A primer to the Hubbard model

Flavio S. Nogueira*

Institut für Theoretische Physik, Freie Universität Berlin,

Arnimallee 14, D-14195 Berlin, Germany

(Dated: Received March 26, 2010)

PACS numbers:

*Electronic address: nogueira@physik.fu-berlin.de

I. THE HUBBARD MODEL

The simplest electronic model of a Mott insulator is provided by the so called Hubbard model:

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} f^{\dagger}_{i\sigma} f_{j\sigma} - \mu \sum_{i,\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $f_{i\sigma}$ is a fermion in the lattice, $n_{i\sigma} \equiv f^{\dagger}_{i\sigma} f_{i\sigma}$, and $\sigma = \uparrow, \downarrow$. In the above Hamiltonian $t, U > 0$, and μ is the chemical potential. In the kinetic term the lattice sum runs only nearest neighbors only. The Hubbard Hamiltonian is exactly solvable in the limits $U = 0$ and $t = 0$. The non-interacting limit corresponds to band theory in the tight-binding approximation, while the $t = 0$ limit corresponds to the atomic limit. Although in the atomic limit the theory is interacting, it is easily diagonalizable, since

$$H_{t=0} = \sum_{i} h_i, \tag{2}$$

where

$$h_i = -\mu \sum_{\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \tag{3}$$

Thus,

$$[h_i, n_{i\alpha}] = 0, \tag{4}$$

and therefore the eigenstates of $n_{i\alpha}$ are also eigenstates of h_i. In this case we can simply omit the lattice sites of any calculation, since the sites are decoupled. The eigenstates of the h are $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$, corresponding to empty, singly occupied (with either up or down spins), and doubly occupied sites, respectively. The corresponding eigenenergies are $\varepsilon_0 = 0$, $\varepsilon_\uparrow = \varepsilon_\downarrow = -\mu$, and $\varepsilon_2 = U - 2\mu$.

Let us consider the example of a half-filled band, i.e., the total number of fermions in the system equals the number of lattice sites L. In this case it can be shown that for a bipartite lattice[10] $\mu = U/2$ *exactly*. This result is straightforwardly checked in the atomic limit. To see that this result is also valid when $t \neq 0$, we just perform a particle-hole transformation $f_{i\sigma} \rightarrow e^{i\mathbf{Q}\cdot\mathbf{R}_i} f^{\dagger}_{i\sigma}$, $f^{\dagger}_{i\sigma} \rightarrow e^{i\mathbf{Q}\cdot\mathbf{R}_i} f_{i\sigma}$, where $\mathbf{Q} = (\pi, ..., \pi)$. When $\mu = U/2$ the Hamiltonian is

invariant under this particle-hole transformation. This implies that the particle density is unity and this corresponds to half-filling.

At half-filling the Hubbard Hamiltonian can be rewritten as

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} f^{\dagger}_{i\sigma} f_{j\sigma} - \frac{2U}{3} \sum_{i} \mathbf{S}_i^2, \tag{5}$$

where

$$\mathbf{S}_i = \frac{1}{2} \sum_{\alpha,\beta} f^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} f_{i\beta}, \tag{6}$$

with $\boldsymbol{\sigma} \equiv (\sigma_1, \sigma_2, \sigma_3)$, σ_i being the Pauli matrices. For $U \gg t$ doubly occupied sites are strongly suppressed and second-order perturbation theory yields the effective Hamiltonian

$$H = \frac{4t^2}{U} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{7}$$

subjected to the local constraint

$$\sum_{\sigma} n_{i\sigma} = 1. \tag{8}$$

Note the subtlety here. The half-filling condition demands that the particle density

$$n = \frac{1}{L} \sum_{i,\sigma} \langle n_{i\sigma} \rangle = 1, \tag{9}$$

which is easily enforced when $\mu = U/2$. This is a global constraint, that simply demands the average site occupation be the unity. However, when $U \gg t$ the average constraint becomes a local one given by the operator equation (8), i.e., double occupation is strictly forbidden.

The effective Hamiltonian (7) is the one of a Heisenberg antiferromagnet. It is rotational invariant in spin space, i.e., it has an $SU(2)$ symmetry. This means that the total spin operator

$$\mathbf{S} = \sum_{i} \mathbf{S}_i, \tag{10}$$

commutes with the Hamiltonian. However, the ground state of the Heisenberg Hamiltonian breaks this symmetry. The most favorable state at zero temperature corresponds to alternating spins in the lattice. This state is pictorially shown for a square lattice in Fig. 2.1.

