Consequently Eq. (21) is an even function of frequency, Eq. (21) an odd function of frequency and Eq. (22) and Eq. (23) even functions of frequencies. The absence of a (real) constant term on the right-hand side of Eq. (21) is therefore forced by symmetry but the absence of constant terms on the right-hand side of Eq. (22) and Eq. (23) is accidental.

**APPROXIMATIONS**

In order to obtain a solution for \( G(i\omega_n) \) we will decouple the equations of motion. We present here a simple, systematic decoupling scheme, which may be applied at any order of the equation of motion. We generalize the decoupling for \( \langle \langle \hat{c}_{1,\sigma} \hat{c}_{0,\sigma} \rangle \rangle \) presented in Eq. (13) by

\[
\langle \langle \hat{U}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle \rightarrow - t G(i\omega_n) \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle
\]

(24)

\[
\langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle \rightarrow t G(i\omega_n) \langle \langle \hat{d}_{1,\sigma} \hat{c}_{0,\sigma} \rangle \rangle.
\]

which may be motivated by considering Eq. (22) and Eq. (23). In contrast to Eq. (13), which is exact in the limit of infinite dimensions, Eq. (24) is an approximation only, valid in the paramagnetic state. In a state with staggered antiferromagnetism the replacement \( G(i\omega_n) \rightarrow G_{-\sigma}(i\omega_n) \) should be made on the right-hand side of Eq. (24). Using Eq. (21) and Eq. (20) we then obtain

\[
[i\omega_n - t^2 G(i\omega_n)] G(i\omega_n) = 1 + \frac{(U/2)^2}{i\omega_n - 3t^2 G(i\omega_n)} G(i\omega_n).
\]

(25)

Comparing Eq. (25) with the Dyson equation of the infinite-dimensional Bethe-lattice, which has the form
\[ [i\omega_n + \mu - \Sigma(i\omega_n) - i\xi^2 G(i\omega_n)] G(i\omega_n) = 1, \]

we find

\[ \Sigma^{(2)}(i\omega_n) - \mu = \frac{(U/2)^2}{i\omega_n - 3 i\xi^2 G(i\omega_n)}. \]

Eq. (27) is the well-known result of the Hubbard-III approximation \textsuperscript{4}. Here we use the index \textsuperscript{2} to indicate that for this approximation to the self-energy the first equation of motion has been retained exactly and that the equation of motion of second order has been decoupled. In order to obtain \( \Sigma^{(3)}(i\omega_n) \) we have to consider the equation of motion of third order, Eq. (22) and Eq. (23). For the decoupling of the terms \( \sim t \) on the respective right-hand sides straightforward generalization of Eq. (24) can be used. For the terms \( \sim U/2 \) we proposed the decoupling scheme

\[
\begin{align*}
\langle \langle \hat{d}_{1,\sigma} \hat{t}_{0,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \langle \langle \hat{c}_{0,\sigma}^\dagger \rangle \rangle &\rightarrow - \frac{2}{U} \langle \langle \hat{J}_{1,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \langle \langle \hat{c}_{0,\sigma} \rangle \rangle \\
\langle \langle \hat{d}_{0,\sigma} \hat{d}_{1,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \langle \langle \hat{c}_{0,\sigma} \rangle \rangle &\rightarrow \frac{2}{U} \langle \langle \hat{J}_{0,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \langle \langle \hat{c}_{0,\sigma} \rangle \rangle,
\end{align*}
\]

valid in the half-filled case, where we have been motivated by Eq. (A1) and Eq. (A2). Eq. (22) and Eq. (23) then become

\[
\begin{align*}
i\omega_n \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle &= t \langle \langle \hat{d}_{0,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle \\
&\quad + 3 i^2 G(i\omega_n) \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle + (\Sigma(i\omega_n) - \mu) \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle \\
i\omega_n \langle \langle \hat{d}_{0,\sigma} \hat{c}_{1,\sigma}^\dagger \rangle \rangle &= t \langle \langle \hat{d}_{0,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle \\
&\quad + 3 i^2 G(i\omega_n) \langle \langle \hat{d}_{0,\sigma} \hat{c}_{1,\sigma}^\dagger \rangle \rangle + (\Sigma(i\omega_n) - \mu) \langle \langle \hat{d}_{0,\sigma} \hat{c}_{1,\sigma}^\dagger \rangle \rangle.
\end{align*}
\]

