Physics Research Project

Tomography of the Superfluid-Mott Transition

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[1] Introduction

In condensed matter physics, the study of quantum many-body systems provides profound insights into the behavior of matter at the nanoscale. The Bose-Hubbard Hamiltonian offering a versatile framework to understand the behavior of ultra-cold atomic gases confined to optical lattices [2, 3, 4]. This Hamiltonian demonstrate the interplay between the kinetic energy of particles hopping between lattice sites and their on-site interactions, creating a rich landscape of quantum phases and transitions.

One particularly intriguing phenomenon that emerges from the Bose-Hubbard Hamiltonian is the Mott transition. The Mott transition represents a fundamental change in the behavior of a quantum many-body system, where a gas of ultra-cold bosonic particles transforms from a superfluid phase characterized by long-range phase coherence to a Mott insulating phase characterized by integer filling of the lattice sites. This transition is driven by the competition between kinetic energy and the on-site repulsive interactions between particles. As the ratio of these two energies changes, the system undergoes a quantum phase transition between the superfluid and Mott insulating phases. The Mott transition regime offers insights into the emergence of collective behavior and topological properties in ultracold atomic gases. This is the regime we focus in this project.

[2] The Model

The project Bose-Hubbard Hamiltonian (BHH) is the simplest model of interacting rotating bosonic system. For a ring of M sites with N bosonic is

$$H = H_U + H_J = \sum_{j=1}^{M} \frac{U}{2}\tilde{n}_j(\tilde{n}_j - 1) - \frac{J}{2}(e^{i\frac{\Phi}{M}}a_{j+1}^\dagger a_j + e^{-i\frac{\Phi}{M}}a_j^\dagger a_{j+1}) \tag{1}$$

Where U is on-site interaction, $\frac{1}{2}\tilde{n}_j(\tilde{n}_j - 1) = \frac{1}{2}a_j^\dagger a_j^\dagger a_j a_j$ is the one site interaction, J is the hopping frequency, Φ is the Sagnac phase that can be regarded as Aharonov-Bohm flux, a_j and $a_j^\dagger$ are the Bosonic annihilation and creation operators.

In this project we use the Fock space as the site basis. Fock space is an algebraic construction of the states of a variable identical particles (Bosons in this context) from a single particle Hilbert space.

$$|\text{indx}\rangle = |\tilde{n_1}, \tilde{n}_2, \tilde{n}_3\rangle = \frac{1}{\sqrt{\tilde{n}_1!\tilde{n}_2!\tilde{n}_3!}}(a_1^\dagger)^{\tilde{n}_1}(a_2^\dagger)^{\tilde{n}_2}(a_3^\dagger)^{\tilde{n}_3}|\rangle, \tag{2}$$

$$\text{indx} = \{1, ..., \frac{(N+M-1)!}{(M-1)!N!}\}, \quad N = \sum_j \tilde{n}_j \tag{3}$$

where $|\rangle$ is the vacuum state, $\tilde{n}_j = a_j^\dagger a_j$ in Eq.1 are the site occupation operators. In this project we focus on $M = 3$ sites, so the site basis is $\tilde{n_1}, \tilde{n_2}, \tilde{n_3}$ and the momentum orbitals are n_0, n_+, n_-. The occupation number is

$$\langle n_\kappa \rangle = \left\langle b_\kappa^\dagger b_\kappa \right\rangle = \frac{1}{M}\sum_{i,j} e^{i\kappa(j-i)}\left\langle a_j^\dagger a_i \right\rangle, \quad \kappa \in \{0, +1, -1\} \tag{4}$$

Next, we define a convenient observable, the orbital occupation imbalance

$$M_\kappa = \langle n_+ \rangle - \langle n_- \rangle \tag{5}$$

The density matrix defined as $\tilde{\rho} = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ where

$$\tilde{\rho}_{ij} = \frac{1}{N}\left\langle a_i^\dagger a_j \right\rangle \tag{6}$$

For a BHH with no site preference (on-site interaction U is equal for all sites) the density matrix is diagonal in the momentum basis,

$$\rho_{\kappa\kappa'} = \frac{1}{N}\left\langle b_\kappa^\dagger b_{\kappa'} \right\rangle = \frac{1}{N}\begin{bmatrix} \langle n_0 \rangle & 0 & 0 \\ 0 & \langle n_+ \rangle & 0 \\ 0 & 0 & \langle n_- \rangle \end{bmatrix} \tag{7}$$

The purity of a state is defined as

$$\text{Purity} = trace(\tilde{\rho}^2) = \sum_{n=1}^{N} P_n^2 \equiv \frac{1}{PN} \tag{8}$$

Where P_n is the distribution of N atoms, $\sum_{n=1}^{N} P_n = 1$. PN is the participant number which demonstrate the number of occupied sites. Note that trace can be taken in every basis such that $trace(\tilde{\rho}^2) = \sum_\kappa (\frac{\langle n_\kappa \rangle}{N})^2 \leq 1$. A pure state has Purity = 1.

Mott State.– When interaction (U) is high, $J << U$. For commensurate N particles will arrange equally between sites, an insulating state. Not a coherent state.

$$|\text{Mott}\rangle = (a_1^\dagger)^{\frac{N}{M}}(a_2^\dagger)^{\frac{N}{M}}...(a_M^\dagger)^{\frac{N}{M}}|\rangle \tag{9}$$

In Fig. 1 and in Fig. 3 these states marked with empty triangular Δ.

Super-Fluid States.– When hopping (J) is high, $J >> U$. Particles will be arranged in momentum orbitals. This is a coherence state. For example the lower momentum orbital is

$$|SF_{\kappa=0}\rangle = (a_1^\dagger + a_2^\dagger + ... + a_M^\dagger)^N |\rangle \tag{10}$$

where $a_1^\dagger + a_2^\dagger + ... + a_M^\dagger|\rangle$ is the $\kappa = 0$ momentum orbital for one particle state. In this region it is easier to work in momentum basis so the state can be rewriten as

$$|\kappa\rangle = |SF_\kappa\rangle = \frac{1}{\sqrt{N!}}(b_\kappa^\dagger)^N\,|\rangle \tag{11}$$

In Fig. 1 and in Fig. 3 these states marked with empty circles ∘.

Self Trapped States.– All particle located at one site, these states are the eigenstates of BHH without hopping ($J = 0$).

$$|\mathrm{ST}_j\rangle = \frac{1}{\sqrt{N!}}(a_j^\dagger)^N\,|\rangle \tag{12}$$

There are M degenerate ST states, so exact diagonalization will lead to cat states, for example the zero momentum ST state is

$$|ST\rangle = \frac{1}{M\sqrt{N!}}[(a_1^\dagger)^N + (a_2^\dagger)^N + ...(a_M^\dagger)^N]\,|\rangle \tag{13}$$

In Fig. 1 and in Fig. 3 these states marked with empty square □.

[3] Main Formulas

The Mott state energy and occupation imbalance are

$$E_{\mathrm{Mott}} = \frac{U}{2}N(\frac{N}{M} - 1), \quad M_{\kappa,\mathrm{Mott}} = 0 \tag{14}$$

The super-fluid states energy and occupation imbalance are

$$E_\kappa = N\epsilon_\kappa + \frac{U}{2M}N(N-1), \quad M_\kappa = N\cdot\kappa, \quad \kappa = \{\pm 1, 0\} \tag{15}$$

The self trapped states energy and occupation imbalance are

$$E_{\mathrm{ST}} = \frac{U}{2}N(N-1), \quad M_{\kappa,\mathrm{ST}} = 0 \tag{16}$$

In the Mott state region, when the interaction is high, $u \gg 1$, we claim the system behaves like hard-core bosons, a system of fermions,with no interaction. We would like to understand how well the lower part of BHH spectrum behaves like excitation from Mott state. We used perturbation theory to analyse the lower levels of the spectrum as a particle excitation from Mott state. Our claim is that the approximation is valid as long the spectra levels don't mix. In this project $M = 3$, we examine the first lowest excited states from Mott state for two scenarios, commensurate and non-commensurate number of particles. For commensurate number of particle $N = 3\bar{n}$ the energy and orbital occupation imbalance for the first excited level of Mott state (contains 6 states) are

$$E_{l=\{\pm,q\}} = \frac{U}{2}\left(3\bar{n}^2 - 3\bar{n} + 2\right) \pm \frac{1}{2}\sqrt{J_{\mathrm{eff},1}^2 + J_{\mathrm{eff},2}^2 + 2J_{\mathrm{eff},1}J_{\mathrm{eff},2}cos(2q)}, \quad q \in \{-\frac{2\pi}{L_{\mathrm{eff}}}, 0, \frac{2\pi}{L_{\mathrm{eff}}}\} \tag{17}$$

$$L_{\mathrm{eff}} = 6, \quad J_{\mathrm{eff},1} = (\bar{n}+1)J, \quad J_{\mathrm{eff},1} = \bar{n}J \tag{18}$$

$$M_{\kappa,l'} = \frac{6\sqrt{3}}{18}\left(\bar{n}sin(\frac{\phi - \pi l'}{3}) + (\bar{n}+1)sin(\frac{\phi + \pi l'}{3})\right), \quad l' \in \{1, .., 6\} \tag{19}$$

For non-commensurate number of particle $N = 3\bar{n}+1$ the energy and orbital occupation imbalance for the first excited level of Mott state (contains 3 states) are

$$E_p = \frac{U}{2}\left(3\bar{n}^2 - \bar{n}\right) - J(\bar{n}+1)\cdot cos\left(\frac{\phi}{3} - \frac{2\pi}{3}p\right), \quad p \in \{1, 2, 3\} \tag{20}$$

$$M_{\kappa,p} = = \frac{2\sqrt{3}(\bar{n}+1)}{9}\left(2sin(\frac{2\pi}{3}p) - sin(2\frac{2\pi}{3}p)\right) \tag{21}$$

[4] Mott Transition

In this project we focus on the quantum phase transition from Super-Fluid to Mott in the lower part of the spectrum. We see in Eq.1 that the relation between U and J will effect on the eigenstates of the system, when $J = 0$, there is no hopping, the eigenstates will be site basis. The lower state of the energy spectrum will be Mott. When a small hopping perturbation ($J << U$) is added, the Mott state won't effect until J is big enough. When $U = 0$, there is no interaction, the momentum basis is better to describe the system.

