Quasi-particle approach for general lattice Hamiltonians

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In many condensed-matter systems, it is very useful to introduce a quasi-particle approach, which is based on some sort of linearization around a suitable background state. In order to be a systematic and controlled approximation, this linearization should be justified by an expansion into powers of some small control parameter. Here, we present a method for general lattice Hamiltonians with large coordination numbers $Z \gg 1$, which is based on an expansion into powers of $1/Z$. In order to demonstrate the generality of our method, we apply it to various spin systems, as well as the Bose and Fermi Hubbard model.

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I. INTRODUCTION

Apart from a few exceptions (mostly in one spatial dimension), the majority of Hamiltonians describing interactions in condensed matter and other fields is not exactly solvable. Thus, it is often very useful to introduce a suitable quasi-particle approach – i.e., to consider linearized excitations (quasi-particles) around a given background (e.g., the ground state). However, in order to avoid neglecting contributions which are of equal magnitude as the terms one keeps (or even larger), such a linearization should be based on the expansion into powers of some small control parameter.

As an example, Bose-Einstein condensates of dilute atomic gases are often described in terms of a mean-field expansion where the full field operator is split up via

$$\Psi(t, r) = \psi_c(t, r) + \delta \Psi(t, r)$$

(1)

into the condensate wave-function $\psi_c(t, r)$ and the remaining (linearized) quantum or thermal fluctuations $\delta \Psi(t, r)$. The above split can be justified if a large number $N \gg 1$ of atoms share the same wave-function $\psi_c(t, r)$, since it scales with $\sqrt{N}$ in this case.\[1, 2\]

As another example, spin systems are often described using the large-$S$ expansion (spin-wave theory)\[13\]. This approximation can be motivated via the Holstein-Primakoff transformation which maps the spin operators to bosonic creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$

$$\hat{S}_+ = \hat{a}^\dagger \sqrt{2S} - \hat{a} \sqrt{2S} + O(1/\sqrt{S})$$

(2)

$$\hat{S}_- = \hat{S}_+^\dagger$$

and $\hat{S}_z = \hat{S}_+^\dagger \hat{S}_+$. For large spins $S$, the system is then approximated by non-interacting bosons. The reliability of the $1/S$-expansion for $S = 1/2$ systems is another question, see Section IV below.

In the following, we present a general formalism for the introduction of quasi-particles for lattice Hamiltonians which is based on an expansion in powers of $1/Z$, where $Z$ is the coordination number of the lattice. The paper is organized as follows. Section II provides the key elements of the $1/Z$ method. In section III we derive the formalism for quasi-particle excitation. We illustrate the usefulness of these concepts for calculating the excitation spectrum and the phase transition boundaries for various known model descriptions: the Heisenberg model in section IV, the Ising model in section V, the Bose-Hubbard model in section VI and the Fermi-Hubbard in section VII. The last section VIII is devoted to the conclusions.

II. BASIC FORMALISM

We consider a general lattice Hamiltonian

$$\hat{H} = \frac{1}{Z} \sum_{\mu\nu} \hat{H}_{\mu\nu} + \sum_\mu \hat{H}_\mu,$$  

(3)

consisting of on-site terms $\hat{H}_\mu$ and two-site coupling or tunneling terms $\hat{H}_{\mu\nu}$ (with $\hat{H}_{\mu\mu} = 0$) where $\mu$ and $\nu$ label the lattices sites. For simplicity, we assume that the $\hat{H}_\mu$ have all the same form (and similarly the $\hat{H}_{\mu\nu}$), i.e., we have (discrete) translational and rotational invariance of the underlying lattice. Finally, the coordination number $Z$ counts the number of tunneling or interaction neighbors $\mu$ of a given lattice site $\nu$ and we consider the limit $Z \gg 1$. The time-evolution of the density matrix $\hat{\rho}$ of the total lattice is given by the von Neumann equation

$$i\partial_t \hat{\rho} = \left[\hat{H}, \hat{\rho}\right] = \frac{1}{Z} \sum_{\mu\nu} \hat{\mathcal{L}}_{\mu\nu} \hat{\rho} + \sum_\mu \hat{\mathcal{L}}_\mu \hat{\rho},$$  