We replace \( \Sigma(i\omega_n) \rightarrow \Sigma^{(3)}(i\omega_n) \) in Eq. (24) and obtain for Eq. (21)

\[
i\omega_n \langle \langle \hat{d}_{0,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle = U/2 G(i\omega_n) + \frac{3 i^2}{i\omega_n - 3 i^2 G(i\omega_n) - (\Sigma^{(3)}(i\omega_n) - \mu)} \langle \langle \hat{d}_{0,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle.
\]

Finally, using Eq. (26) and Eq. (28) we obtain

\[ \Sigma^{(3)}(i\omega_n) - \mu = \frac{(U/2)^2}{i\omega_n - 3 i^2 G(i\omega_n) - (\Sigma^{(3)}(i\omega_n) - \mu)}, \]

with \( \mu = U/2 \) at half-filling. In Appendix A we derive the expression for \( \Sigma^{(4)}(i\omega_n) \), see Eq. (A11). Considering the self-energy expanded in powers of \( (U/2)^2 \) and of \( i^2 \), we see that \( \Sigma^{(2)}(i\omega_n) \) is exact up to \( i^2 \) and all powers of \( (U/2)^2 \). Similary \( \Sigma^{(3)}(i\omega_n) \) is exact up to \( i^4 \) and \( \Sigma^{(4)}(i\omega_n) \) up to \( i^6 \).

**RESULTS**

The solution for the retarded Green’s function, \( G(\omega) \), is given by Eq. (24) together with the respective self-energy, see Eq. (27), Eq. (30) and Eq. (A11). For small \( U \)’s the solution is metallic, for large \( U \)’s insulating. The transition point can be calculated from a small-\( \omega \) expansion, by noting that in the insulating state the Laurent-series of the self-energy starts by a \( 1/\omega \) divergence \textsuperscript{1}: \( \Sigma(\omega) \sim \alpha/\omega + \ldots \). From Dyson’s equation, Eq. (24), it follows that that \( G(\omega) \sim -\omega/\alpha + \ldots \). We find then that
\[ \alpha^{(2)} = \alpha^{(3)} = \frac{1}{4} \left( U^2 - 12 t^2 \right) \]
\[ \alpha^{(4)} = \frac{1}{4} \frac{U^2 - 160 t^4 / U^2}{1 + 8 t^2 / U^2}, \]
where \( \alpha^{(4)} \) has been calculated in Appendix A (see Eq. (A12)). It can be shown \[ \Box \], considering the spectral representation of \( G(\omega) \), that the coefficient \( \alpha \geq 0 \). The \( U_c \) for the Mott-Hubbard transition is then given by the \( \alpha = 0 \) condition in Eq. (32). We then find \( U_c^{(2)} = U_c^{(3)} = \sqrt{12} \tilde{t} \) and \( U_c^{(4)} = \sqrt{100} \tilde{t} \). From now on we use the scaling \( \tilde{t} = 1/\sqrt{2} \). We have

\[ U_c^{(2)} = U_c^{(3)} = \sqrt{6} \sim 2.4495 \]
\[ U_c^{(4)} = \sqrt{40} \sim 2.5149. \]

The \( U_c \) given in Eq. (32) has been denoted \[ \Box \] \( U_{c1} \), being the critical interaction strength at with the insulating solution becomes stable. A \( U_{c2} \) has also been defined \[ \Box \] as the critical interaction strength at with the metallic solution becomes unstable, i.e. when \( \text{Im} \ G(0) = 0 \). We will discuss further below that the equation of motion solutions always yield \( U_c^{(n)} = U_{c1}^{(n)} = U_{c2}^{(n)} \) as given by Eq. (32), for \( n = 2, 3, 4 \).