Dimensionless Parameters.– The BHH parameters are M, N, U, J, Φ. The classical dimensionless parameter is

$$u_M = M\frac{NU}{J} = Mu \tag{22}$$

In the Matlab simulation the control parameter is $u = \frac{NU}{J}$ and $J = 1$ by definition, such that for number of particle N, U is determined. The quantum parameter is

$$\gamma_M = \frac{u_M}{N^2} \tag{23}$$

Roughly speaking when $u_M = 1$, $u = \frac{1}{M}$, self trapping appear and when $\gamma_M = 1, u_M = N^2, u = MN^2$, Mott transition appears. Namely, we expect to see the Mott transition appears at $u \sim N^2$

First, lets see what happens to a system of $N = 30$ particles when u getting larger, see Fig.1. (For more information about the simulation process see Appendix A,B,C). The code for this part is N30MottTransition.m.

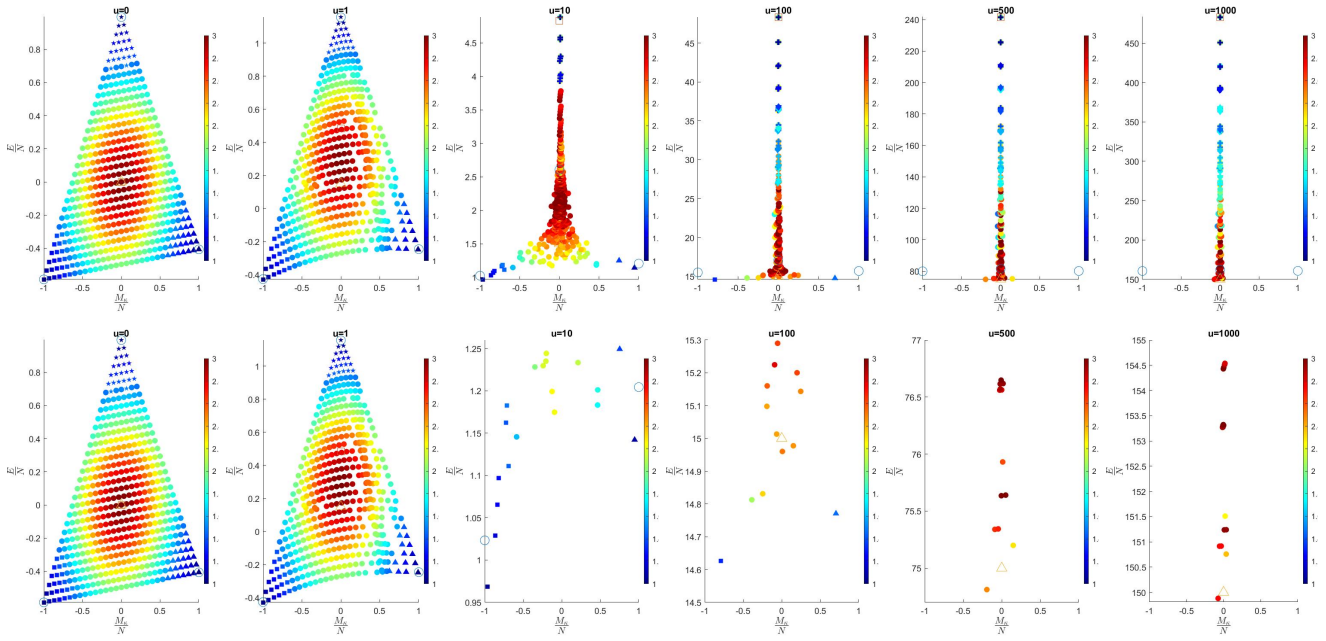


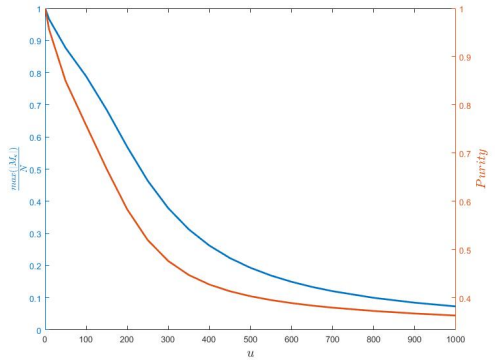
FIG. 1: $E(M_\kappa)$ for $N = 30, \phi = 3.1\pi$ and $u = 0$ to $u = 1000$, second raw is zoom to the lower part of the spectra for $u > 1$ values. The color is the participant number (PN).

In order to classify the states of this system we used specific marker for each condense state as mention bellow.

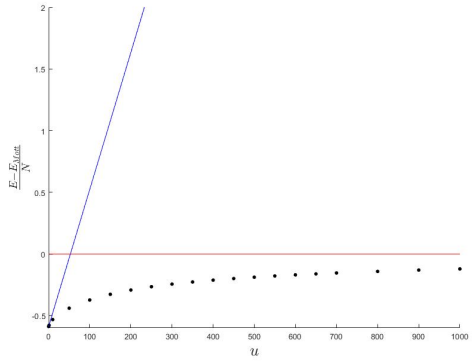
- $\diamond$ condensation $\langle \tilde{n}_3 \rangle \geq 0.7N$ at site 3.
- $\triangledown$ condensation $\langle \tilde{n}_2 \rangle \geq 0.7N$ at site 2.
- $+$ condensation $\langle \tilde{n}_1 \rangle \geq 0.7N$ at site 1.
- $\star$ condensation $\langle n_0 \rangle \geq 0.8N$ at momentum orbital $\kappa = 0$.
- Δ condensation $\langle n_+ \rangle \geq 0.8N$ at momentum orbital $\kappa = +1$.
- $\square$ condensation $\langle n_- \rangle \geq 0.8N$ at momentum orbital $\kappa = -1$.

We can see that at $u \approx 500$ the Mott state appears, as expected $u \sim N^2$. In order to find the exact u value, u_c in which the Mott transition appear we will check when the ground-state crosses the $M_\kappa = 0$ and see how the purity of the ground-state changes as u increases, see Fig.2a. The code for this is max_Mk_u.m. We see the phase transition is a second order phase transition so the M_κ is not a good criteria and we cant get a u_c from this. However, we saw in Fig.1 the levels formation appears in the spectrum already at $u = 500$.

Next, we will look at another graph that will emphasize the Mott transition, see Fig.2b. The code for this is E_u_SF_GS_Mott.m.



(a) $\max(|M_\kappa|)$ and purity as function of u for $N = 30, \phi = 3.1\pi$



(b) Energy $E(u)$ for $N = 30, \phi = 3.1\pi$. Black marker is the numerical ground state, red line is analytical Mott, blue line is analytical SF

FIG. 2: Ground state properties as u increase

Further on, we will examine what happens to the first excited level from Mott state, namely, the states at the bottom of the spectra. We will see what happens to them as u decreased from Mott region, when does the level formation stops and how well this part of the spectrum can be described with perturbation theory.

In Fig.3 we see the difference between two cases. For commensurate number of particles we see the ground state is the Mott state. For non-commensurate we see the ground state is excitation from Mott.

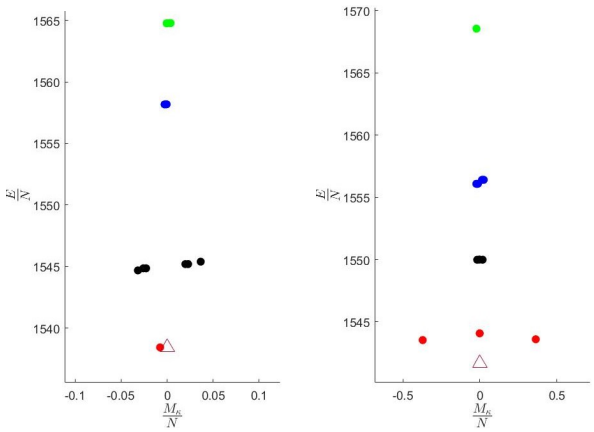


FIG. 3: Lowest part of $E(M_\kappa)$ when $\phi = 3.1\pi, u = 10000$. First level (red), second level (black), third level (blue) and forth level (green). **Left figure:** $N = 39$, commensurate number of particles. First level is Mott ground state, second level is the first excitation from Mott state. **Right figure:** $N = 40$, non-commensurate number of particles. First level is the first excitation from Mott state.

For commensurate number of particle $N = 3\bar{n}$, the first excitation from Mott state are the first level above the ground-state, the level includes 6 states, see Fig.4. We checked what happens for $N = 39, \bar{n} = 13$. For range of u from $u = 10000$ to $u = 550$. It is clear that when u decreases the analytical calculation using perturbation theory can't describe the first level of excitation. We see that as u decreased the analytical calculation and the numerical exact calculation separate. When we took the parameter $u < 550$, the 6 states jumped to different place in the spectrum, as a result of the levels mixing. At $u_c \approx 500$ the levels start to mix. The code for this part is Mott_exceed_u.m.

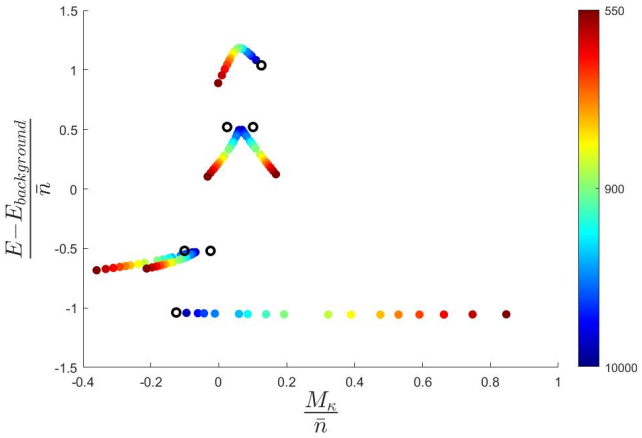


FIG. 4: E(M_k) for exceeding u and for $N = 39$,the flux is $\phi = 3.1\pi$, the color bar is u, the black circles are the analytical calculation for this $\bar{n}$ according to Eq.17,19

For non-commensurate number of particle $N = 3\bar{n} + 1$, the first excitation from Mott state is the lowest level of the spectrum contains 3 states, see Fig.5. We checked what happens for $N = 40, \bar{n} = 13$ For exceeding u from $u = 10000$ to $u = 550$. It is clear that again when u decreases the analytical calculation using perturbation theory can't describe the first level and also here $u_c \approx 500$.