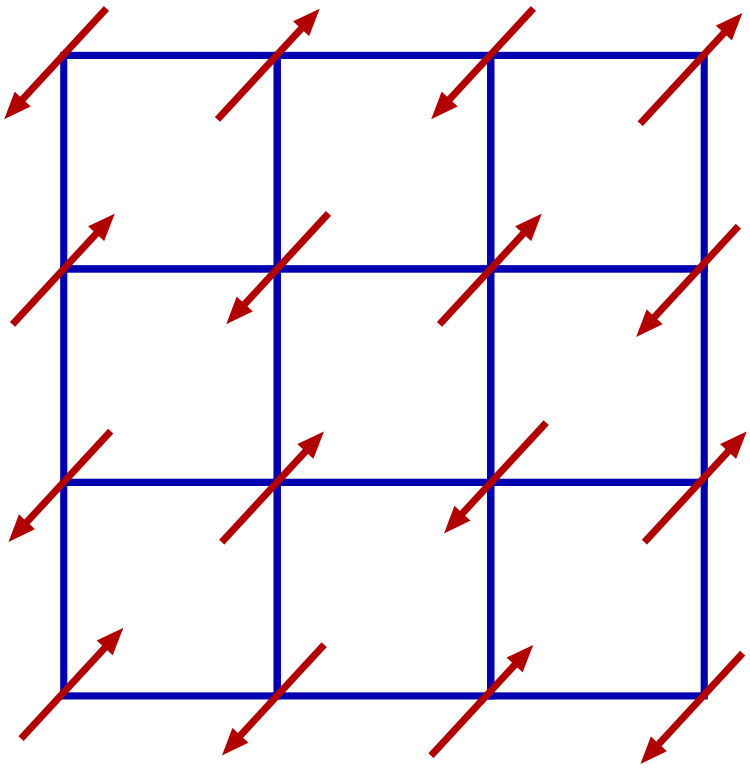

FIG. 1: Mean-field ground state for a Heisenberg antiferromagnet, the so called Néel state.

The antiferromagnetic state shown in the figure is actually a mean-field state for the Heisenberg model, the so called Néel state. This state is also a mean-field state of the Hubbard model at half-filling. Incidentally, the total spin operator (10) obviously commutes with the Hubbard Hamiltonian, showing that the Hubbard model is $SU(2)$ symmetric, as expected physically.

Let us perform the mean-field theory for the Hubbard model in a d-dimensional cubic lattice explicitly. In orderr to do this, we introduce an auxiliary field via a Hubbard-Stratonovich transformation:

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} f^{\dagger}_{i\sigma} f_{j\sigma} - U \sum_{i} \mathbf{m}_i \cdot \mathbf{S}_i + \frac{3U}{8} \sum_{i} \mathbf{m}_i^2. \tag{11}$$

We are looking for a mean-field state with a staggered magnetic moment

$$\mathbf{m}_i = e^{i\mathbf{Q}\cdot\mathbf{R}_i} \mathbf{m}, \tag{12}$$

where the vector $\mathbf{m}$ is uniform. Rotational invariance allows us to fix a direction for $\mathbf{m}$. We

will choose the quantization axis to be along the z-direction. Thus, $\mathbf{m} = m\mathbf{e}_z$. Let us define

$$f_{i\sigma} = \begin{cases} c_{i\sigma}, & i \in A \\ \bar{c}_{i\sigma}, & i \in B \end{cases} \tag{13}$$

The mean-field Hamiltonian can be written as

$$H_{\mathrm{MF}} = \sum_{\mathbf{k},\sigma} \psi^{\dagger}_{\mathbf{k}\sigma} M_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma} + \frac{3UL}{8} m^2, \tag{14}$$

where

$$\psi_{\mathbf{k}\sigma} = \begin{bmatrix} c_{\mathbf{k}\sigma} \\ \bar{c}_{\mathbf{k}\sigma} \end{bmatrix}, \qquad \psi^{\dagger}_{\mathbf{k}\sigma} = \begin{bmatrix} c^{\dagger}_{\mathbf{k}\sigma} & \bar{c}^{\dagger}_{\mathbf{k}\sigma} \end{bmatrix}, \tag{15}$$

and

$$M_{\mathbf{k}\sigma} = \begin{bmatrix} -\frac{\sigma U m}{2} & \varepsilon_{\mathbf{k}} \\ \varepsilon_{\mathbf{k}} & \frac{\sigma U m}{2} \end{bmatrix}, \tag{16}$$

with the tight-binding dispersion

$$\varepsilon_{\mathbf{k}} = -2t \sum_{a=1}^{d} \cos k_a. \tag{17}$$

The mean-field Hamiltonian is easily diagonalized and leads to the energy spectrum

$$E^{\pm}_{\mathbf{k}} = \pm \sqrt{\varepsilon^2_{\mathbf{k}} + \frac{U^2 m^2}{4}}, \tag{18}$$

and we see that the electronic spectrum is gapped. Thus, the mean-field ground state energy per site is

$$E_0 = -\frac{2}{L} \sum_{\mathbf{k}}{}' E^{+}_{\mathbf{k}} + \frac{3U}{8} m^2, \tag{19}$$

where the prime on the sum over $\mathbf{k}$ is to denote that we are summing over the upper half of the Brillouin zone. Let us specialize to two dimensions. By minimizing the above equation with respect to m, we obtain the gap equation,

$$\frac{3}{2U} = \int_0^{\pi} \frac{dk_x}{2\pi} \int_0^{\pi} \frac{dk_y}{2\pi} \frac{1}{E^{+}_{\mathbf{k}}}. \tag{20}$$