In Fig. (a) we have plotted \( \alpha^{(3)} \) and \( \alpha^{(4)} \) as given by Eq. (31). For comparison we have included in Fig. (a) the results obtained by an exact diagonalization study \[ \Box \], where the symbol \( S(1) \) denotes the so-called Hubbard star \[ \Box \] and the symbol \( S(2) \) the so-called star of the stars. In general, the symbol \( S(n) \) denotes clusters which are truncated Bethe-lattices of order \( n \). For instance, \( S(1) \) is the cluster containing a central site with its n.n. sites. As the \( S(n) \) are finite clusters, no true Mott-Hubbard transition is observed, only a crossover. Nevertheless, good agreement between the \( S(2) \) cluster and the equation of motion results if found for \( U \geq 3 \), indicating that \( U_c \leq 3 \).

In Fig. (b) we have plotted the \( Z \)-factor, as defined by the second term in the Laurent expansion for the self-energy, \( \Sigma(\omega) \sim \alpha/\omega + (1 - 1/Z) \omega + \ldots \), which we calculate in Appendix B. In a Fermi-liquid state \( \alpha = 0 \) the \( Z \)-factor would have the meaning of the inverse effective mass, \( Z = m/m^* \), but in the insulating state \( \alpha > 0 \) considered in Fig. (b) the \( Z \)-factor is just a parameter. \( Z \) vanishes at \( U_c \) for all three equation of motion solutions in the same fashion. To see this we note that \( \alpha^{(n)} \sim U - U_c^{(n)} \) (for \( U - U_c^{(n)} \ll U_c^{(n)} \) and \( n = 2, 3, 4 \), see Eq. (31)) and \( Z^{(n)} \sim |\alpha^{(n)}|^2 \) for small \( \alpha^{(n)} \) (see Eq. (33) and Eq. (34)). We then obtain

\[ Z^{(n)} \sim (U - U_c^{(n)})^2 \]

for \( n = 2, 3, 4 \) and \( U_c^{(n)} \) given by Eq. (32).

In Fig. (b) and Fig. (c) we present the equation of motion results for the density of states, \(-\text{Im} \, G^{(n)}(\omega + i\delta)\), for a small \( \delta = 0.0001 \). The results for \( U = 1 \) and \( U = 2 \) are in the metallic state and for \( U = 3 \) and \( U = 4 \) in the insulating state. The magnitude of the gap changes little with \( n = 1, 2, 3 \), but the shapes of the Hubbard bands change somewhat and side bands appear at higher energies.

In Fig. (c) we present the results for the density of states at the Fermi level, \(-\text{Im} \, G^{(n)}(0)\), and the self-energy at the Fermi level, \(-\text{Im} \, \Sigma^{(n)}(0)\), in the metallic state, as a function of \( U \). Both quantities are related via \( \Sigma^{(n)}(0) = \mu - G^{(n)}(0)/2 - 1/G^{(n)}(0) \), compare Eq. (36), with \( \text{Re} \, \Sigma^{(n)}(0) = \mu \). Analytically we find

\[ -\text{Im} \, G^{(2)}(0) = \sqrt{\frac{12 t^2 - U^2}{12 t^4}}, \]
\[ -\text{Im} \, G^{(3)}(0) = \sqrt{\frac{12 t^2 - U^2}{12 t^4 (t^2 + 3/2(U/2)^2)}}, \]

where \( \mu \) is the chemical potential.

\[ \Box \]
In a Fermi-liquid state $Im \Sigma(0) \equiv 0$ and $-Im G(0) = \sqrt{2}$, independent of interaction strength, $U$. As we see from Fig. 4 $-Im G^{(n)}(0) < \sqrt{2}$ and the $-Im \Sigma^{(n)}(0) > 0$. The equation of motion solutions do not describe a Fermi liquid. Indeed, in the equation of motion solutions the divergence

$$\lim_{U \to U_c} -Im \Sigma^{(n)}(0) \sim \frac{1}{\sqrt{U^{(n)}_c - U}} \to \infty$$

(34)

drives the Mott-Hubbard transition. Here we have derived Eq. (34) from Eq. (33) for $n = 2, 3$ and verified it for $n = 4$ from a small $G(0)$-expansion of Eq. (A1). We note that the metallic solution becomes unstable, as seen from Eq. (34), at exactly the same $U^{(n)}_c$ at which the insulating solution becomes stable, compare Eq. (32). In an alternative approach to the Mott-Hubbard transition on the Bethe lattice in infinite dimensions [8] it has been proposed that the metallic solution might remain stable up to a much higher $U^{(n)}_c \sim 4.2 - 4.7$.