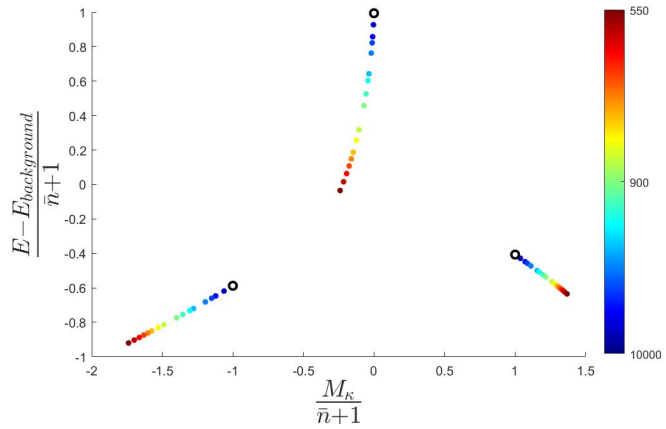


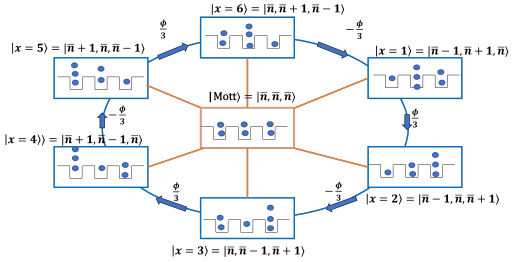
FIG. 5: E(M_k) for exceeding u and for $N = 40$,the flux is $\phi = 3.1\pi$, the color bar is u, the black circles are the analytical calculation for this $\bar{n}$ according to Eq.20,21

In the following sections we explain the use of perturbation theory as a way to analyse the first excitation from Mott state for both cases.

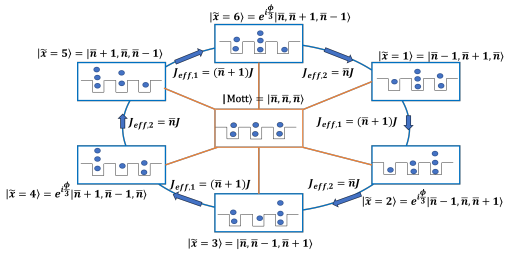
[5] Commensurate Number of Particles

We chose the flux to be $\phi = 3.1\pi$. The highest level of the spectrum is the ST states, the lowest level of the spectrum is the Mott state. At the middle there are levels that relate to the particle excitation. We analyze the second floor (from bottom) of the spectrum, hence the one particle excitation, namely the states of the form: $|x\rangle = |\bar{n}, \bar{n}-1, \bar{n}+1\rangle$, there are 6 states of this form. When $J = 0$ and there is no tilt (no site preference) in the Hamilotnian, those 6 states are degenerate states. When U is big, the site basis supposed to win but there is degeneracy, so it is like a ring of Fock states, see Fig.6a. One can treat the six degenerate states with perturbation theory, meaning the 6 degenerate states will produce 6 momentum states. In our simulation $J \neq 0$, the hopping term should remove degeneracy.

In order to find the energies and momentum occupation, M_κ, of these Fock-momentum states, we need to understand what is the effective Hamiltonian of the 6 degenerate states. Notice, the phase between those state is not constant,



(a) States diagram of the one particle excitation for arbitrary $\bar{n}$. For example in this figure $\bar{n} = 2$.



(b) Effective diagram of the one particle excitation for arbitrary $\bar{n}$. Notice, the figure has specific $\bar{n} = 2$ to emphasize.

FIG. 6: Diagram of the one particle excitation level

so we gauge the flux into the states:

$$|\tilde{x}=1\rangle = |\bar{n}-1, \bar{n}+1, \bar{n}\rangle \qquad |\tilde{x}=3\rangle = |\bar{n}, \bar{n}-1, \bar{n}+1\rangle \qquad |\tilde{x}=5\rangle = |\bar{n}+1, \bar{n}, \bar{n}-1\rangle \tag{24}$$
$$|\tilde{x}=2\rangle = e^{i\frac{\phi}{3}}|\bar{n}-1, \bar{n}, \bar{n}+1\rangle \qquad |\tilde{x}=4\rangle = e^{i\frac{\phi}{3}}|\bar{n}+1, \bar{n}-1, \bar{n}\rangle \qquad |\tilde{x}=6\rangle = e^{i\frac{\phi}{3}}|\bar{n}, \bar{n}+1, \bar{n}-1\rangle$$

Now there is a translation symmetry in the ring so the eigenstates are the Fock-momentum states. The effective Hamiltonian of this Fock-ring includes $L_{\text{eff}} = 6$ and the effective hopping coefficient, J_{eff} defined as the matrix elements between those states. There is different hopping coefficient for a transition from even to odd state or from odd to even state,

$$\langle\tilde{x}=6|H|\tilde{x}=5\rangle = -\frac{J}{2}\cdot(\bar{n}+1) \quad \langle\tilde{x}=3|H|\tilde{x}=2\rangle = -\frac{J}{2}\cdot\bar{n} \tag{25}$$

So, the effective hopping coefficients are $J_{\text{eff},1} = (\bar{n}+1)J, J_{\text{eff},2} = \bar{n}J$. Finally the effective system is shown in Fig.6b. The background energy is the interaction energy of these states (the height of the excited level),

$$E_{\text{background}} = \frac{U}{2}\left(3\bar{n}^2 - 3\bar{n} + 2\right) \tag{26}$$

According to Bloch's theorem, the eigen-energies of the effective systems are:

$$E_\pm = E_{\text{background}} \pm \frac{1}{2}\sqrt{J_{\text{eff},1}^2 + J_{\text{eff},2}^2 + 2J_{\text{eff},1}J_{\text{eff},2}cos(2q)}, \quad q \in \{-\frac{2\pi}{L_{\text{eff}}}, 0, \frac{2\pi}{L_{\text{eff}}}\} \tag{27}$$

Next, we calculate the orbital occupation number using another approximation $J_{\text{eff},1} = J_{\text{eff},2}$ which is valid for large N, such that the approximates eigen-states are the Fock momentum states,

$$|l\rangle = \frac{1}{\sqrt{L_{\text{eff}}}}\sum_{\tilde{x}=1,\ldots,6} e^{iq\tilde{x}}|\tilde{x}\rangle \tag{28}$$

We mark the momentum states with the letter $q = \frac{2\pi}{L_{\text{eff}}}\cdot l$, $l \in \{1,2,3,4,5,6\}$. Now we can calculate analytically the approximated orbital occupation number M_κ. The orbital occupation number of these $|l\rangle$ states using Eq.4 is

$$\langle n_\kappa \rangle = \bar{n} + \frac{1}{18}\left(4\bar{n}cos(\frac{-2\pi\kappa+\phi-\pi l}{3}) + 4(\bar{n}+1)cos(\frac{-2\pi\kappa+\phi+\pi l}{3}) + 2\bar{n}cos(\frac{4\pi\kappa+\phi-\pi l}{3}) + 2(\bar{n}+1)cos(\frac{4\pi\kappa+\phi+\pi l}{3})\right) \tag{29}$$

So, the orbital occupation imbalance is

$$M_\kappa = \langle n_{\kappa=1}\rangle - \langle n_{\kappa=-1}\rangle = \frac{6\sqrt{3}}{18}\left(\bar{n}sin(\frac{\phi-\pi l}{3}) + (\bar{n}+1)sin(\frac{\phi+\pi l}{3})\right) \tag{30}$$

We see there is no good normalization in this case so we chose to normalized by $\bar{n}$. The full analytical calculation can be found in Appendix E.

To see better what happens at the lower part of the spectrum, we plot the 6 states Fock ring for exceeding number of particles, from $\bar{n} = 1$ to $\bar{n} = 17$, see Fig.7.

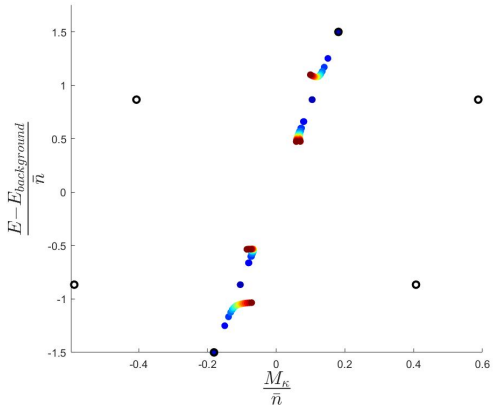


FIG. 7: E(M_k) for exceeding $\bar{n}$ and for $u = 10000$, blue for $\bar{n} = 1$ and red is for $\bar{n} = 17$. Black circles are the analytical calculation for $\bar{n} = 1$

Notice the 4 black circle in the middle seem to be wrong, however, since these states are degenerate the computer removes the degeneracy spontaneously. The code for this part is fock_ring_analytical.m and Mott_exceed_N.m.

In order to find the region of validity for the approximation using perturbation theory to analysis the effective system, we need to check the small parameter. Using perturbation theory assumes the first excited level from Mott is far enough from the ground state (Mott) and from the next excited level (excited). The level we look at contains states of the form $|\bar{n}-1, \bar{n}, \bar{n}+1\rangle$, has a background energy as mention in Eq.26, and the Mott energy is E_{Mott}, see Fig.8. The distance between the first two levels is $\Delta_1 = E_{\text{background}} - E_{\text{Mott}} = U \sim \frac{Nu}{J}$. Remember that $J_{\text{eff}} \sim NJ$. The

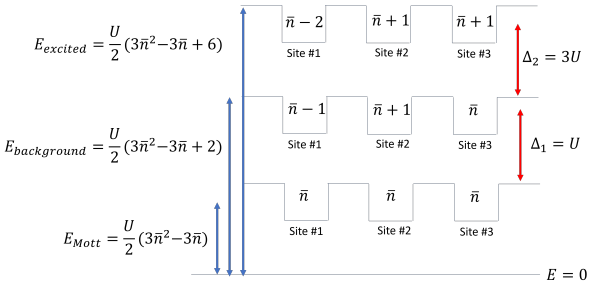


FIG. 8: The lower levels of the spectrum for $N = 3\bar{n}$

next excited state contains states of the form $|\bar{n}-2, \bar{n}+1, \bar{n}+1\rangle$, has an excited energy $E_{\text{excited}} = \frac{U}{2}(3\bar{n}^2 - 3\bar{n} + 6)$, the distance between the next excited level is $\Delta_2 = E_{\text{excited}} - E_{\text{background}} = 3U \sim \frac{Nu}{J}$. Finally we got $\Delta_1 \approx \Delta_2 \sim U$, the small parameter is define as

$$\frac{J_{\text{eff}}}{\Delta} \sim \frac{J^2}{u} \tag{31}$$

We see there is no N dependence. Moreover, since $J = 1$ we see that the small parameter for the usage of perturbation theory is $\frac{1}{u}$ as it is the parameter that control the Mott transition. So we conclude that when u is big enough for Mott regime it is valid to use perturbation theory to analyse the spectrum. The code for an arbitrary $\bar{n}$ is Mott_specific_nbarM3.m.