(4)

with the Liouville super-operators $\hat{\mathcal{L}}_{\mu\nu} \hat{\rho} = [\hat{H}_{\mu\nu}, \hat{\rho}]$ and $\hat{\mathcal{L}}_\mu \hat{\rho} = [\hat{H}_\mu, \hat{\rho}]$. Now we introduce the reduced density matrices $\hat{\rho}_\mu$ (or $\hat{\rho}_{\mu\nu}$) of a given lattice site $\mu$ (or $\mu, \nu$) by tracing over all sites except $\mu$ (or $\mu, \nu$)

$$\hat{\rho}_\mu = \text{Tr}_\nu \{\hat{\rho}\}, \quad \hat{\rho}_{\mu\nu} = \text{Tr}_\mu \{\hat{\rho}\}, \quad \text{etc.}$$  

(5)

Note that $\hat{\rho}_\mu$ is a linear operator acting on the Hilbert space $\mathcal{H}_\mu$ of one lattice site $\mu$ while $\hat{\rho}_{\mu\nu}$ is a linear operator acting on $\mathcal{H}_\mu \otimes \mathcal{H}_\nu$ etc. Now we may split up those matrices into correlated and uncorrelated parts

$$\hat{\rho}_{\mu\nu} = \hat{\rho}_{\mu\nu}^{\text{corr}} + \hat{\rho}_{\mu\nu}^{\text{uncorr}},$$  

(6)
and \( \hat{\rho}_{\mu\lambda} = \rho_{\mu\lambda} + \rho_{\mu\lambda}^{\text{corr}} \rho_{\lambda} + \rho_{\lambda\mu}^{\text{corr}} \rho_{\mu} + \rho_{\mu\rho} \rho_{\rho} \). From Eq. (4), we get the equation of motion for the reduced density matrix \( \hat{\rho}_{\mu} \)

\[
i \partial_t \hat{\rho}_{\mu} = \frac{1}{Z} \sum_{\kappa \neq \mu} \text{Tr}_{\kappa} \left\{ \hat{L}_{\mu\kappa}^{\text{S}} (\hat{\rho}_{\mu\kappa} + \hat{\rho}_{\kappa\mu}) + \hat{\rho}_{\mu\kappa} \right\}.
\]

where \( \hat{L}_{\mu\kappa}^{\text{S}} = \hat{L}_{\mu\kappa} + \hat{L}_{\kappa\mu} \).

The above equation is still exact – but in order to solve it and to obtain \( \hat{\rho}_{\mu} \), we would need the correlations \( \rho_{\mu\kappa}^{\text{corr}} \). Similarly, the equation for the two-point correlations \( \rho_{\mu\nu}^{\text{corr}} \) contains the three-point correlator \( \rho_{\mu\kappa}^{\text{corr}} \) and so on. However, for large coordination numbers \( Z \gg 1 \), one can solve this set of equations approximately and iteratively. If we start in a separable (i.e., uncorrelated) initial state, the correlations satisfy – at least for a finite period of time – the following hierarchy [3, 9]:

\[
\hat{\rho}_{\mu} = \mathcal{O} \left( Z^0 \right), \quad \rho_{\mu\nu}^{\text{corr}} = \mathcal{O} \left( 1/Z \right), \quad \rho_{\mu\kappa}^{\text{cor}} = \mathcal{O} \left( 1/Z^2 \right) \quad (8)
\]

and so on. This allows us to obtain the approximate equation for the on-site density matrix

\[
i \partial_t \hat{\rho}_{\mu} = \frac{1}{Z} \sum_{\kappa \neq \mu} \text{Tr}_{\kappa} \left\{ \hat{L}_{\mu\kappa}^{\text{S}} \hat{\rho}_{\mu\kappa} + \hat{\rho}_{\mu\kappa} \right\} + \mathcal{O}(1/Z) \quad (9)
\]