**CONCLUSIONS**

We have considered the equation of motion approach to the Hubbard model on the infinite-dimensional Bethe-lattice and shown that it is possible to evaluate higher-order Green’s function by a simple decoupling scheme. We presented analytic and numerical results for the half-filled case in the paramagnetic sector. We found the critical $U_c \sim 2.5$ for the Mott-Hubbard transition to change only little with the order of the approximation. The metallic state is a non-Fermi-liquid, with a finite imaginary part of the self-energy at the Fermi-level, diverging at the Mott-Hubbard transition. The metallic state does not show, surprisingly, any tendency to become more Fermi-liquid like with increasing order of approximation.

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**APPENDIX A:**

Here we present the equations of motion of fourth order for the six new Green’s functions created by the third-order equations of motion, Eq. (16) and Eq. (19). The first one is

\[
(i\omega_n + \Delta \mu) \langle \langle \hat{d}_{0,-\sigma}\hat{d}_{1,-\sigma}\hat{c}_{1,\sigma}^\dagger;\hat{c}_{0,\sigma}^\dagger \rangle \rangle = \frac{U}{2} \langle \langle \hat{d}_{0,-\sigma}\hat{c}_{1,\sigma};\hat{c}_{0,\sigma}^\dagger \rangle \rangle + 2t \Delta n_{1,-\sigma} \langle \langle \hat{d}_{0,-\sigma}\hat{c}_{0,\sigma};\hat{c}_{0,\sigma}^\dagger \rangle \rangle + zt \langle \langle \hat{d}_{0,-\sigma}\hat{d}_{1,-\sigma}\hat{c}_{2,\sigma};\hat{c}_{0,\sigma}^\dagger \rangle \rangle - 2zt \langle \langle \hat{j}_{1,0,-\sigma}\hat{d}_{1,-\sigma}\hat{c}_{1,\sigma};\hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]

(A1)

where we have used the exact decoupling

\[
\langle \langle \hat{d}_{0,-\sigma}\hat{d}_{1,-\sigma}\hat{c}_{1,\sigma}^\dagger;\hat{c}_{0,\sigma}^\dagger \rangle \rangle \rightarrow <\hat{d}_{1,-\sigma}> \langle \langle \hat{d}_{0,-\sigma}\hat{c}_{0,\sigma};\hat{c}_{0,\sigma}^\dagger \rangle \rangle
\]

with $<\hat{d}_{1,-\sigma}> = 2\Delta n_{1,-\sigma}$. Note, that the n.n. site 2 occuring in the last term of the right-hand side of Eq. (A1) in $\hat{j}_{2,1,-\sigma}$ could in finite dimensions also be the central site, 0, but not in infinite dimensions. The second equation of motion in fourth order is
Due to particle-hole symmetry the real part of Eq. (A2) is an odd function of frequency at half filling, where $\Delta = 0$. The third equation of motion in fourth order is

\[
(i\omega_n + \Delta \mu) \langle \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{\sigma,0}^\dagger \rangle \rangle = \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \rangle - U/2 \langle \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{\sigma,0}^\dagger \rangle \rangle + zt \langle \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{\sigma,0}^\dagger \rangle \rangle - 2zt \langle \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{\sigma,0}^\dagger \hat{c}_{\sigma,0} \rangle \rangle + zt \langle \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{\sigma,0}^\dagger \rangle \rangle + zt \langle \langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{\sigma,0}^\dagger \hat{c}_{\sigma,0} \rangle \rangle.
\]

where we have used, besides others, the commutator relation $[\hat{t}_{1,0,-\sigma}, \hat{t}_{1,0,-\sigma}] = 0$. The fourth equation of motion in fourth order is

\[
(i\omega_n + \Delta \mu) \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{2,\sigma}^\dagger \rangle \rangle = t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle + zt \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{3,\sigma} \rangle \rangle + 2zt \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{2,\sigma} \hat{c}_{0,\sigma} \rangle \rangle + U/2 \langle \langle \hat{d}_{0,-\sigma} \hat{d}_{2,-\sigma} \hat{c}_{2,\sigma} \rangle \rangle.
\]