Lets see what happens to the second level of the excited states for $N = 39$ and same range of u as before, see Fig.9 When we take u to even smaller values the second level leaks to the area of the first level (the second level drifts to

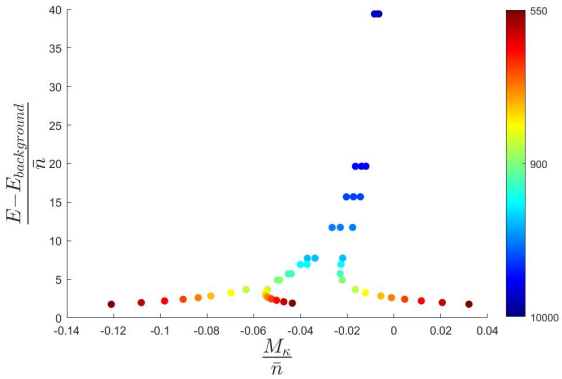


FIG. 9: E(M_k) for second level of excitation for exceeding u and for $N = 39$ where the color bar is u.

the $\frac{E-E_{\text{background}}}{\bar{n}} = 1$ where the first level located), this happens at $u_c \approx 500$.

[6] Non-commensurate Number of Particles

We chose the flux to be $\phi = 3.1\pi$. The lower excitation of Mott state are three states of the form $|x\rangle = |\bar{n}+1, \bar{n}, \bar{n}\rangle$. Our technique is to simulate an effective Hamiltonian that will represent the lower part of the spectrum, near the Mott state. Namely, a ring system with 3 states $|x\rangle$.

$$H_{\text{eff}} = H_{J,\text{eff}} + E_{\text{background}} \tag{32}$$

The effective hopping coefficient can be found:

$$\left\langle \bar{n}, \bar{n}+1, \bar{n} \middle| a_2^\dagger a_1 \middle| \bar{n}+1, \bar{n}, \bar{n} \right\rangle = (\bar{n}+1) \tag{33}$$

Such that

$$J_{\text{eff}} = J(\bar{n}+1) \tag{34}$$

The hopping coefficient for each transition is $c = \frac{J_{\text{eff}}}{2} e^{i\frac{\phi}{3}}$. The constant background energy for arbitrary $\bar{n}$ can be found from interaction part in Eq.1,

$$E_{\text{background}} = \frac{U}{2}\left(3\bar{n}^2 - \bar{n}\right) \tag{35}$$

There are 3 degenerate states of the one particle excitation with the same hopping coefficient connecting them, hence, the system has a translation symmetry and breaking the symmetry yields 3 momentum states $|p\rangle$ of the form:

$$|p\rangle = \frac{1}{\sqrt{3}} \sum_{x=\{1,2,3\}} e^{iPx} |x\rangle, \quad P = \frac{2\pi}{3} p, p \in \{1,2,3\} \tag{36}$$

Finally the energy for these Fock-momentum states is immediate

$$E_p = \langle p|H|p\rangle = E_{\text{background}} - J_{\text{eff}} \cdot cos\left(\frac{\phi}{3} - \frac{2\pi}{3} p\right) \tag{37}$$

The momentum occupation number for these states using Eq.4,

$$\langle n_\kappa \rangle = \frac{1}{9}\left(3(3\bar{n}+1) + (\bar{n}+1)\left[4cos\left(\frac{2\pi(p-\kappa)}{3}\right) + 2cos\left(\frac{4\pi(p-\kappa)}{3}\right)\right]\right) \tag{38}$$

And the orbital occupation imbalance is

$$M_\kappa = \langle n_{\kappa=1}\rangle - \langle n_{\kappa=-1}\rangle = \frac{2\sqrt{3}(\bar{n}+1)}{9}\left(2sin(\frac{2\pi p}{3}) - sin(2\frac{2\pi p}{3})\right) \tag{39}$$

Finally, we see that the right normalization for this scenario is not the total number of particle N but $\bar{n}+1$. The full analytical calculation can be found in Appendix F.

To see better what happens at the lower part of the spectrum, we plot the 3 excited states from Mott for exceeding number of particles, shown in Fig.10.

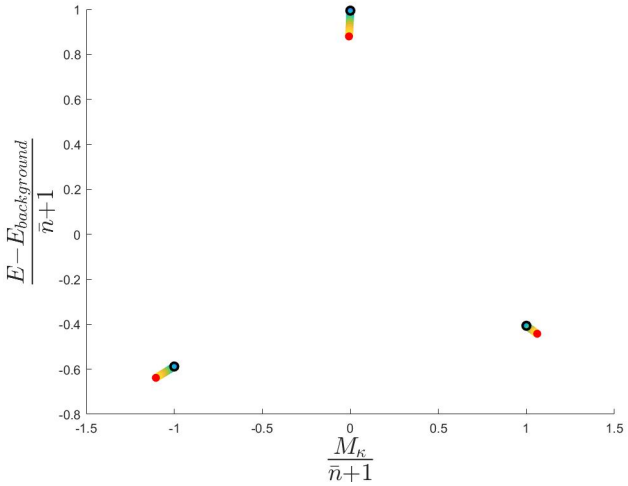


FIG. 10: E(M_k) for exceeding $\bar{n} = 1:17$ and for $u = 10000$, blue for $\bar{n} = 1$ and red is for $\bar{n} = 17$. Black circles are the analytical calculation for $\bar{n} = 1$

We see that the approximation doesn't depend on N, the analytical and numerical calculation stay at the same region of the spectrum. The codes for this part are Jeff_1par_exc.m and one_par_exceed_N.m.

In order to find the region of validity for this approximation (using perturbation theory) we need to check the small parameter. We claim that this approximation is valid as long the spectrum levels don't mix, meaning the second excited states (excited) is far from the one-particle-level we looked at, see Fig.11. The second excited states are of

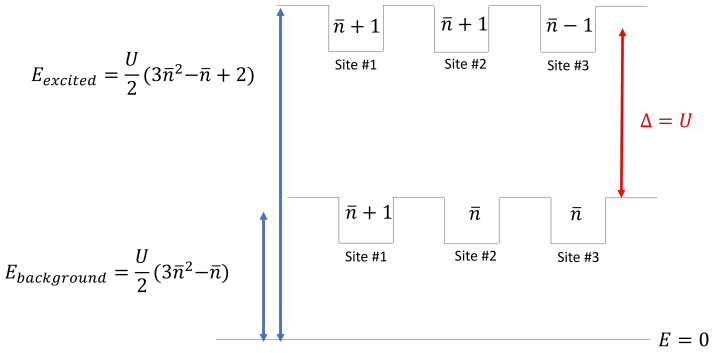


FIG. 11: The distance between the lower level of the spectrum for $N = 3\bar{n}+1$

the form $|\bar{n}-1, \bar{n}+1, \bar{n}+1\rangle$ and the excited energies are

$$E_{\text{excited}} = \frac{U}{2}\langle \bar{n}-1, \bar{n}+1, \bar{n}+1|H_U|\bar{n}-1, \bar{n}+1, \bar{n}+1\rangle = \frac{U}{2}\left(3\bar{n}^2 - \bar{n} + 2\right) \tag{40}$$

The distance between the first two levels is $\Delta = E_{\text{excited}} - E_{\text{background}} = U \sim \frac{Nu}{J}$. The small parameter is define as

$$\frac{J_{\text{eff}}}{\Delta} \sim \frac{J^2}{u} \tag{41}$$

so we see there is no N dependence. The code for an arbitrary $\bar{n}$ is one_par_specific_N.m.

Lets see what happens to the second level of the excited states of the form $|\bar{n}+1, \bar{n}+1, \bar{n}-1\rangle$, for $N = 40$ and same range of u as before, see Fig.12.

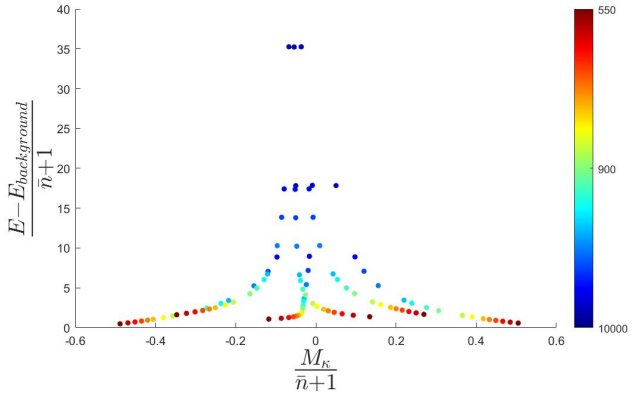


FIG. 12: E(M_k) for second level of excitation for exceeding u and for $N = 40$ where the color bar is u.

When u decreases the second level leaks to the area of the first level (the second level drifts to the region of $\frac{E-E_{\text{background}}}{\bar{n}+1} = 1$ where the first level located), this happens at $u_c \approx 500$.

[7] Conclusions

This project places significant emphasis on the usage of perturbation theory as a tool for characterization of the lower segment of the Bose-Hubbard Hamiltonian in the context of Mott state excitations. The criteria governing this analysis is the parameter $u = \frac{JU}{N}$. The perturbation theory works well when we can see levels forming in the spectrum of the system. When u attains sufficient magnitude, the phenomena of level formation appears, subsequently enabling perturbation theory to effectively characterize the Mott excitation states. It has been observed that this criterion remains invariant (same u_c value) for both commensurate and non-commensurate particle numbers.

[A] Matlab Simulations Process

First, lets explain the basic concepts of spectrum analysis of a system in Matlab. We need to understand how to build the BHH in the Fock site basis.

1. Building the Fock basis for N particles in $M = 3$ sites, meaning $|\tilde{n}_1, \tilde{n}_2, \tilde{n}_3\rangle$. In this code the matrix's name that holds this basis is "nsite" and it holds all possible configurations of the particles in the three sites. The code for this part is FockBasis_M3.m.

2. Building the operators $a_j^\dagger a_i$. Notice, when $i = j$: $a_j^\dagger a_j = \tilde{n}_j$ which we use for the interaction term and when $i \neq j$: we get the jump operators of the hopping term. In Matlab, these operators are actually matrices. The matrices elements $\left\langle a_j^\dagger a_i \right\rangle$ evaluate through $J_{21} = \left\langle \tilde{n}_1 - 1, \tilde{n}_2, \tilde{n}_3 \middle| a_2^\dagger a_1 \middle| \tilde{n}_1, \tilde{n}_2 - 1, \tilde{n}_3 \right\rangle = \sqrt{\tilde{n}_1 \tilde{n}_2}$. The code for this part is FockBasis_M3.m.