The zeroth-order solution \( \rho_{\mu}^{0} \) of this equation corresponds to the local (e.g., Gutzwiller) mean-field ansatz. Inserting this solution and performing an analogous procedure for two sites, we get

\[
i \partial_t \rho_{\mu\nu}^{\text{corr}} = \hat{L}_{\mu\nu} \rho_{\mu\nu}^{\text{corr}} + \frac{1}{Z} \sum_{\kappa} \text{Tr}_{\kappa} \left\{ \hat{L}_{\mu\kappa}^{\text{S}} \rho_{\mu\nu}^{\text{corr}} \rho_{\nu\kappa}^{0} + \rho_{\mu\nu}^{\text{corr}} \rho_{\nu\kappa}^{0} \right\} + \mathcal{O}(1/Z^2).
\]

This equation determines the quantum fluctuations around the background solution \( \rho_{\mu}^{0} \) and will be the starting point for our quasi-particle picture.

### III. FACTORIZATION

As it turns out, Eq. (10) can be simplified considerably by effectively factorizing it. To this end, let us introduce the propagator \( \hat{W}_{\mu}^{\nu}(t, t_0) \) from an initial lattice site \( \nu \) at time \( t_0 \) to a final lattice site \( \mu \) at time \( t \) which corresponds to the mapping

\[
\hat{A}_{\nu}(t_0) \to \hat{A}_{\mu}(t) = \sum_{\mu} \text{Tr}_{\mu} \left\{ \hat{W}_{\mu}^{\nu}(t, t_0) \hat{A}_{\nu}(t_0) \right\}.
\]

Here \( \hat{W}_{\mu}^{\nu}(t, t_0) \) is a linear operator acting on \( \mathcal{H}_{\mu} \otimes \mathcal{H}_{\nu} \) where \( \mathcal{H}_{\mu} \) and \( \mathcal{H}_{\nu} \) are two different Hilbert spaces (initial and final lattice sites) even for \( \mu = \nu \).

To achieve consistency for \( t = t_0 \), we impose the initial condition

\[
\langle n_{\alpha}, n_{\mu} | \hat{W}_{\mu}^{\nu}(t, t) | m_{\alpha}, m_{\mu} \rangle = \delta_{\mu}^{\alpha} \delta_{n_{\nu}}^{m_{\nu}} \delta_{m_{\mu}}^{n_{\mu}}, \quad (12)
\]

where the \( | n_{\mu} \rangle \) form a complete basis of \( \mathcal{H}_{\mu} \) and similarly the \( | n_{\alpha} \rangle \) for \( \mathcal{H}_{\alpha} \). If we now postulate the following effective equation of motion for the propagator

\[
i \partial_t \hat{W}_{\mu}^{\nu}(t, t_0) = \hat{L}_{\mu} \hat{W}_{\mu}^{\nu}(t, t_0) + \frac{1}{Z} \sum_{\kappa} \text{Tr}_{\kappa} \left\{ \hat{L}_{\kappa} \hat{W}_{\mu}^{\nu}(t, t_0) + \hat{W}_{\kappa}^{\alpha}(t, t_0) \rho_{\nu}^{0} \right\} + \mathcal{O}(1/Z).
\]

and insert it into the factorization ansatz

\[
\hat{\rho}_{\mu\nu}^{\text{corr}}(t) = \sum_{\alpha\beta} \text{Tr}_{\alpha\beta} \left\{ \hat{W}_{\mu}^{\alpha}(t, t_0) \hat{W}_{\nu}^{\beta}(t, t_0) \rho_{\alpha\beta}^{0} \right\} + \sum_{\nu} \text{Tr}_{\nu} \left\{ \hat{L}_{\nu} \hat{W}_{\nu}^{\alpha}(t, t_0) \rho_{\alpha}^{0} \right\} + i \frac{1}{Z} \sum_{\alpha\beta} \text{Tr}_{\alpha\beta} \left\{ \hat{L}_{\alpha} \hat{W}_{\alpha}^{\beta}(t, t_0) \hat{W}_{\beta}^{\alpha}(t, t_0) + \hat{W}_{\alpha}^{\beta}(t, t_0) \hat{W}_{\beta}^{\alpha}(t, t_0) \right\} + \mathcal{O}(1/Z^2)
\]

which \( Q_{\alpha\beta} \) denotes the sources term in Eq. (10).