In two dimensions it is not a too bad approximation, at least for more qualitative purposes, to use a square density of states to evaluate the above momentum integral,

$$\rho(\varepsilon) = \frac{1}{W}\theta\left(\frac{W}{2} - |\varepsilon|\right), \tag{21}$$

where $W = 4t$ is the bandwidth and $\theta(x)$ is the Heaviside function. This yields the magnetization,

$$m = \frac{2W}{U}\frac{e^{-\frac{3W}{2U}}}{1 - e^{-\frac{3W}{U}}}. \tag{22}$$

II. THE BOSE-HUBBARD MODEL

The Hamiltonian of the so called Bose-Hubbard model [1] is given by

$$\hat{H} = -J\sum_{\langle i,j\rangle}\hat{b}_i^\dagger\hat{b}_j - \mu\sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1), \tag{23}$$

where $U, J > 0$, $\hat{n}_i \equiv \hat{b}_i^\dagger\hat{b}_i$ and μ is the chemical potential. The summations are over the sites of a cubic lattice and the symbol $\langle i, j\rangle$ means a sum over nearest neighbors. The operators b_i obey the usual bosonic commutation relations, i.e., $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$ and $[\hat{b}_i, \hat{b}_j] = [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0$.

The aim of this tutorial is to provide an introduction to the theory of the Bose-Hubbard model, which in the last years gained considerable experimental relevance in the context of Bose-Einstein condensation (BEC) [2].

What kind of phases we expect for the above model? Firstly, let us note that the Hamiltonian (23) is simply a lattice version of the interacting Bose gas Hamiltonian. Indeed, the hopping term is just a lattice derivative. Thus, for small enough U we expect to obtain a superfluid featuring the well known Bogoliubov spectrum. To see this, just write

$$\hat{b}_i = b_0 + \delta\hat{b}_i, \qquad \hat{b}_i^\dagger = b_0^* + \delta\hat{b}_i^\dagger, \tag{24}$$

where b_0 represents the condensate and minimize the Hamiltonian, and $\delta\hat{b}_i$ are small fluctuations around the condensate. By keeping just the quadratic fluctuations, it is easy to see that the Hamiltonian can be approximately written as $\hat{H} = LE_0 + \delta\hat{H}$ (L is the number of lattice sites), with

$$E_0 = -\left(2dJ + \mu + \frac{U}{2}\right)n_0 + \frac{U}{2}n_0^2, \tag{25}$$

$$\delta\hat{H} = \frac{1}{2}\sum_{\mathbf{k}\neq 0} \hat{\Psi}^{\dagger}_{\mathbf{k}} \hat{\mathbf{M}}_{\mathbf{k}} \hat{\Psi}_{\mathbf{k}}, \tag{26}$$

where we have performed a Fourier transformation in the lattice and

$$\hat{\Psi}^{\dagger}_{\mathbf{k}} = \left[\begin{array}{cc} \delta\hat{b}^{\dagger}_{\mathbf{k}} & \delta\hat{b}_{-\mathbf{k}} \end{array} \right], \qquad \hat{\Psi}_{\mathbf{k}} = \left[\begin{array}{c} \delta\hat{b}_{\mathbf{k}} \\ \delta\hat{b}^{\dagger}_{-\mathbf{k}} \end{array} \right], \tag{27}$$

$$\hat{\mathbf{M}}_{\mathbf{k}} = \left[\begin{array}{cc} \varepsilon_{\mathbf{k}} - \mu - U/2 + 2Un_0 & Ub_0 \\ U(b_0^*)^2 & \varepsilon_{\mathbf{k}} - \mu - U/2 + 2Un_0 \end{array} \right], \tag{28}$$

with $\varepsilon_{\mathbf{k}} = -2J\sum_{a=1}^{d}\cos k_a$ and $n_0 \equiv |b_0|^2$. Due to the minimization condition we have

$$\mu = -2dJ - \frac{U}{2} + Un_0. \tag{29}$$

The above result follows easily by demanding that the linear terms in both $\delta\hat{b}_i$ and $\delta\hat{b}^{\dagger}_i$ vanish. Alternatively it may be derived by simply minimizing E_0 with respect to n_0. The energy spectrum can be obtained by simply solving the Heisenberg equations of motion. To this end we need the equations

$$i\partial_t \delta\hat{b}_{\mathbf{k}} = [\delta\hat{b}_{\mathbf{k}}, \delta\hat{H}], \qquad i\partial_t \delta\hat{b}^{\dagger}_{-\mathbf{k}} = [\delta\hat{b}^{\dagger}_{-\mathbf{k}}, \delta\hat{H}]. \tag{30}$$

After straightforward evaluation of the commutators, we can rewrite the two equations above as a single matrix equation:

$$i\hat{\sigma}_3 \partial_t \hat{\Psi}_{\mathbf{k}} = \frac{1}{2}\hat{\mathbf{M}}_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}, \tag{31}$$

where $\hat{\sigma}_3$ is the third Pauli matrix. The Ansatz

$$\hat{\Psi}_{\mathbf{k}}(t) = e^{-iE_{\mathbf{k}}t/2}\hat{\Psi}_{\mathbf{k}}(0) \tag{32}$$

solves Eq. (31) provided $\det(E_{\mathbf{k}}\hat{\sigma}_3 - \hat{\mathbf{M}}_{\mathbf{k}}) = 0$, or

$$E_{\mathbf{k}} = \pm\sqrt{(\varepsilon_{\mathbf{k}} - \mu - U/2 + 2Un_0)^2 - U^2 n_0^2}. \tag{33}$$

Note that due to the form of the chemical potential (29), the above spectrum is gapless, i.e., $E_{\mathbf{k}=0} = 0$, as required by superfluidity.