3. Building the BHH using Eq.1 and calculate the following elements:

   - Diagonlization of the Hamiltonian matrix and find its eigen-energies and eigen-states. The code for this part is spectrum.m.
   - Calculate the site occupation numbers, $\tilde{n}_1, \tilde{n}_2, \tilde{n}_3$ when $\tilde{n}_i = \left\langle a_i^\dagger a_i \right\rangle$ and the $\langle\rangle$ is over the eigenstate found previously. The code for this part is occupations.m.
   - Calculate the orbital occupation numbers, n_0, n_1, n_{-1} using Eq.4 where $\langle\rangle$ is over the eigenstates found previously. The code for this part is occupations.m.
   - Build density matrix $\tilde{\rho}$ of each eigenstate by using Eq.6 and calculate the participant number of each state by using $\frac{1}{trace(\tilde{\rho}^2)}$, The code for this part is rho_purity.m.
   - Calculate the occupation imbalances $M_k = \langle n_+ \rangle - \langle n_- \rangle$,$M_x = \langle \tilde{n}_1 \rangle - \langle \tilde{n}_3 \rangle$ and the modify imbalance $m = M_x + M_k$

4. Another useful code in this project is a function that plots the spectrum of the system as function of site occupation number or momentum occupation number ore modify occupation number. The code for this part is marker4plot.m and plot_spec.m.

In the Matlab simulation, to see the separation between ST states, a small tilt is added to the Hamiltonian. Tilt between the sites is actually site preference, the on-site interaction isn't equal for all sites. So there is a degeneracy removal of the ST states. The tilt Interaction term for small t is of the form

$$\frac{U}{2} \sum_{j=1,2,3} t_j \tilde{n}_j (\tilde{n}_j - 1), \quad t_j = \begin{cases} 1, j = 1 \\ 0, j = 2 \\ -1, j = 3 \end{cases} \tag{A42}$$

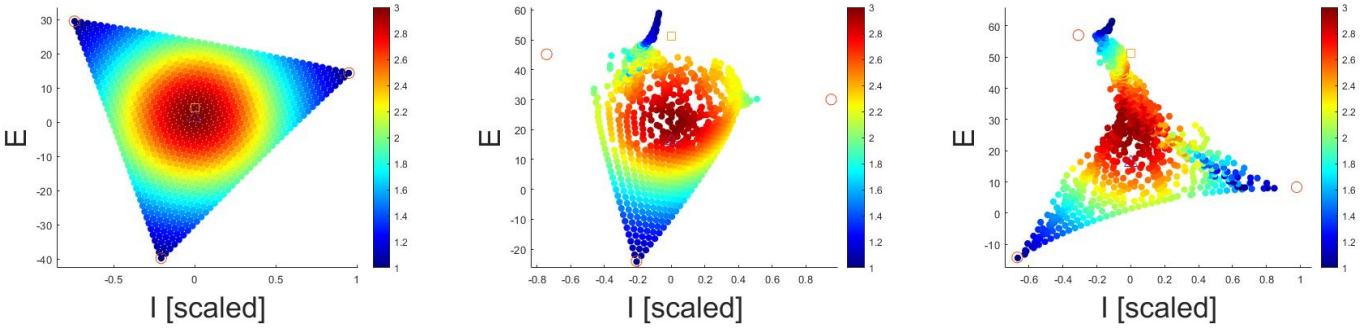
[B] Redoing Past Simulations

First, we re-simulated past simulation done by Geva Arwas in his thesis "Superfluidity and Quantum Chaos in Bose Condensed Systems" [1]. First we got the same graphs as Geva Arwas did, see Fig.13.

In these simulations we added a tilt to the Hamiltonian and got the same results as in Geva's article 'Triangular Bose-Hubbard trimer as a minimal model for a superfluid circuit'. The differences can be seen at the edges of the spectrum close to SF states in Fig.13(b).

My next purpose was to improve these figures. In order to classify the states of this system we used specific marker for each state.

- $\diamond$- condensation $\langle \tilde{n}_3 \rangle \geq 0.7N$ at site 3.
- $\triangledown$ -condensation $\langle \tilde{n}_2 \rangle \geq 0.7N$ at site 2.
- $+$ - condensation $\langle \tilde{n}_1 \rangle \geq 0.7N$ at site 1.
- $\star$ - condensation $\langle n_0 \rangle \geq 0.8N$ at momentum orbital $\kappa = 0$.
- Δ - condensation $\langle n_+ \rangle \geq 0.8N$ at momentum orbital $\kappa = +1$.
- $\square$- condensation $\langle n_- \rangle \geq 0.8N$ at momentum orbital $\kappa = -1$.



(a) $M = 3, N = 42, \Phi = 0.2\pi, u = 0.2$ (b) $M = 3, N = 42, \Phi = 0.2\pi, u = 2.5$ (c) $M = 3, N = 42, \Phi = 0.7\pi, u = 2.5$

(d) $M = 3, N = 42, \Phi = 0.6\pi, u = 8.5$ (e) $M = 3, N = 42, \Phi = 0.6\pi, u = 1470$

FIG. 13: $E(I)$ - Redoing Past Simulations

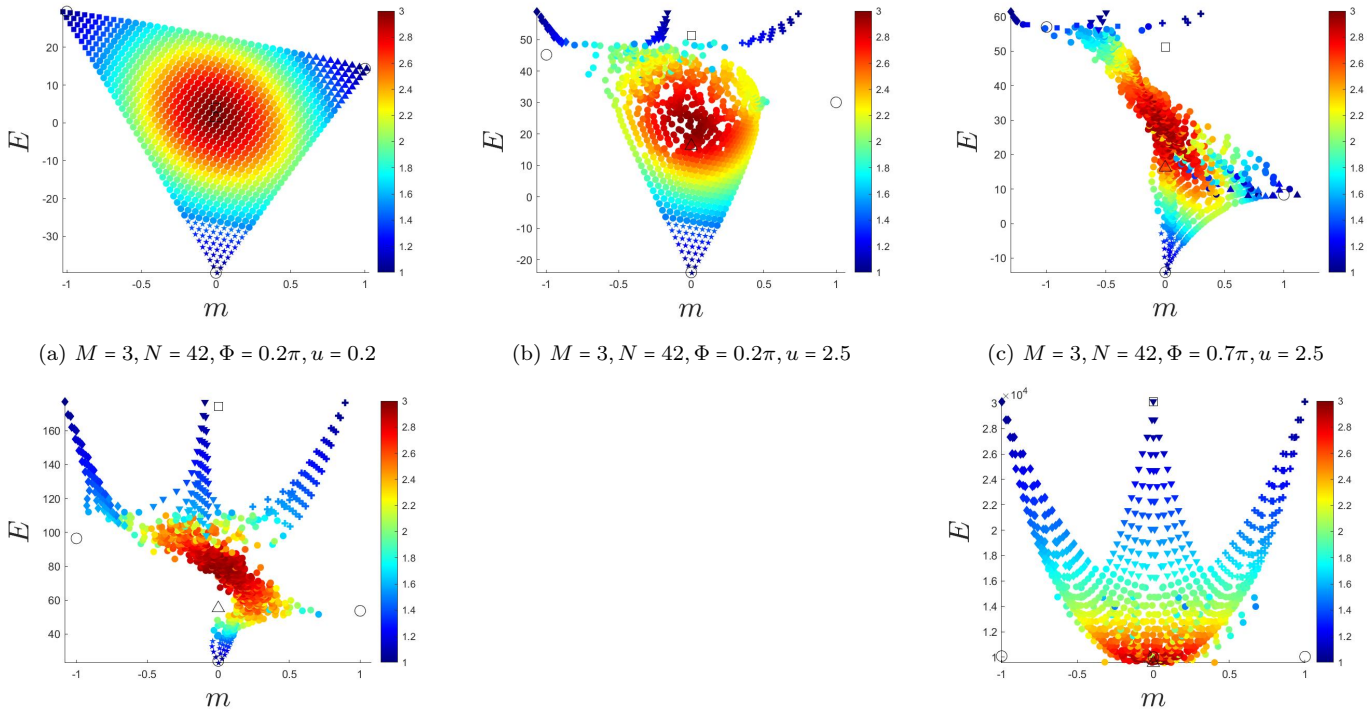
Note: The site condensation was define as $\langle \tilde{n}_j \rangle > 0.7$ while orbital condensation was define as $\langle n_\kappa \rangle > 0.8$.

Moreover, to see better what happens at the upper spectrum I changed the X-axis to modify occupation number. The modify occupation imbalance defined as $m = \sum_\kappa \langle n_\kappa \rangle \kappa + \sum_x \langle \tilde{n}_x \rangle x$ where $\langle \tilde{n}_x \rangle = \langle a_x^\dagger a_x \rangle$. The reason to do so is that the current, I is related to orbital occupation, M_κ. In order to see the self-trapped states separation we need to take into consideration the site occupation as well, as can be seen in Fig.14. Now we can see more clearly that the spectrum upward is actually sites condensation.

Lets note a few observations:

- As u exceeds the ST state getting closer to the analytically ST state (empty square).
- Notice Fig.14(c). It might look that there is eigenstate with occupation number bigger than the the (coherent) SF state. Moreover, if we look closely we see that its value is bigger than 1 (which mean more than N, total number of particles). However, it happened because we used the modify occupation number. When we added a tilt to the Hamiltonian, M_κ can get a value bigger then N.
- It seems that the lower energies aren't in the same place. In Fig.13 the lower eigenstates is at $I < 0$, while in Fig.14 the lower eigenstates are at $M = 0$. This can be explained since when $I = 0$ the modify occupation number $m \neq 0$ since it includes M_x and M_k while the current, I includes only M_k.

The code for this section is Geva.m.