\[
\hat{Q}_{\alpha\beta} = i \frac{\rho_{\alpha}^{0}}{Z} \text{Tr}_{\alpha\beta} \left\{ \hat{L}_{\alpha} \rho_{\beta}^{0} + \hat{L}_{\beta} \rho_{\alpha}^{0} \right\} - i \frac{1}{Z} \hat{L}_{\alpha\beta} \rho_{\alpha}^{0} \rho_{\beta}^{0}
\]

we find that we obtain the solution of Eq. (10) to first order in \( 1/Z \). Ergo, instead of solving Eq. (10) directly, we may solve the simpler equation (13) instead and recover the correlations \( \rho_{\mu\nu}^{\text{corr}}(t) \) as a bilinear combination (14). Interestingly, the effective equation (13) for fixed \( \alpha \) (the initial lattice site) is formally equivalent to a direct linearization of the on-site equation (9). To see that, let us set \( \hat{\rho}_{\mu} = \rho_{\mu} + \delta \hat{\rho}_{\mu} \) and linearize around the stationary solution \( \rho_{\mu}^{0} \). The resulting equation

\[
i \partial_t \delta \hat{\rho}_{\mu} = \hat{L}_{\mu} \delta \hat{\rho}_{\mu} + \frac{1}{Z} \sum_{\kappa} \text{Tr}_{\kappa} \left\{ \hat{L}_{\kappa} \delta \hat{\rho}_{\mu} + \delta \hat{\rho}_{\mu} \rho_{\kappa}^{0} \right\}
\]

is formally equivalent to (13). Accordingly, the solution of this equation is given by (11).

\[
\delta \hat{\rho}_{\mu}(t) = \sum_{\nu} \text{Tr}_{\nu} \left\{ \hat{W}_{\nu}^{\mu}(t, t_0) \delta \hat{\rho}_{\nu}(t_0) \right\},
\]

which confirms that \( \hat{W}_{\mu}^{\nu}(t, t_0) \) is the propagator.

### IV. HEISENBERG MODEL

The Heisenberg model is the first basic lattice model to which the \( 1/Z \) approach applies. The Hamiltonian is

\[
\hat{H} = -\frac{J}{Z} \sum_{\mu\nu} T_{\mu\nu} \hat{S}_{\mu} \cdot \hat{S}_{\nu}
\]

Here \( \hat{S}_{\mu} = \left( \hat{S}_{\mu}^{x}, \hat{S}_{\mu}^{y}, \hat{S}_{\mu}^{z} \right) \) are spin operators at the lattice site \( \mu \) satisfying the usual \( SU(2) \) commutation relations

\[
[S_{\mu}^{a}, S_{\nu}^{b}] = i \epsilon_{abc} S_{\nu}^{c}, \quad J \text{ denotes the coupling strength.}
\]

The lattice structure is encoded in the adjacency matrix \( T_{\mu\nu} \) which equals unity if \( \mu \) and \( \nu \) are tunnelling neighbours (i.e., if a particle hops from \( \mu \) to \( \nu \)) and zero otherwise. For simplicity, we restrict ourselves to spin \( S = 1/2 \) systems, but our results can be generalized easily.
A. Ferromagnetic case $J > 0$