The above results are valid for U small, i.e., $U \ll J$. So, what happens now in the opposite limit, when $U \gg J$? This is a subtle question. In the continuum limit *exact* arguments [3, 4] involving the Ward identities show that at zero temperature the superfluid

density is identical to the particle density, and this for *for all* values of U. This means that at zero temperature the whole system is in a superfluid state, although not every particle is condensed, since the condensate is depleted due to interaction effects. Does this exact result also holds in the lattice? The answer is: it depends on whether the particle density $\langle\hat{n}\rangle$ is integer or not! For noninteger particle density, approaching the strong coupling limit from the weak coupling one by varying J/U essentially does not change the superfluid characteristics of the system. Thus, in this situation the system is still a superfluid for $U \gg J$. However, for $\langle\hat{n}\rangle = \nu_0 \in \mathbb{N}$ the situation is different. In this case the bosons will localize for large enough U and the system will become an insulator, whose ground state has ν_0 particles per site. In order to better understand how it actually works, let us consider the eigenstates of the number operator (we omit the site index for simplicity)

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{b}^\dagger)^n|0\rangle, \tag{34}$$

and the coherent state

$$\begin{aligned} |z\rangle &= e^{-|z|^2/2}\exp(z\hat{b}^\dagger)|0\rangle \\ &= e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle. \end{aligned} \tag{35}$$

Recall that for a coherent state $\hat{b}|z\rangle = z|z\rangle$. Let us consider for simplicity a two-site problem. For this case let us assume that the system is in the coherent state

$$|\Phi\rangle = \frac{1}{\sqrt{2}}(|z_1\rangle \otimes |z_2\rangle + |z_2\rangle \otimes |z_1\rangle). \tag{36}$$

The expectation value of the Hamiltonian in this state is the energy

$$E(z_1, z_2) \equiv \langle\Phi|\hat{H}|\Phi\rangle = -2J(z_1^* z_2 + z_2^* z_1) + \sum_{i=1,2}\left[-\mu|z_i|^2 + \frac{U}{2}|z_i|^2(|z_i|^2 - 1)\right]. \tag{37}$$

In terms of $z_i = \sqrt{\bar{n}_i}e^{i\varphi_i}$, where $\bar{n}_i$ is the mean particle number at the site i, Eq. (37) becomes

$$E_{\bar{n}_1,\bar{n}_2}(\varphi_1, \varphi_2) = -4J\sqrt{\bar{n}_1\bar{n}_2}\cos(\varphi_1 - \varphi_2) + \sum_{i=1,2}\left[-\mu\bar{n}_i + \frac{U}{2}\bar{n}_i(\bar{n}_i - 1)\right]. \tag{38}$$

The above energy is similar to the classical Hamiltonian of a Josephson junction [6]. In order to explore this similarity further, we rewrite Eq. (38) as

$$E(\Delta\bar{n}, \Delta\varphi) = -2J\sqrt{N^2 - (\Delta\bar{n})^2}\cos\Delta\varphi + \frac{U}{4}(\Delta\bar{n})^2 + E_N, \tag{39}$$

where $N = \bar{n}_1 + \bar{n}_2$ is the total number of particles of the system, $\Delta\bar{n} \equiv \bar{n}_1 - \bar{n}_2$, $\Delta\varphi \equiv \varphi_1 - \varphi_2$, and

$$E_N = -\left(\mu + \frac{U}{2}\right) N + \frac{U}{4} N^2. \tag{40}$$

The energy (39) corresponds precisely to the Hamiltonian describing a two-level Bose-Einstein condensate via a Josephson junction as discussed by Leggett [7]. In this case the variable $\Delta\bar{n}$ plays the role of the momentum conjugated to $\Delta\varphi$. Therefore, the Josephson current is given by

$$\partial_t \Delta\bar{n} = -2J\sqrt{N^2 - (\Delta\bar{n})^2}\sin\Delta\varphi. \tag{41}$$

The so called Josephson "phase-voltage" relation is here generalized to

$$\partial_t \Delta\varphi = \frac{U}{2}\Delta\bar{n} + \frac{2J\Delta\bar{n}}{\sqrt{N^2 - (\Delta\bar{n})^2}}\cos\Delta\varphi. \tag{42}$$

Recall that in the case of superconductors we have $\partial_t \Delta\varphi = 2eV/\hbar$, where the voltage V the same as the difference of chemical potential across the junction. In the above equation the role of $2eV/\hbar$ is played by $U\Delta\bar{n}/2$. The second term is absent in the Josephson relation. This term appears in the context of Josephson junctions in Bose-Einstein condensates [5].