(a) $M = 3, N = 42, \Phi = 0.2\pi, u = 0.2$

(b) $M = 3, N = 42, \Phi = 0.2\pi, u = 2.5$

(c) $M = 3, N = 42, \Phi = 0.7\pi, u = 2.5$

(d) $M = 3, N = 42, \Phi = 0.6\pi, u = 8.5$

(e) $M = 3, N = 42, \Phi = 0.6\pi, u = 1470$

FIG. 14: Energy as function of the normalized (by N) modify occupation imbalance

[C] Stability Gallery

In the next gallery we explored the stability of the system as the flux changes. The simulation parameters are

$$N = 42, \quad M = 3, \quad u = 2.3$$

In $M = 3$ system the modify occupation imbalance defined as

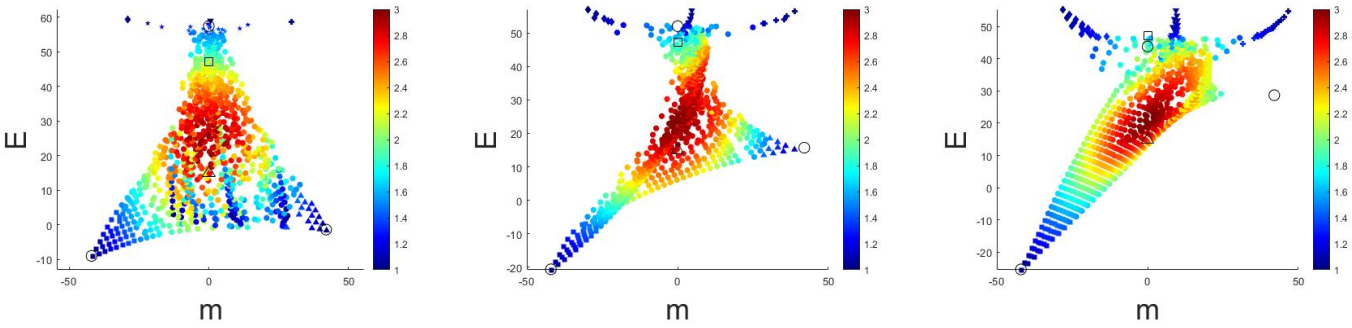
$$m = \sum_{\kappa=(-1,0,1)} \langle n_\kappa \rangle \, \kappa + \sum_{\substack{x=(-1,0,1) \\ [1\to 1, 2\to 0, 3\to -1]}} \langle \tilde{n}_x \rangle \, x = n_{+1} - n_{-1} + \tilde{n}_1 - \tilde{n}_3 \tag{C43}$$

Namely, when $m = 0$ there is condensation at $\kappa = 0$ or at $\tilde{n}_2$, when $m = N$ there is condensation at n_{+1} ($\kappa = +1$) or at $\tilde{n}_1$ and when $m = -N$ there is condensation at n_{-1} ($\kappa = -1$) or at $\tilde{n}_3$.

In Fig.15(a) we see that there are condensation states at $\kappa = +1$ and $\kappa = -1$. There is also condensation states at $\kappa = 0$ although the SF state is empty. At the top we can see three ST states. The ST state I calculated analytically (marked with empty square) has lower energy than the ST states I mentioned above since there is hopping term.

In Fig.15(b) we see that the SF state at $\kappa = -1$ is empty but the system still has some amount of condensation near it. There is still SF state at $\kappa = +1$ There is no condensation states at $\kappa = 0$. at the top we see that there are more ST condensation states than the Landau stability regime.

In Fig.15(c) we can see that there are condensation states at $\kappa = +1$ and that there is a SF state. There is no longer a condensation at $\kappa = -1$ (lost stability). At the top of the spectrum there are more ST condensation states than before. Notice at the middle of the spectra in Fig.15 there are the chaotic states. The code for this section is Stability_Gallery.m



(a) **Landau Stability** $\Phi = 3.1\pi$ (b) **Dynamical Stability** $\Phi = 3.5\pi$ (c) **No Stability** $\Phi = 3.8\pi$

FIG. 15: Stability Gallery not normalized modify occupation number

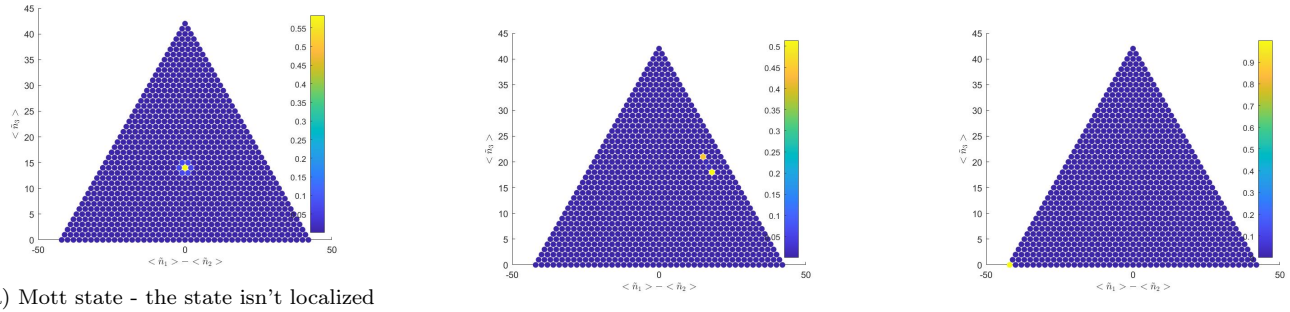
[D] Drawing Wave Functions

In order to understand better the eigen-states of the BHH in different regimes we drew some wave functions in site space, namely, in the configuration space (projection on r space). The points of the triangular are the site basis states, the color determined by $|\psi|^2$. It is quite good toll to observe Mott, ST and SF states. However these methods has limited information for the chaotic states. In this section we used the code probability_density.m.

The simulations parameters:

$$N = 42, \quad M = 3, \quad \Phi = 0.2\pi, \quad K = 1$$

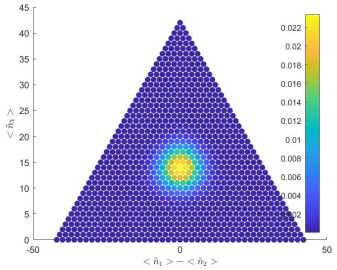
- In Fig.16 we can see some wave-functions in r space for $U >> K$, since the interaction is high the states are localized in a bound region in the configuration space. The site basis is a good basis.



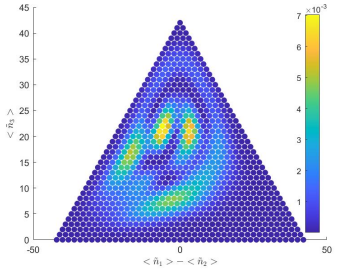
(a) Mott state - the state isn't localized at a particular site (b) An arbitrary state. (c) Self trapped state at $\tilde{n}_- = \tilde{n}_1$

FIG. 16: **Wave functions for** $U >> K$

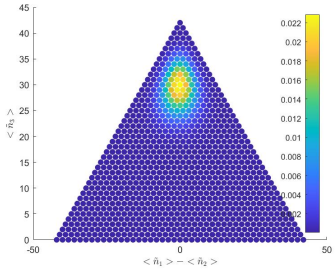
- In Fig.17 we can see some wave-functions in r space for $NU = K$.The interaction and hopping terms both contribute to BHH.
- In Fig.18 we can see some wave-functions in r space for $U << K$.The hopping term is dominant so the momentum site is a natural basis. We can see that the configuration (site) basis isn't very informative



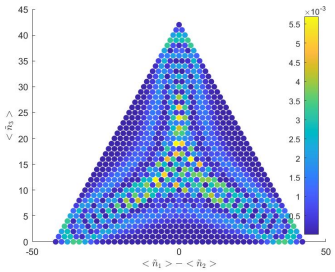
(a) SF state - The state isn't localized at a particular site.



(b) The state with $\max(M_k)$, we see an unlocated state

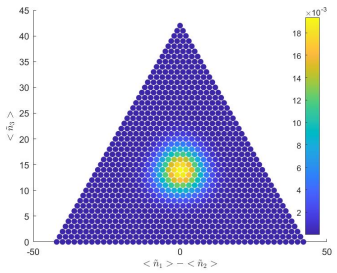


(c) The state with $\max(M_x)$, most located state at site 3

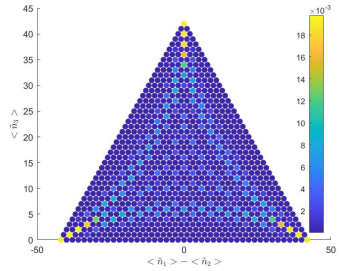


(d) A chaotic state - not an informative picture (although beautiful).

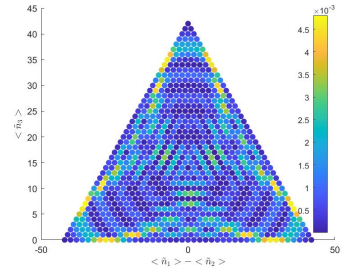
FIG. 17: **Wave functions for $NU = K$:**



(a) SF state



(b) The state with $\min(M_k)$, the closest to Mott state



(c) A chaotic state - not an informative picture although beautiful

FIG. 18: **Wave functions for $U << K$**

[E] Calculation for Commensurate Number of Particles

Using Eq.1 the hopping term for transition from an odd state to even state (for example: $\tilde{x} = 5$ to $\tilde{x} = 6$):

$$\begin{aligned}
\langle \tilde{x}=6|H|\tilde{x}=5\rangle &= \left\langle \tilde{x}=6\left|\sum_{i=j}^{3}\frac{U}{2}\tilde{n}_j(\tilde{n}_j-1)\right|\tilde{x}=5\right\rangle - \left\langle \tilde{x}=6\left|\frac{J}{2}\left(e^{i\frac{\Phi}{3}}a_{j+1}^{\dagger}a_j + e^{-i\frac{\Phi}{3}}a_j^{\dagger}a_{j+1}\right)\right|\tilde{x}=5\right\rangle \\
&= 2\frac{U}{2}\langle \tilde{x}=6|\tilde{x}=5\rangle - \left\langle \tilde{x}=6\left|\frac{J}{2}\left(e^{i\frac{\Phi}{3}}a_2^{\dagger}a_1 + e^{-i\frac{\Phi}{3}}a_1^{\dagger}a_2 + e^{i\frac{\Phi}{3}}a_3^{\dagger}a_2 + e^{-i\frac{\Phi}{3}}a_2^{\dagger}a_3 + e^{i\frac{\Phi}{3}}a_1^{\dagger}a_3 + e^{-i\frac{\Phi}{3}}a_3^{\dagger}a_1\right)\right|\tilde{x}=5\right\rangle \\
&= -\frac{J}{2}\left(e^{i\frac{\Phi}{3}}\left\langle \tilde{x}=6\left|a_2^{\dagger}a_1 + a_3^{\dagger}a_2 + a_1^{\dagger}a_3\right|\tilde{x}=5\right\rangle + e^{-i\frac{\Phi}{3}}\left\langle \tilde{x}=6\left|a_1^{\dagger}a_2 + a_2^{\dagger}a_3 + a_3^{\dagger}a_1\right|\tilde{x}=5\right\rangle\right) \\
&= -\frac{J}{2}\left(e^{i\frac{\Phi}{3}}\left\langle \tilde{x}=6\left|a_2^{\dagger}a_1\right|\tilde{x}=5\right\rangle\right) = -\frac{J}{2}\left(e^{i\frac{\Phi}{3}}e^{-i\frac{\phi}{3}}\left\langle x=6\left|a_2^{\dagger}a_1\right|x=5\right\rangle\right) = -\frac{J}{2}\cdot(\bar{n}+1)
\end{aligned} \tag{E44}$$