The fourth equation of motion in fourth order is

\[
(i\omega_n + \Delta \mu) \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{1,\sigma} \rangle \rangle = t \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + zt \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{2,\sigma} \rangle \rangle + 2zt \langle \langle \hat{J}_{1,0,-\sigma} \hat{c}_{1,\sigma} \hat{c}_{0,\sigma} \rangle \rangle + U/2 \langle \langle \hat{J}_{1,0,-\sigma} \hat{d}_{2,\sigma} \rangle \rangle + U/2 \langle \langle \hat{J}_{1,0,-\sigma} \hat{d}_{-1,\sigma} \hat{c}_{1,\sigma} \rangle \rangle.
\]

where we used the exact relation

\[
2t \langle \langle \hat{n}_{1,0,-\sigma} \hat{n}_{0,-\sigma} \rangle \rangle = 2t \langle \langle \hat{c}_{1,\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle + 2t \Delta n_{1,0,-\sigma} \langle \langle \hat{c}_{1,\sigma} \rangle \rangle - t \langle \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle,
\]

similar to one valid in Eq. (16) and Eq. (18). The fifth equation of motion in fourth order is

\[
(i\omega_n + \Delta \mu) \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle = \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \rangle + t \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle - \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle - zt \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + zt \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle + zt \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + U/2 \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle + U/2 \langle \langle \hat{t}_{1,\sigma} \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle.
\]

which might be further simplified due to $t \langle \langle \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle - \langle \langle \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle = 2t \langle \langle \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle$ and $-zt \langle \langle \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + zt \langle \langle \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle = -2zt \langle \langle \hat{t}_{1,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle$. Finally, the sixth equation of motion in fourth order is

\[
(i\omega_n + \Delta \mu) \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle = \langle \hat{t}_{2,0,-\sigma} \rangle - \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle - zt \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + zt \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle + U/2 \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma} \rangle \rangle + U/2 \langle \langle \hat{t}_{2,0,-\sigma} \hat{c}_{0,\sigma}^\dagger \rangle \rangle.
\]

Due to particle-hole symmetry the real part of Eq. (A2) is an odd function of frequency at half filling, where $\Delta = 0$. Therefore the constant term of the right-hand side of Eq. (A2), $\langle \hat{d}_{1,\sigma} \hat{t}_{1,0,-\sigma} \rangle$, has to vanish at half-filling, and it
With the introduction of another decoupling rule, namely the self-energy \( \Sigma(\omega) \) created in the third-order equation of motion, Eq. (A3), and that therefore the difference of the constant terms on the right-hand side of Eq. (A5) and Eq. (A6) respectively, namely \( \langle \hat{t}_{1,1',-\sigma} \rangle - \langle \hat{t}_{2,0,-\sigma} \rangle \) has to vanish at half-filling, and it does.

Now we derive \( \Sigma^{(3)}(i\omega_n) \) at half-filling. Generalizing the decoupling schemes Eq. (24) and Eq. (28) we define

\[
\begin{align*}
\frac{a(i\omega_n)}{\omega_n} &= \frac{U/2}{\omega_n - 5\tilde{t}^2 G(i\omega_n)} \\
\frac{b(i\omega_n)}{\omega_n} &= \frac{t}{\omega_n - (\Sigma(i\omega) - \mu) - 3\tilde{t}^2 G(i\omega_n)}
\end{align*}
\]

and find

\[
\begin{align*}
\langle \hat{d}_{0,-\sigma} \hat{d}^\dagger_{1,\sigma}\rangle &= a(i\omega_n) \langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{1,\sigma}\rangle \\
\langle \hat{d}_{1',\sigma} \hat{d}^\dagger_{0,\sigma}\rangle &= -a(i\omega_n) \langle \hat{d}_{1',\sigma} \hat{c}^\dagger_{0,\sigma}\rangle \\
\langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{1,\sigma}\rangle &= b(i\omega_n) \langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{1,\sigma}\rangle \\
\langle \hat{d}_{1',\sigma} \hat{c}^\dagger_{0,\sigma}\rangle &= b(i\omega_n) \langle \hat{d}_{1',\sigma} \hat{c}^\dagger_{0,\sigma}\rangle \\
\langle \hat{c}_{1,\sigma} \hat{c}^\dagger_{0,\sigma}\rangle &= 2b(i\omega_n) \langle \hat{c}_{1,\sigma} \hat{c}^\dagger_{0,\sigma}\rangle.
\end{align*}
\]