The Josephson effect implies superfluidity. Semiclassically, since $\Delta\bar{n}$ and $\Delta\varphi$ are canonically conjugated, we have the uncertainty relation [6]

$$\Delta\bar{n}\Delta\varphi \sim 1. \tag{43}$$

If $U \gg J$, the second term in Eq. (39) will constraint $\bar{n}_1 \approx \bar{n}_2$ and a commensurate situation $\bar{n}_1 = \bar{n}_2 = n = 1, 2, 3, \ldots$ will be favored. It is then clear that the current will be zero and we have an insulator.

Now we will solve the full model approximately using a Green function method. The aim is to compute the Green function

$$G_{ij}(t) = -i\langle T[\hat{b}_i(t)\hat{b}_j^\dagger(0)]\rangle, \tag{44}$$

where $T[\hat{b}_i(t_1)\hat{b}_j^\dagger(t_2)] = \theta(t_1 - t_2)\hat{b}_i(t_1)\hat{b}_j^\dagger(t_2) + \theta(t_2 - t_1)\hat{b}_j^\dagger(t_2)\hat{b}_i(t_1)$ and $\theta(t)$ is the Heaviside function. The Green function can be calculated exactly in both limit cases $J = 0$ and $U = 0$. We will consider a solution that corresponds to a perturbation expansion in J/U, i.e., around the limit case $J = 0$. Thus, we have to compute the exact Green function in this limit in order to proceed.

The $J = 0$ limit is actually a single-site system, since the Hamiltonian can be written as a sum of single-site Hamiltonians:

$$\hat{H}_{J=0} = \sum_i \hat{h}_i, \tag{45}$$

where

$$\hat{h}_i = -\mu \hat{n}_i + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1). \tag{46}$$

In this case it is enough to compute the Green function for the single-site Hamiltonian $\hat{h}_i$ and the site index can even be omitted. Since $[\hat{h}, \hat{n}] = 0$, the eigenstates $|n\rangle$ of $\hat{n}$ are the exact eigenstates of $\hat{h}$ with eigenvalues

$$E_n = -\mu n + \frac{U}{2} n(n-1). \tag{47}$$

We want to compute

$$\begin{aligned} \mathcal{G}(t) &= -i\langle T[\hat{b}(t)\hat{b}^\dagger(0)]\rangle \\ &= -i[\theta(t)\langle \hat{b}(t)\hat{b}^\dagger(0)\rangle + \theta(-t)\langle \hat{b}^\dagger(0)\hat{b}(t)\rangle]. \end{aligned} \tag{48}$$

Let us assume a ground state with $n \in \mathbb{N}$ particles per site. Then we have

$$\begin{aligned} \langle \hat{b}(t)\hat{b}^\dagger(0)\rangle &= \langle n|\hat{b}(t)\hat{b}^\dagger(0)|n\rangle \\ &= \sqrt{n+1}\langle n|e^{i\hat{h}t}\hat{b}(0)e^{-i\hat{h}t}|n+1\rangle \\ &= (n+1)e^{i(E_n - E_{n+1})t} \end{aligned} \tag{49}$$

Similarly we find

$$\langle \hat{b}(0)^\dagger \hat{b}(t)\rangle = n e^{i(E_{n-1} - E_n)t}. \tag{50}$$

Therefore,

$$\mathcal{G}(t) = -i[\theta(t)(n+1)e^{i(E_n - E_{n+1})t} + \theta(-t) n e^{i(E_{n-1} - E_n)t}], \tag{51}$$

such that the Fourier transformation

$$\mathcal{G}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \mathcal{G}(t) \tag{52}$$

reads

$$\begin{aligned} \mathcal{G}(\omega) &= \frac{n+1}{\omega + E_n - E_{n+1} + i\delta} - \frac{n}{\omega + E_{n-1} - E_n - i\delta} \\ &= \frac{n+1}{\omega + \mu - Un + i\delta} - \frac{n}{\omega + \mu - U(n-1) - i\delta}, \end{aligned} \tag{53}$$

where $\delta \to 0^+$. Note that in order to perform the Fourier transformation of (51) a convergence factor $e^{-\delta t}$ was used for the first term, while for the second term a convergence factor $e^{\delta t}$ was needed.

The approximation we are going to employ is equivalent to a well known mean-field theory approach to solve the Bose-Hubbard model [8]. Instead performing a mean-field theory in the Hamiltonian, we will compute the Green function approximately using an expansion on the hopping. Thus, the unperturbed Green function will be given by Eq. (53). In order to better motivate the method of solution, let us show how it can be used to solve the exactly solvable limit $U = 0$. For this particular case the Hamiltonian is easily diagonalized by a Fourier transformation:

$$\hat{H}_{U=0} = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu)\hat{n}_{\mathbf{k}}, \tag{54}$$

where $\hat{n}_{\mathbf{k}} = \hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}}$. The exact Green function is obviously given by

$$G(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} + i\delta}. \tag{55}$$

Let us derive the above Green function in a less direct way, namely, via the hopping expansion. It will be a more or less complicate way to derive a straightforward result, but it will serve the purpose of illustrating the strategy to solve the Bose-Hubbard model approximately.