So, the effective hopping coefficient is $J_{\text{eff},1} = (\bar{n}+1)J$

However, the hopping term for transition from an even state to odd state (for example, transition from $\tilde{x} = 2$ to $\tilde{x} = 3$:

$$\begin{aligned}
\langle \tilde{x}=3|H|\tilde{x}=2\rangle &= \left\langle \tilde{x}=3\left|\sum_{i=j}^{3}\frac{U}{2}\tilde{n}_j(\tilde{n}_j-1)\right|\tilde{x}=2\right\rangle - \left\langle \tilde{x}=3\left|\frac{J}{2}\left(e^{i\frac{\Phi}{3}}a_{j+1}^{\dagger}a_j+e^{-i\frac{\Phi}{3}}a_j^{\dagger}a_{j+1}\right)\right|\tilde{x}=2\right\rangle \\
&= 2\frac{U}{2}\langle \tilde{x}=3|\tilde{x}=2\rangle - \left\langle \tilde{x}=3\left|\frac{J}{2}\left(e^{i\frac{\Phi}{3}}a_2^{\dagger}a_1+e^{-i\frac{\Phi}{3}}a_1^{\dagger}a_2+e^{i\frac{\Phi}{3}}a_3^{\dagger}a_2+e^{-i\frac{\Phi}{3}}a_2^{\dagger}a_3+e^{i\frac{\Phi}{3}}a_1^{\dagger}a_3+e^{-i\frac{\Phi}{3}}a_3^{\dagger}a_1\right)\right|\tilde{x}=2\right\rangle \\
&= -\frac{J}{2}\left(e^{i\frac{\Phi}{3}}\left\langle \tilde{x}=3\left|a_2^{\dagger}a_1+a_3^{\dagger}a_2+a_1^{\dagger}a_3\right|\tilde{x}=2\right\rangle + e^{-i\frac{\Phi}{3}}\left\langle \tilde{x}=3\left|a_1^{\dagger}a_2+a_2^{\dagger}a_3+a_3^{\dagger}a_1\right|\tilde{x}=2\right\rangle\right) \\
&= -\frac{J}{2}\left(e^{-i\frac{\Phi}{3}}\left\langle \tilde{x}=3\left|a_1^{\dagger}a_2\right|\tilde{x}=2\right\rangle\right) = -\frac{J}{2}\left(e^{-i\frac{\Phi}{3}}e^{i\frac{\phi}{3}}\left\langle x=3\left|a_1^{\dagger}a_2\right|x=2\right\rangle\right) = -\frac{J}{2}\cdot\bar{n}
\end{aligned} \tag{E45}$$

So, the effective hopping coefficient is $J_{\text{eff},2}=\bar{n}J$. Finally the effective system is shown in Fig.6b.

The background energy can be calculate from

$$\begin{aligned}
E_{\text{background}} &= \langle|\, a_1^{\dagger\bar{n}-1}a_2^{\dagger\bar{n}+1}a_3^{\dagger\bar{n}}|H|a_1^{\dagger\bar{n}-1}a_2^{\dagger\bar{n}+1}a_3^{\dagger\bar{n}}\,|\rangle = \langle|\, a_1^{\dagger\bar{n}-1}a_2^{\dagger\bar{n}+1}a_3^{\dagger\bar{n}}|\sum_{i=1}^{3}\frac{U}{2}\tilde{n}_i(\tilde{n}_i-1)|a_1^{\dagger\bar{n}-1}a_2^{\dagger\bar{n}+1}a_3^{\dagger\bar{n}}\,|\rangle \\
&= \frac{U}{2}\left((\bar{n}-1)(\bar{n}-2)+(\bar{n}+1)\bar{n}+\bar{n}(\bar{n}-1)\right) \\
E_{\text{background}} &= \frac{U}{2}\left(3\bar{n}^2-\bar{n}+4\right)
\end{aligned} \tag{E46}$$

The effective Hamiltonian of the Fock-ring is shown in Fig.19 with $c_1=\frac{J_{\text{eff},1}}{2}$ and $c_2=\frac{J_{\text{eff},2}}{2}$. where

$$\begin{bmatrix} U & c_1 & 0 & 0 & 0 & c_2 \\ c_1 & U & c_2 & 0 & 0 & 0 \\ 0 & c_2 & U & c_1 & 0 & 0 \\ 0 & 0 & c_1 & U & c_2 & 0 \\ 0 & 0 & 0 & c_2 & U & c_1 \\ c_2 & 0 & 0 & 0 & c_1 & U \end{bmatrix} \cdot \begin{bmatrix} \psi_{1a} \\ \psi_{1b} \\ \psi_{2a} \\ \psi_{2b} \\ \psi_{3a} \\ \psi_{3b} \end{bmatrix} = \mathrm{E} \begin{bmatrix} \psi_{1a} \\ \psi_{1b} \\ \psi_{2a} \\ \psi_{2b} \\ \psi_{3a} \\ \psi_{3b} \end{bmatrix}$$

FIG. 19: Effective Hamiltonian for the Fock ring

$$\begin{aligned}
\psi_{2a} &= \psi_{1a}e^{i(2q)} & \psi_{3a} &= \psi_{1a}e^{-i(2q)} \\
\psi_{2b} &= \psi_{1b}e^{i(2q)} & \psi_{3b} &= \psi_{1b}e^{-i(2q)}
\end{aligned} \tag{E47}$$

Next we want to calculate the orbital occupation number. In this part we used another approximation $J_{\text{eff},1}=J_{\text{eff},2}$. This approximation is valid for large N. such that the approximates eigen-states are the Fock momentum states

$$|l\rangle = \frac{1}{\sqrt{L_{\text{eff}}}}\sum_{\tilde{x}=1,\ldots,6}e^{iq\tilde{x}}\,|\tilde{x}\rangle \tag{E48}$$

We mark the momentum states with the letter $q=\frac{2\pi}{L_{\text{eff}}}\cdot l$, $l\in\{1,2,3,4,5,6\}$. Now we can calculate analytically the approximated orbital occupation number M_κ.

The orbital occupation number of these $|l\rangle$ states using Eq.4

$$\begin{aligned}
\langle n_\kappa\rangle &= \langle l|b_\kappa^{\dagger}b_\kappa|l\rangle = \frac{1}{3}\sum_{j,g=1}^{3}e^{i\frac{2\pi}{3}\kappa(j-g)}\langle l|a_j^{\dagger}a_g|l\rangle \\
&= \frac{1}{3}\Big[\langle l|a_1^{\dagger}a_1|l\rangle + e^{-i\frac{2\pi}{3}\kappa}\langle l|a_1^{\dagger}a_2|l\rangle + e^{-2i\frac{2\pi}{3}\kappa}\langle l|a_1^{\dagger}a_3|l\rangle + e^{i\frac{2\pi}{3}\kappa}\langle l|a_2^{\dagger}a_1|l\rangle \\
&\quad + \langle l|a_2^{\dagger}a_2|l\rangle + e^{-i\frac{2\pi}{3}\kappa}\langle l|a_2^{\dagger}a_3|l\rangle + e^{2i\frac{2\pi}{3}\kappa}\langle l|a_3^{\dagger}a_1|l\rangle + e^{i\frac{2\pi}{3}\kappa}\langle l|a_3^{\dagger}a_2|l\rangle + \langle l|a_3^{\dagger}a_3|l\rangle\Big]
\end{aligned} \tag{E49}$$

	$\|\tilde{x}=1\rangle$	$\|\tilde{x}=2\rangle$	$\|\tilde{x}=3\rangle$	$\|\tilde{x}=4\rangle$	$\|\tilde{x}=5\rangle$	$\|\tilde{x}=6\rangle$
$\langle\tilde{x}=1\|$	$a_i^\dagger a_i$	$a_2^\dagger a_3$	–	–	–	$a_3^\dagger a_1$
$\langle\tilde{x}=2\|$	$a_3^\dagger a_2$	$a_i^\dagger a_i$	$a_2^\dagger a_1$	–	–	–
$\langle\tilde{x}=3\|$	–	$a_1^\dagger a_2$	$a_i^\dagger a_i$	$a_3^\dagger a_1$	–	–
$\langle\tilde{x}=4\|$	–	–	$a_1^\dagger a_3$	$a_i^\dagger a_i$	$a_3^\dagger a_2$	–
$\langle\tilde{x}=5\|$	–	–	–	$a_2^\dagger a_3$	$a_i^\dagger a_i$	$a_1^\dagger a_2$
$\langle\tilde{x}=6\|$	$a_1^\dagger a_3$	–	–	–	$a_2^\dagger a_1$	$a_i^\dagger a_i$

FIG. 20: Table that emphasize which $\langle\tilde{x}'|a_i^\dagger a_j|\tilde{x}\rangle \neq 0$