The Heisenberg model \([17]\) is invariant under internal (spin) rotations, but its ground state breaks this symmetry spontaneously, i.e., we have a set of degenerate ground states. For positive $J$, any state where all the spins point into the same direction is an exact ground state. For simplicity, let us take the spin-up state:

$$\tilde{\rho}^0_{\mu} = |\uparrow\rangle_{\mu} \langle \uparrow|$$

Introducing the time-propagated spin operator

$$\hat{S}_\nu(t) = \sum_{\mu} T_{\mu\nu} \left\{ \hat{W}^\nu_{\mu}(t, t_0) \hat{S}_\mu(t_0) \right\},$$

according to \([11]\), we obtain the following closed operatorial equation of motion:

$$i\partial_t \hat{S}^\pm_\mu = 0,$$

$$i\partial_t + J) \hat{S}^\pm_\mu = \pm \sum_{\nu} \frac{J_{T\mu\nu}}{Z} \hat{S}^\pm_\nu,$$

where we have used the notation $\hat{S}^\pm_\mu = \hat{S}^x_\mu \pm i\hat{S}^y_\mu$. Assuming (discrete) translational symmetry of our lattice, we may Fourier transform these equations

$$\left(\omega \mp J[1-T_k]\right) \hat{S}^\pm_{k,\omega} = 0,$$

where $T_k$ is the Fourier transform of the adjacency matrix $T_{\mu\nu}$ with the normalization $T_{k=0} = 1$. From the above equation, we may directly read off the spectrum

$$\omega_k = \pm J(1-T_k).$$

As expected, the magnons in the ferromagnetic phase are gapless (Goldstone modes) and their spectrum scales as $\omega_k \sim k^2$ for small $k$. Note that the same spectrum can be derived via the $1/S$-expansion \([13]\) mentioned in the Introduction. However, for $S = 1/2$, the $1/2$-expansion appears better justified than the $1/S$-expansion.

The positive frequency associated to the excitation operator $\hat{S}^+_{k,\omega}$ means that it costs energy to flip one spin up. On the contrary, $\hat{S}^-_{k,\omega}$ has a negative energy which means that adding a spin up to a spin polarized magnet liberates energy. This process is not possible because already all the spin are up. Therefore, such a release of energy is possible provided excitations are created in pair: a creation of positive energy followed by a creation of negative energy so that the net energy is positive. A switch in the sign of $J$ changes the sign of the frequencies and announces the change to the antiferromagnetism phase. In this case, the system becomes instable because energy is released by changing a spin up into a spin down.

B. Anti-ferromagnetic case $J < 0$

For negative $J = -J_A$, the ground state(s) cannot be determined exactly in general. Nevertheless, under certain conditions, we can get a good approximation. In order to avoid problems with frustration, we assume that we have a bi-partite lattice, i.e., that we can divide the lattice into two sublattices $A$ and $B$ such that for each site $\mu \in A$ all the adjacent neighbouring sites $\nu$ belong to $B$ and vice versa. Then, for large $Z$, we may approximate the anti-ferromagnetic ground state by the Néel state \([12]\)

$$\tilde{\rho}^0_{\mu} = \left\{ \begin{array}{l} |\uparrow\rangle_{\mu} \langle \uparrow| \quad \mu \in A, \\ |\uparrow\rangle_{\mu} \langle \downarrow| \quad \mu \in B. \end{array} \right.$$

A similar reasoning as in the ferromagnetic case leads to the following operatorial equations

$$i\partial_t \hat{S}^\pm_\mu = 0,$$

$$(i\partial_t \mp J_A) \hat{S}^\pm_\mu = \mp \sum_{\nu} \frac{J_A T_{\mu\nu}}{Z} \hat{S}^\pm_\nu \quad \text{if} \quad \mu \in A, \quad (25)$$

$$(i\partial_t \pm J_A) \hat{S}^\pm_\mu = \mp \sum_{\nu} \frac{J_A T_{\mu\nu}}{Z} \hat{S}^\pm_\nu \quad \text{if} \quad \mu \in B. \quad (26)$$

After a Fourier transform, we deduce the following spectrum for the magnons in the anti-ferromagnetic case

$$\omega_k = \pm J_A \sqrt{1-T_k^2}.$$  

As expected, the spectrum is still gapless but scales as $\omega_k \sim |k|$ for small $k$. Again, the same spectrum can be derived via the $1/S$-expansion \([13]\).