The $U = 0$ Hamiltonian can be decomposed in the following way:

$$\hat{H}_{U=0} = \hat{H}_0 + \hat{H}_1, \tag{56}$$

where

$$\hat{H}_0 = -\mu \sum_i \hat{n}_i, \tag{57}$$

is the unperturbed Hamiltonian, and

$$\hat{H}_1 = -J \sum_{\langle i,j \rangle} \hat{b}^\dagger_i \hat{b}_j, \tag{58}$$

is the perturbation. The unperturbed Green function is given by

$$\mathcal{G}_0(\omega) = \frac{1}{\omega + \mu + i\delta}. \tag{59}$$

The exact Green function can be obtained by performing the infinite sum of diagrams shown in Fig. 2.2. The continuum line represents the local Green function (59) at a lattice site i,

while the dashed line represents a hopping process between two neighboring sites. The exact Green function gives the response of the system to a boson propagating from a site i at some time t to another site j at an earlier time t'. The diagrams of the figure illustrate all the possible processes for a quadratic Hamiltonian. In this case only tree diagrams contribute are nonzero, since $U = 0$. The perturbation expansion reads simply

$$G_{ij}(\omega) = \mathcal{G}_0(\omega)\delta_{ij} + \mathcal{G}_0(\omega)J_{ij}\mathcal{G}_0(\omega) + \mathcal{G}_0(\omega)\sum_l J_{il}\mathcal{G}_0(\omega)J_{lj}\mathcal{G}_0(\omega) + \ldots, \tag{60}$$

where $J_{ij} = -J$ if (i, j) are nearest neighbors and zero otherwise. This has the structure of a geometric series and can be rewritten as

$$\begin{aligned} G_{ij}(\omega) &= \mathcal{G}_0(\omega)\delta_{ij} + \mathcal{G}_0(\omega)\sum_l J_{il}\left[\delta_{lj}\mathcal{G}_0(\omega) + \mathcal{G}_0(\omega)J_{lj}\mathcal{G}_0(\omega) + \ldots\right] \\ &= \mathcal{G}_0(\omega)\delta_{ij} + \mathcal{G}_0(\omega)\sum_l J_{il}G_{lj}(\omega). \end{aligned} \tag{61}$$

The Fourier representations

$$J_{ij} = \frac{1}{L}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}\varepsilon_{\mathbf{k}}, \tag{62}$$

$$G_{ij}(\omega) = \frac{1}{L}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}G(\mathbf{k}, \omega), \tag{63}$$

$$\delta_{ij} = \frac{1}{L}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}, \tag{64}$$

allow us to rewrite Eq. (61) in the simpler form:

$$G(\mathbf{k}, \omega) = \mathcal{G}_0(\omega) + \mathcal{G}_0(\omega)\varepsilon_{\mathbf{k}}G(\mathbf{k}, \omega), \tag{65}$$

which can easily be solved to obtain once more the exact Green function for $U = 0$:

$$\begin{aligned} G(\mathbf{k}, \omega) &= \frac{1}{\mathcal{G}_0^{-1}(\omega) - \varepsilon_{\mathbf{k}}} \\ &= \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} + i\delta}. \end{aligned} \tag{66}$$

Unfortunately, when $U \neq 0$ the series of diagrams given in Fig. 2.2 do not lead to the exact Green function, since *loop* diagrams containing higher order local Green functions (higher order cumulants) are missing. The latter vanish when $U = 0$. Nevertheless, the diagrams of Fig. 2.2 still give a good approximation, especially in three dimensions. Thus,

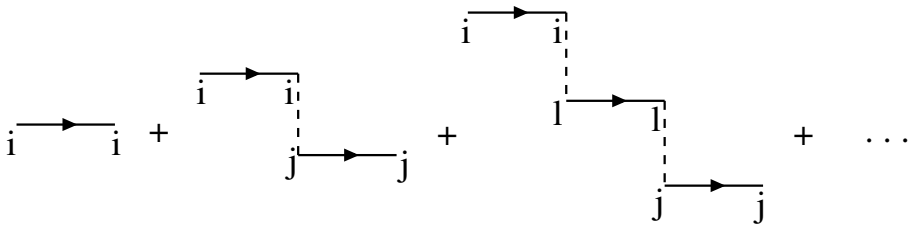

FIG. 2: Hopping expansion for the Green function.

we can approximate the Green function for the Bose-Hubbard model using Eq. (61) with $\mathcal{G}_0(\omega)$ replaced by $\mathcal{G}(\omega)$ given in Eq. (53), i.e.,

$$G(\mathbf{k},\omega) = \frac{1}{\mathcal{G}^{-1}(\omega) - \varepsilon_{\mathbf{k}}}. \tag{67}$$

The energy spectrum is given by the poles of the above Green function:

$$E_{\pm}(\mathbf{k}) = -\mu + \frac{1}{2}[\varepsilon_{\mathbf{k}} + (2n-1)U] \pm \frac{1}{2}\sqrt{\varepsilon_{\mathbf{k}}^2 + 2(2n+1)U\varepsilon_{\mathbf{k}} + U^2}. \tag{68}$$