Here we have introduced another decoupling rule, namely the self-energy \( \Sigma(i\omega_n) \) comes in definitions Eq. (A7) only with the prefactor zero or minus one. We substitute Eq. (A8) into Eq. (22) and Eq. (23). We find

\[
\begin{align*}
A(i\omega_n) \langle \hat{d}_{1',0,-\sigma} \hat{c}_{0,\sigma}\rangle + B(i\omega_n) \langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{1,\sigma}\rangle &= -t \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}\rangle \\
2B(i\omega_n) \langle \hat{d}_{1',0,-\sigma} \hat{c}^\dagger_{0,\sigma}\rangle + A(i\omega_n) \langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{1,\sigma}\rangle &= t \langle \hat{d}_{0,-\sigma} \hat{c}_{0,\sigma}\rangle,
\end{align*}
\]

with \( B(i\omega_n) = zt b(i\omega_n) \) and \( A(i\omega_n) = i\omega_n - U/2 a(i\omega_n) - 3zt b(i\omega_n) \), with \( a(i\omega_n) \) and \( b(i\omega_n) \) given by Eq. (A7). Inverting Eq. (A9) we obtain

\[
\begin{align*}
\langle \hat{d}_{1',0,-\sigma} \hat{c}_{0,\sigma}\rangle &= -t \frac{A(i\omega_n) + B(i\omega_n)}{A^2(i\omega_n) - 2B^2(i\omega_n)} \langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{0,\sigma}\rangle \\
\langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{1,\sigma}\rangle &= t \frac{A(i\omega_n) + 2B(i\omega_n)}{A^2(i\omega_n) - 2B^2(i\omega_n)} \langle \hat{d}_{0,-\sigma} \hat{c}^\dagger_{0,\sigma}\rangle.
\end{align*}
\]

Finnall, using Eq. (24), Eq. (28) and Eq. (26) we obtain

\[
\Sigma^{(4)}(i\omega_n) = \mu - \frac{(U/2)^2}{\omega_n - \tilde{t}^2 \frac{2A(i\omega_n) + 3B(i\omega_n)}{A^2(i\omega_n) - 2B^2(i\omega_n)}}.
\]

The critical interaction strength, \( U_c^{(4)} \), at zero temperature may by be obtained from Eq. (A11) by considering the insulating state. For small real frequencies \( \omega \) the self energy starts like \( \Sigma(\omega) = \alpha/\omega + O(\omega) \) and the Green’s function like \( G(\omega) = -\omega/\alpha + O(\omega^3) \), which leads to \( B(\omega) \sim -\omega \tilde{t}^2 / \alpha, A(\omega) \sim -(\alpha/\omega)(U/2)^2/2t^2 \) and \( \Sigma^{(4)}(\omega) \sim (U/2)^2/(\omega_n - 2\tilde{t}^2/A(\omega)) \). One then obtains

\[
\alpha^{(4)} = \frac{U^2/4 - 40\tilde{t}^4/U^2}{1 + 8\tilde{t}^2/U^2}.
\]

Since \( \alpha \geq 0 \) Eq. (A12) is valid only for \( U > U_c^{(4)} = \sqrt{160} \tilde{t} \). For the usual scaling \( \tilde{t} = 1/\sqrt{2} \) the critical \( U_c^{(4)} = \sqrt{40} \approx 2.5149 \), which compares to \( U_c^{(2)} = U_c^{(3)} = \sqrt{6} \approx 2.4495 \). (compare Eq. (24)).
APPENDIX B:

Here we consider the insulating state, in which the Laurent expansion of the retarded self-energy starts like

\[ \Sigma(\omega) = \frac{\alpha}{\omega} + \mu + (1 - \frac{1}{Z}) \omega + \ldots \]
\[ G(\omega) = -\frac{\omega}{\alpha} - \left( \frac{1}{\alpha} \right)^2 \left( \frac{1}{Z} \right) \omega^3 + \ldots, \]

where we have used Eq. (26) for self-consistency. In order to calculate \( Z \) we need

\[ \frac{1}{\Sigma(\omega) - \mu} = \frac{\omega}{\alpha} - (1 - 1/Z) \omega^3/\alpha^2 + \ldots \]
\[ \frac{1}{\omega + \mu - \Sigma(\omega) - 3 t^2 G(\omega)} = -\frac{\omega}{\alpha} - (1/Z + 3 t^2/\alpha) \omega^3/\alpha^2 + \ldots \]
\[ \frac{1}{\omega - 5 t^2 G(\omega)} = \frac{\alpha}{(\alpha + 5 t^2)\omega} - 5 \tilde{t}^2 \frac{1/Z + t^2/\alpha}{(\alpha + 5 t^2)^2} \omega + \ldots. \]

Using Eq. (27), Eq. (30) together with Eq. (26) and Eq. (B2) one finds

\[ Z^{(2)} = \frac{[\alpha^{(2)}]^2}{[(\alpha/2)^2 + 3 \tilde{t}^4]} \]
\[ Z^{(3)} = \frac{[\alpha^{(3)}]^2}{[(\alpha/2)^2 + 9 \tilde{t}^4]} \]

For the evaluation of \( Z^{(4)} \) we need

\[ \frac{2 A(\omega) + 3 B(\omega)}{A^2(\omega) - 2 B^2(\omega)} = -2 \frac{\alpha + 5 \tilde{t}^2}{\alpha(U/2)^2} \omega - 10 \frac{t^2}{\alpha^2(U/2)^2} (1/Z + \tilde{t}^2/\alpha) \omega^3 + \ldots. \]

Finally obtain

\[ \frac{\alpha^{(4)}}{Z^{(4)}} \left[ 1 + 8 \tilde{t}^2/U^2 \right] = (U/2)^2 + \tilde{t}^2 \frac{(\alpha^{(4)} + 5 \tilde{t}^2)^2}{(U/2)^4} \left[ 2 + 9 \tilde{t}^2/\alpha^{(4)} \right] + \frac{10 \tilde{t}^2}{(U/2)^2 \alpha^{(4)}}. \]

from which we may obtain \( Z^{(4)} \), with Eq. (A12) for \( \alpha^{(4)} \).

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FIG. 1. (a) The coefficient $\alpha$ and (b) the coefficient $Z$ of the self-energy, $\Sigma(\omega) \sim \alpha/\omega + U/2 + (1 - 1/Z)\omega + \ldots$, in the insulating state at half-filling, as a function of $U$. Shown are the results for $\Sigma^{(2)}(\omega)$ (dotted line), $\Sigma^{(3)}(\omega)$ (dashed line) and $\Sigma^{(4)}(\omega)$ (solid line). For comparison, the corresponding results obtained by exactly diagonalizing the Hubbard star, S(1) and the star of the stars, S(2), are given.

FIG. 2. The density of states, $-Im G^{(2)}(\omega)$ (dotted line), $-Im G^{(3)}(\omega)$ (dashed line) and $-Im G^{(4)}(\omega)$ (solid line) in the metallic state at half-filling for (a) $U = 1$ and (b) $U = 2$.

FIG. 3. The density of states, $-Im G^{(2)}(\omega)$ (dotted line), $-Im G^{(3)}(\omega)$ (dashed line) and $-Im G^{(4)}(\omega)$ (solid line) in the insulating state at half-filling for (a) $U = 3$ and (b) $U = 4$.

FIG. 4. (a) The density of states at the Fermi level in the half-filled metallic state, $-Im G^{(2)}(0)$ (dotted line), $-Im G^{(3)}(0)$ (dashed line) and $-Im G^{(4)}(0)$ (solid line) as a function of $U$ and (b) the self-energy at the Fermi level, $-Im \Sigma^{(2)}(0)$ (dotted line), $-Im \Sigma^{(3)}(0)$ (dashed line) and $-Im \Sigma^{(4)}(0)$ (solid line).