Also the frequencies go to zero at the antiferromagnetism-ferromagnetism transition. At the difference of ferromagnetism, it costs energy to change the spin up from spin down in sublattice $A$ and the other way around for sublattice $B$. But this process reverses once the frequencies go to zero at the antiferromagnetism-ferromagnetism transition.

V. QUANTUM ISING MODEL

As our second example, let us investigate the quantum Ising model in a transverse field with the Hamiltonian

$$\hat{H} = -\frac{J}{Z} \sum_{\mu\nu} T_{\mu\nu} \hat{S}^z_\mu \hat{S}^z_\nu - B \sum_{\mu} \hat{S}^x_\mu.$$

This model displays a quantum transition from the paramagnetic phase (where the transversal magnetic field $B$ dominates) to the ferromagnetic or anti-ferromagnetic phase, which breaks the $Z_2$ spin-flip symmetry.

To lowest order in $1/Z$, we employ the following variational ansatz for the ground state

$$E_0 = \sum_{\mu} \text{Tr}_\mu \left\{ \hat{H} \tilde{\rho}^0_\mu \right\} + \frac{1}{Z} \sum_{\mu\nu} \text{Tr}_{\mu\nu} \left\{ \hat{H} \tilde{\rho}^0_\mu \tilde{\rho}^0_\nu \right\}$$

where the reduced density matrix is given by a pure state $\tilde{\rho}^0_\mu = |\psi\rangle_\mu \langle \psi|$ with $|\psi\rangle_\mu = c_\uparrow |\uparrow\rangle_\mu + c_\downarrow |\downarrow\rangle_\mu$. The variational ground state energy $E_0$ per site reads

$$E_0 \frac{1}{N} = -\frac{J}{4} (|c_\uparrow|^2 - |c_\downarrow|^2)^2 - \frac{B}{2} (c_\uparrow^* c_\downarrow + c_\downarrow^* c_\uparrow).$$
Minimizing this energy, we find that the ground state always has $\langle \hat{S}_\mu^z \rangle_0 = 0$, i.e., we can choose the amplitudes $c_t$ and $c_j$ to be real. To lowest order in $1/Z$, the critical point is at $J = B$. For $J < B$, the magnetic field controls the orientation of the spin so that the state is paramagnetic with $\langle \hat{S}_\mu^z \rangle = 0$ and $\langle \hat{S}_\mu^z \rangle = 1/2$ (assuming $B > 0$). For $J > B$, on the other hand, the ferromagnetism case is associated to a permanent magnetization with a non-vanishing ferromagnetic order parameter $\langle \hat{S}_\mu^z \rangle = \pm \sqrt{1 - B^2 / J^2}$.

In complete analogy the Heisenberg model, we may derive the effective quasi-particle equations

$$i \partial_t \hat{S}_\mu^+ = \pm B \hat{S}_\mu^z + \frac{2Jt_{\mu\nu}}{Z} \left( \hat{S}_\mu^+ \langle \hat{S}_\nu^- \rangle_0 + \hat{S}_\nu^- \langle \hat{S}_\mu^+ \rangle_0 \right),$$

$$i \partial_t \hat{S}_\mu^- = \frac{B}{2} (\hat{S}_\mu^+ - \hat{S}_\mu^-).$$

This gives the excitation spectrum

$$\omega_k = \pm \sqrt{4J^2 \langle \hat{S}_\nu^- \rangle_0^2 + B^2 - 2BJT_k \langle \hat{S}_\nu^- \rangle_0}. \quad (33)$$

For the paramagnetic phase, this simplifies to

$$\omega_k = \pm \sqrt{B^2 - BJT_k}. \quad (34)$$

At the difference of the Heisenberg models, here transition occurs for $J = B$ when the frequencies becomes imaginary. For comparison, the spectrum in 1D obtained from exact diagonalisation is given by

$$\omega_{1D} = \pm \sqrt{B^2 - BJT_k + J^2 / 4} \quad (35)$$

and is well approximated by the lowest order result Eq.\[34\] for large $B$. In 1D however transition occurs for a zero frequency at $B = J/2$. Let us note here that, although the $1/Z$ expansion is supposed to work very well in the limit of large dimensions, it gives nevertheless qualitatively good results for 1D.