For large enough U there is an energy gap Δ between the $+$ and $-$ branches of the spectrum, which is given by

$$\begin{aligned} \Delta &= E_+(0) - E_-(0) \\ &= \sqrt{(2dJ)^2 - 4d(2n+1)UJ + U^2}. \end{aligned} \tag{69}$$

The presence of the energy gap indicates that the system is an insulator. As U gets smaller, it will eventually attains a critical value U_c below which the system becomes a superfluid. This critical value of U is found by demanding that the gap vanishes for $U = U_c$. The condition $\Delta = 0$ yields

$$U_c^{\pm} = 2dJ\left[2n + 1 \pm 2\sqrt{n(n+1)}\right]. \tag{70}$$

Note that both solutions are positive. In order to know what is the right one we have to plot the phase diagram and study it more carefully. The transition from the insulating phase to the superfluid phase occurs when the bosons condense. This happens when the Green function is singular for $\omega = 0$ and $\mathbf{k} = 0$, since the bosons condense at $\mathbf{k} = 0$. Thus, the phase diagram is given by the equation

$$\mathcal{G}(0) = \frac{1}{\varepsilon_{\mathbf{k}=0}}, \tag{71}$$

or

$$\frac{n}{\mu/U + 1 - n} - \frac{n+1}{\mu/U - n} = \frac{U}{2dJ}. \tag{72}$$

In Fig. 2.3 we plot the phase diagram for $d = 3$ and $n = 1, 2, 3, 4$. It features the so called Mott lobes [1]. The phase inside the Mott lobes is an insulating one. Outside them we have a superfluid phase. Each Mott lobe corresponds to a Mott-insulating phase with n paricles per site. Thus, the largest lobe, corresponding to $0 \leq \mu/U \leq 1$ has $n = 1$. The next one, in the interval $1 \leq \mu/U \leq 2$ has $n = 2$, and so on. The tips of the lobes correspond to the points where the upper and lower bands of the spectrum meet for $\mathbf{k} = 0$, thus closing the gap. The coordinates of the tips can be easily obtained by extremizing Eq. (72) with respect to μ/U. The tip of a Mott lobe corresponds to the maximum value of J/U for a given value of n. Extremization gives the results:

$$\left(\frac{\mu}{U}\right)_c = \sqrt{n(n+1)} - 1, \tag{73}$$

$$U_c = 2dJ\left[2n + 1 + 2\sqrt{n(n+1)}\right], \tag{74}$$

and we see that U_c corresponds to the solution U_c^+ of the equation $\Delta = 0$.

Let us compare the above results with recent highly precise Monte Carlo (MC) simulations for the $n = 1$ case [9]. There it is obtained that $J/U_c \approx 0.03408$. On the other hand, our formula (74) for $d = 3$ and $n = 1$ gives

$$\frac{J}{U_c} = \frac{1}{6(3 + 2\sqrt{2})} \approx 0.0286. \tag{75}$$

Near the tip of the Mott lobe, which corresponds to the quantum critical regime, our approximation is very bad. This is to be expected, since our approach is equivalent to mean-field theory. In Fig. 2.4 we compare our result for $n = 1$ with the MC phase diagram of Ref. [9]. Indeed, the MC points agree with the mean-field curve only far away of the critical point, i.e., for small J/U.

Acknowledgments

I would like to thank Hagen Kleinert for many interesting discussions. Special thanks to Barbara Capogrosso-Sansone and Nikolay V. Prokof'ev for sending me the Monte Carlo data of the phase diagram in their paper, Ref. [9].

---

[1] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).