In the ferromagnetic case, the spectrum is

$$\omega = \pm \sqrt{J^2 - B^2 T_k} \quad (36)$$

and corresponds in the limit of weak $B$ to two kink excitation $2\omega_{1D}$ of the exact 1D spectrum Eq.\[35\].

VI. BOSE-HUBBARD MODEL

After discussing two examples for spin systems, let us apply the hierarchy discussed above to the Bose-Hubbard model, see also \[8, 9\]. This model describes (identical) bosons hopping on a lattice with the tunnelling rate $J$. If two (or more) bosons occupy the same lattice site, they repel each other with the interaction energy $U$. Altogether, the Hamiltonian reads

$$\hat{H} = -\frac{J}{Z} \sum_{\mu\nu} T_{\mu\nu} \hat{b}_\mu \hat{b}_\nu + \frac{U}{2} \sum_\mu \hat{n}_\mu (\hat{n}_\mu - 1). \quad (37)$$

Here $\hat{b}_\mu$ and $\hat{b}_\nu$ are creation and annihilation operators at the lattice sites $\mu$ and $\nu$, respectively, satisfying the bosonic commutation relations $[\hat{b}_\mu, \hat{b}_\nu'] = \delta_{\mu\nu'}$ and $[\hat{b}_\mu, \hat{b}_\nu'] = [\hat{b}_\mu, \hat{b}_\nu] = 0$. As before, the lattice structure is encoded in the adjacency matrix $T_{\mu\nu}$ which equals unity if $\mu$ and $\nu$ are tunnelling neighbours (i.e., if a particle can hop from $\mu$ to $\nu$) and zero otherwise. Finally, $\hat{n}_\mu = \hat{b}_\mu^\dagger \hat{b}_\mu$ is the number operator and we assume the Mott phase $\hat{\rho}_\mu^0 = |1\rangle_\mu \langle 1|$ in the following.

In complete analogy to the spin operators in the previous Sections, we may define effective particle and hole operators via $\hat{h}_\mu = |0\rangle_\mu \langle 1|$ and $\hat{p}_\mu = |1\rangle_\mu \langle 0|$. Time-propagating these operators according to \[11\], we deduce the following operatorial equations \[9\]:

$$i \partial_t \hat{h}_\mu = \frac{J}{Z} \sum_{\nu} T_{\mu\nu} \left[ \hat{h}_\nu + \sqrt{2} \hat{p}_\nu \right],$$

$$[i \partial_t - U] \hat{p}_\mu = -\frac{J}{Z} \sum_{\nu} T_{\mu\nu} \left[ 2 \hat{p}_\nu + \sqrt{2} \hat{h}_\nu \right]. \quad (38)$$

Thus, the eigenvalues obtained from this system are

$$\omega_k^\pm = \frac{U - J T_k \pm \sqrt{U^2 - 6 J U T_k + J^2 T_k^2}}{2}. \quad (39)$$

They correspond to the ones obtained in the random phase approximation \[1, 11\]. Inspection of the frequencies shows that they become imaginary for $J/U = 3 - 2\sqrt{2}$ indicating the onset of instability of the Mott state towards a superfluid state.

VII. FERMI-HUBBARD MODEL

As our final example, let us consider the Fermi-Hubbard model, which is somewhat similar to the Bose-Hubbard model, but significantly more complicated. The Hamiltonian has a quite similar form as above

$$\hat{H} = -\frac{J}{Z} \sum_{\mu\nu} T_{\mu\nu} \hat{c}_\mu^\dagger \hat{c}_\nu + U \sum_\mu \hat{n}_\mu^\dagger \hat{n}_\mu, \quad (40)$$

but now the $\hat{c}_\mu^\dagger$ and $\hat{c}_\nu$ are fermionic creation and annihilation operators and we have two different fermion species labeled by their spin $s = \uparrow$ and $s = \downarrow$. Depending on the values of $J$ and $U$ as well as the filling factors $\langle \hat{n}_\mu^\dagger \rangle$ and $\langle \hat{n}_\mu \rangle$, there are various phases which all require a different ansatz for $\hat{\rho}_\mu^0$.

Let us consider the case of large and positive $U$ with small fillings $\langle \hat{n}_\mu^\dagger \rangle \ll 1$ and $\langle \hat{n}_\mu \rangle \ll 1$ and where the temperature $T$ satisfies $U \gg T \gg J$. In this case, double occupancy $\langle \downarrow \downarrow \rangle_\mu = \hat{c}_\mu^\dagger \hat{c}_\mu^\dagger \hat{c}_\mu \hat{c}_\mu$ can be neglected and any possible spin ordering is washed out thermally. We may then use the following ansatz

$$\hat{\rho}_\mu^0 = p_0 |0\rangle_\mu \langle 0| + p_+ |\downarrow \rangle_\mu \langle \downarrow | + p_\uparrow |\uparrow \rangle_\mu \langle \uparrow |, \quad (41)$$

where $p_0 + p_+ + p_\uparrow = 1$ with $\langle \hat{n}_\mu^\dagger \rangle = p_\uparrow$ and $\langle \hat{n}_\mu \rangle = p_\downarrow$. 

This ansatz provides a solution of the lowest (zeroth) order in $1/Z$ and we find that the quasi-particle modes decouple into two branches for the two spin degrees of freedom. Let us analyze the spin-up excitation (the results for the other spin-down branch are analogous). The relevant perturbations part of the density matrix read

$$\delta \hat{\rho}_\mu = u_{\mu,\uparrow} \hat{\rho}^{\dagger}_{\mu,\uparrow} (|0\rangle \langle 0 | + v_{\mu,\uparrow} | \uparrow \downarrow \rangle \langle \uparrow | + v_{\mu,\downarrow} | \downarrow \uparrow \rangle \langle \downarrow |)
= u_{\mu,\uparrow} \hat{h}^\dagger_{\mu,\uparrow} + v_{\mu,\uparrow} \hat{p}^\dagger_{\mu,\uparrow},$$

(42)

where $\hat{h}_{\mu,\uparrow} = \hat{c}_{\mu,\uparrow} (1 - \hat{n}_{\mu,\downarrow})$ and $\hat{p}_{\mu,\uparrow} = \hat{c}_{\mu,\uparrow} \hat{n}_{\mu,\downarrow}$ are effective particle and hole operators respectively. Using this ansatz in Eq. (16) for the Hamiltonian (40), we obtain the following set of equations

$$i \partial_t u_{\mu,\uparrow} = - \frac{J}{Z} \sum_\kappa T_{\mu \kappa} (p_\uparrow + p_\uparrow) (u_{\kappa,\uparrow} + v_{\kappa,\uparrow})$$

$$(i \partial_t - U) v_{\mu,\uparrow} = - \frac{J}{Z} \sum_\kappa T_{\mu \kappa} p_\downarrow (u_{\kappa,\uparrow} + v_{\kappa,\uparrow}).$$

(43)

After a Fourier transform, we obtain the following Hubbard expression for the eigen-frequencies

$$\omega_k^\uparrow = \frac{U - JT_k}{2} \pm \frac{1}{2} \sqrt{(U + JT_k)^2 - 4UJT_k p_\downarrow}.$$  

(44)

VIII. CONCLUSIONS

Via a controlled expansion into inverse powers of the coordination number $1/Z$ leading to a hierarchy of correlations, we establish a simple and elegant way to obtain quasi-particle operators and spectra. We demonstrated the general applicability of this method by means of several examples such as spin systems, the Bose and Fermi-Hubbard model. Even though some of the results can also be obtained by other means – such as the $1/S$-expansion – the $1/Z$-expansion developed here is in several cases (such as for $S = 1/2$) better justified than the $1/S$-expansion, for example.

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