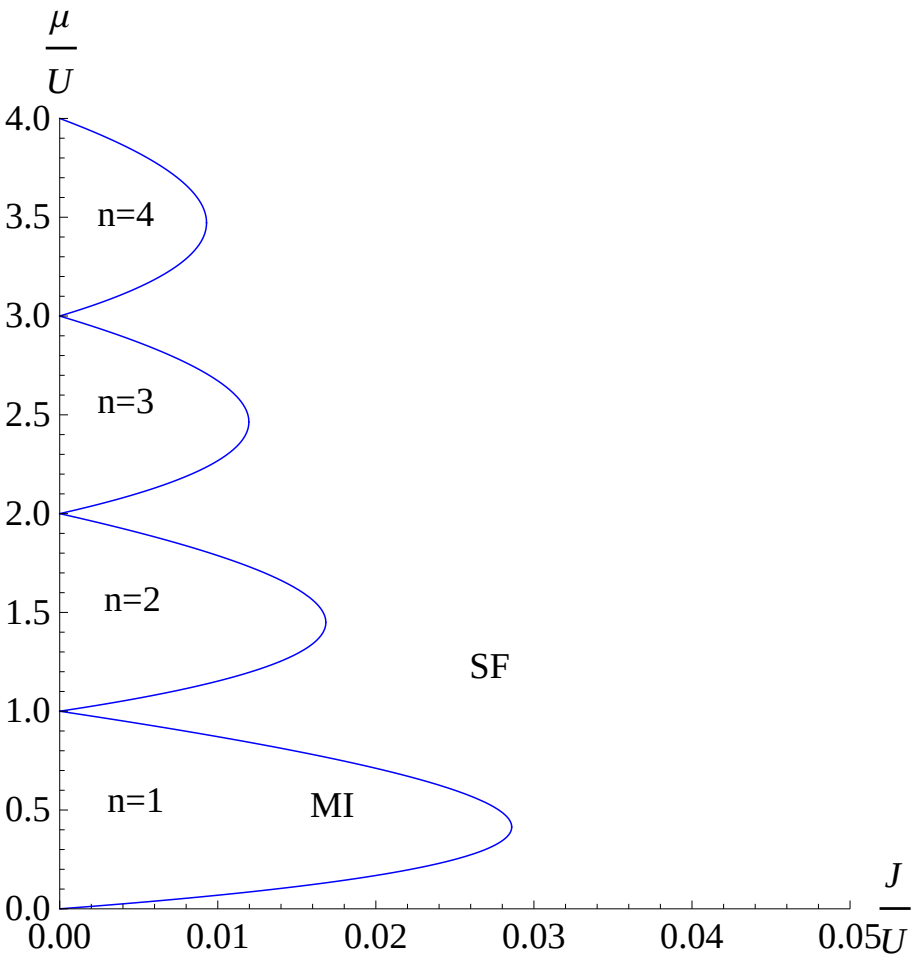

FIG. 3: Phase diagram of the Bose-Hubbard model.

[2] M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch, Nature **415**, 39 (2002).

[3] J. Gavoret and P. Nozières, Ann. Phys. (N.Y.) **28**, 349 (1964).

[4] P. C. Hohenberg and P. C. Martin, Ann. Phys. (N.Y.) **34**, 291 (1965).

[5] A. Smerzi, S. Fantoni, S. Giovanazzi, and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997).

[6] P.W. Anderson, in: *Lectures on the Many-Body Problem*, E.R. Caianello (Ed.) (Academic Press, New York, 1964).

[7] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).

[8] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, 1999).

[9] B. Capogrosso-Sansone, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. B **75**, 134302 (2007).

[10] This means that the lattice can be viewed as being made of two interpenetrating sublattices. One simple example is the cubic lattice

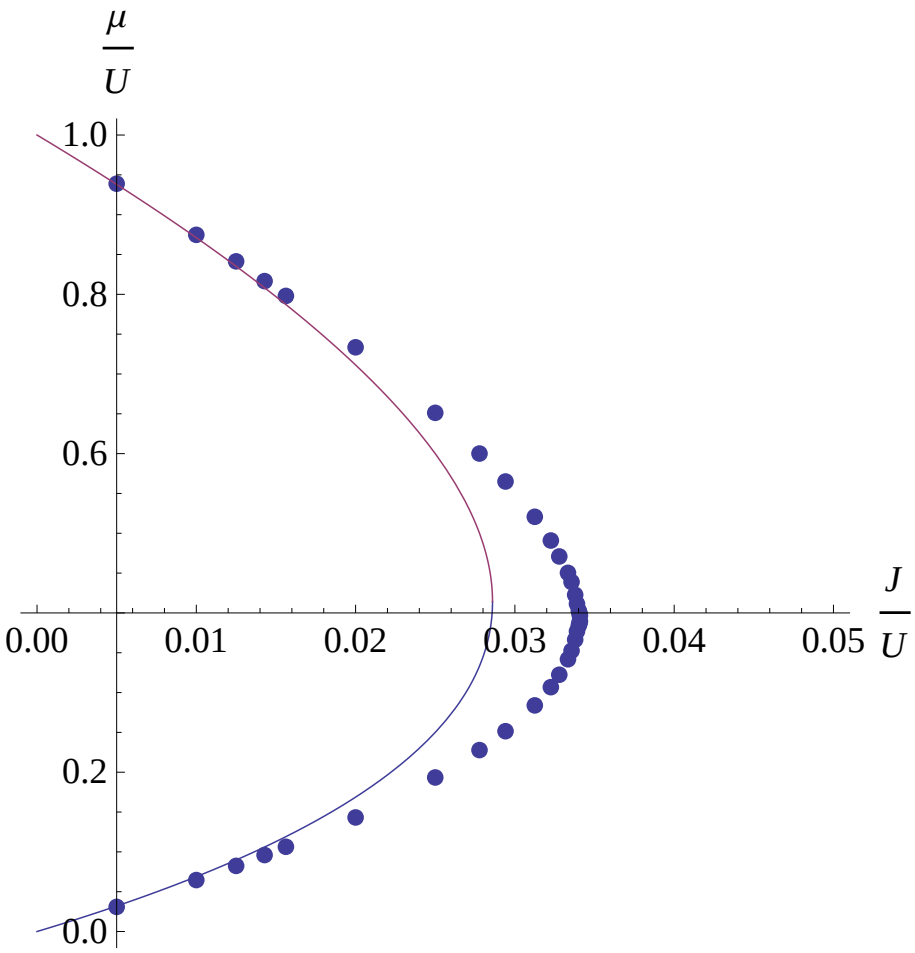

FIG. 4: Phase diagram for $n = 1$. The Black circles are Monte Carlo points from Ref. [9]. The continuous line is the mean-field result.