Lets check each element contribution using Fig.20:

$$\langle l|a_1^\dagger a_1|l\rangle = \frac{1}{6}\sum_{\tilde{x}=1}^{6}\langle\tilde{x}|a_1^\dagger a_1|\tilde{x}\rangle = \frac{1}{6}2(\bar{n}-1+\bar{n}+\bar{n}+1) = \bar{n} \tag{E50}$$

$$\langle l|a_1^\dagger a_2|l\rangle = \frac{1}{6}\left(e^{-iq}\langle\tilde{x}=3|a_1^\dagger a_2|\tilde{x}=2\rangle + e^{iq}\langle\tilde{x}=5|a_1^\dagger a_2|\tilde{x}=6\rangle\right) = \frac{1}{6}e^{i\frac{\phi}{3}}\left(\bar{n}e^{-iq}+(\bar{n}+1)e^{iq}\right) \tag{E51}$$

$$\langle l|a_1^\dagger a_3|l\rangle = \frac{1}{6}\left(e^{-5\cdot iq}\langle\tilde{x}=6|a_1^\dagger a_3|\tilde{x}=1\rangle + e^{-iq}\langle\tilde{x}=4|a_1^\dagger a_3|\tilde{x}=3\rangle\right) = \frac{1}{6}e^{-i\frac{\phi}{3}}\left(\bar{n}e^{iq}+(\bar{n}+1)e^{-iq}\right) \tag{E52}$$

$$\langle l|a_2^\dagger a_1|l\rangle = \frac{1}{6}\left(e^{iq}\langle\tilde{x}=2|a_2^\dagger a_1|\tilde{x}=3\rangle + e^{-iq}\langle\tilde{x}=6|a_2^\dagger a_1|\tilde{x}=5\rangle\right) = \frac{1}{6}e^{-i\frac{\phi}{3}}\left(\bar{n}e^{iq}+(\bar{n}+1)e^{-iq}\right) \tag{E53}$$

$$\langle l|a_2^\dagger a_2|l\rangle = \frac{1}{6}\sum_{\tilde{x}=1}^{6}\langle\tilde{x}|a_2^\dagger a_2|\tilde{x}\rangle = \frac{1}{6}2(\bar{n}-1+\bar{n}+\bar{n}+1) = \bar{n} \tag{E54}$$

$$\langle l|a_2^\dagger a_3|l\rangle = \frac{1}{6}\left(e^{iq}\langle\tilde{x}=1|a_2^\dagger a_3|\tilde{x}=2\rangle + e^{-iq}\langle\tilde{x}=5|a_2^\dagger a_3|\tilde{x}=4\rangle\right) = \frac{1}{6}e^{i\frac{\phi}{3}}\left((\bar{n}+1)e^{iq}+\bar{n}e^{-iq}\right) \tag{E55}$$

$$\langle l|a_3^\dagger a_1|l\rangle = \frac{1}{6}\left(e^{iq}\langle\tilde{x}=3|a_3^\dagger a_1|\tilde{x}=4\rangle + e^{5\cdot iq}\langle\tilde{x}=1|a_3^\dagger a_1|\tilde{x}=6\rangle\right) = \frac{1}{6}e^{i\frac{\phi}{3}}\left((\bar{n}+1)e^{iq}+\bar{n}e^{-iq}\right) \tag{E56}$$

$$\langle l|a_3^\dagger a_2|l\rangle = \frac{1}{6}\left(e^{-iq}\langle\tilde{x}=2|a_3^\dagger a_2|\tilde{x}=1\rangle + e^{iq}\langle\tilde{x}=4|a_3^\dagger a_2|\tilde{x}=5\rangle\right) = \frac{1}{6}e^{-i\frac{\phi}{3}}\left((\bar{n}+1)e^{-iq}+\bar{n}e^{iq}\right) \tag{E57}$$

$$\langle l|a_3^\dagger a_3|l\rangle = \frac{1}{6}\sum_{\tilde{x}=1}^{6}\langle\tilde{x}|a_1^\dagger a_1|\tilde{x}\rangle = \frac{1}{6}2(\bar{n}-1+\bar{n}+\bar{n}+1) = \bar{n} \tag{E58}$$

So Eq.E49 reduces to

$$\langle n_\kappa\rangle = \langle l|b_\kappa^\dagger b_\kappa|l\rangle = \frac{1}{18}\Big[3(6\bar{n}) + e^{-i\frac{2\pi}{3}\kappa}e^{i\frac{\phi}{3}}\left(\bar{n}e^{-iq}+(\bar{n}+1)e^{iq}\right) + e^{-2i\frac{2\pi}{3}\kappa}e^{-i\frac{\phi}{3}}\left(\bar{n}e^{iq}+(\bar{n}+1)e^{-iq}\right) + e^{i\frac{2\pi}{3}\kappa}e^{-i\frac{\phi}{3}}\left(\bar{n}e^{iq}+(\bar{n}+1)e^{-iq}\right)$$
$$+ e^{-i\frac{2\pi}{3}\kappa}e^{i\frac{\phi}{3}}\left((\bar{n}+1)e^{iq}+\bar{n}e^{-iq}\right) + e^{2i\frac{2\pi}{3}\kappa}e^{i\frac{\phi}{3}}\left((\bar{n}+1)e^{iq}+\bar{n}e^{-iq}\right) + e^{i\frac{2\pi}{3}\kappa}e^{-i\frac{\phi}{3}}\left((\bar{n}+1)e^{-iq}+\bar{n}e^{iq}\right)\Big]$$

$$\langle n_\kappa\rangle = \bar{n} + \frac{1}{18}\left(4\bar{n}cos(\frac{-2\pi}{3}\kappa+\frac{\phi}{3}-q)+4(\bar{n}+1)cos(-\frac{2\pi}{3}\kappa+\frac{\phi}{3}+q)+2\bar{n}cos(4\frac{2\pi}{3}\kappa+\frac{\phi}{3}-q)+2(\bar{n}+1)cos(4\frac{2\pi}{3}\kappa+\frac{\phi}{3}+q)\right) \tag{E59}$$

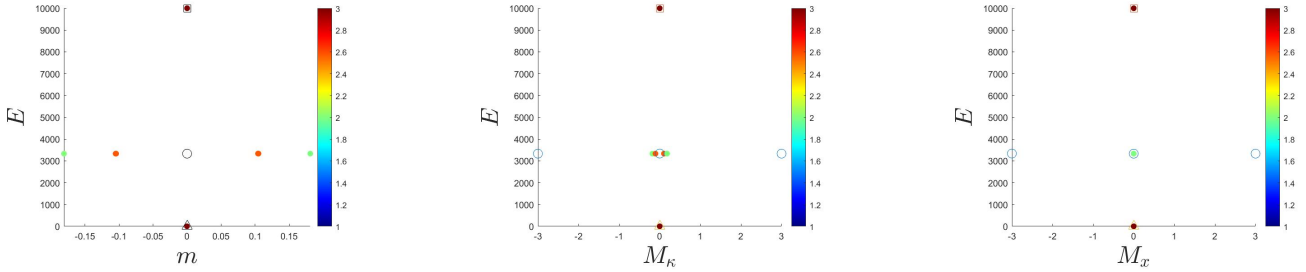
Finally, the momentum occupation numbers for the $|l\rangle$ states are

$$\langle n_\kappa\rangle = \bar{n} + \frac{1}{18}\left(4\bar{n}cos(\frac{-2\pi\kappa+\phi-\pi l}{3}) + 4(\bar{n}+1)cos(\frac{-2\pi\kappa+\phi+\pi l}{3}) + 2\bar{n}cos(\frac{4\pi\kappa+\phi-\pi l}{3}) + 2(\bar{n}+1)cos(\frac{4\pi\kappa+\phi+\pi l}{3})\right) \tag{E60}$$

Remember, the orbital occupation imbalance is define by

$$M_\kappa = \langle n_{\kappa=1}\rangle - \langle n_{\kappa=-1}\rangle = \frac{6\sqrt{3}}{18}\left(\bar{n}sin(\frac{\phi-\pi l}{3}) + (\bar{n}+1)sin(\frac{\phi+\pi l}{3})\right) \tag{E61}$$

As an example, see the case of $N = 3$ particles, namely, $\bar{n} = 1$. The full spectrum is shown in Fig. 21. There are 10 eigenstates: the upper states is actually three self trapped states, the lower state is the Mott state and in the middle there are 6 excitation states (the orange points contains 2 states). Zoom in helps us see better the middle floor, these



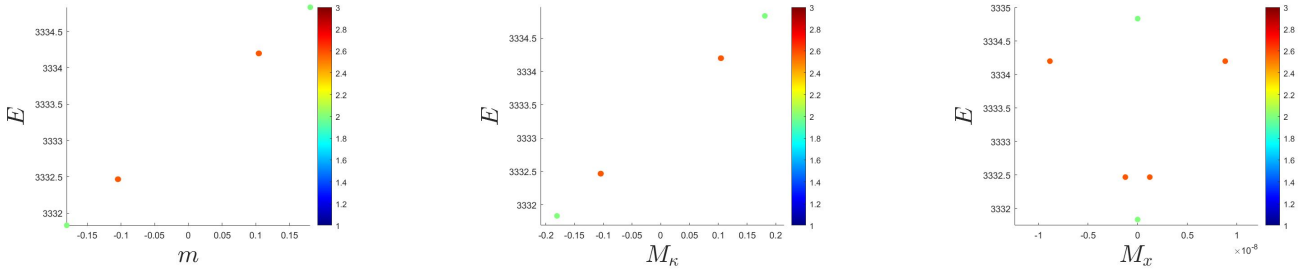
(a) Spectrum as function of modify occupation number $m = M_x + M_\kappa$

(b) Spectrum as function of momentum occupation number M_κ

(c) Spectrum as function of site occupation number M_x

FIG. 21: $M = 3, N = 3, \Phi = 3.1\pi, u = 10000$

six states, see Fig.22. We would like to connect the 6 states to the one particle excitation from Mott state. In order



(a) Modify occupation number m

(b) Momentum occupation number M_κ

(c) Site occupation number M_x

FIG. 22: **Zoom in of the middle floor of the spectrum in Fig.21**

to understand the phase space of the system, I drew the same diagram as Fig.6a, see Fig.23, the six middle states in the full spectrum are actually the momentum states of the blue ring in the diagram. We will define $|x\rangle$ as the 6 states in the Fock-space ring:

$$|x = 1\rangle = |0, 2, 1\rangle \qquad |x = 4\rangle = |2, 0, 1\rangle \tag{E62}$$
$$|x = 2\rangle = |0, 1, 2\rangle \qquad |x = 5\rangle = |2, 1, 0\rangle \tag{E63}$$
$$|x = 3\rangle = |1, 0, 2\rangle \qquad |x = 6\rangle = |1, 2, 0\rangle \tag{E64}$$

The 6 states are degenerate states which correspond to the site basis states where there are 2 particles in one site and another particle at a second site, see blue states in Fig.23. Through perturbation theory, the 6 degenerate states produce 6 momentum states which obey $M_x = 0$, see Fig.21c. We see that M_x spectrum, Fig.22c is symmetric as a result of the site symmetry, see Fig.22c. Moreover, the two green points has the smallest M_x value and the highest $|M_\kappa|$.

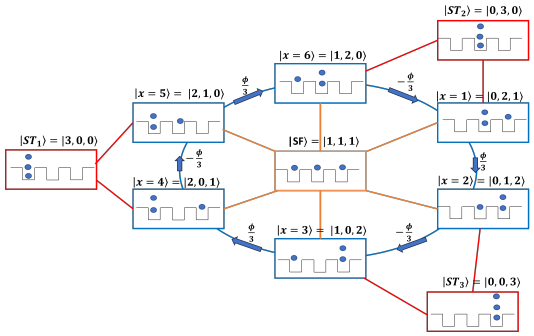
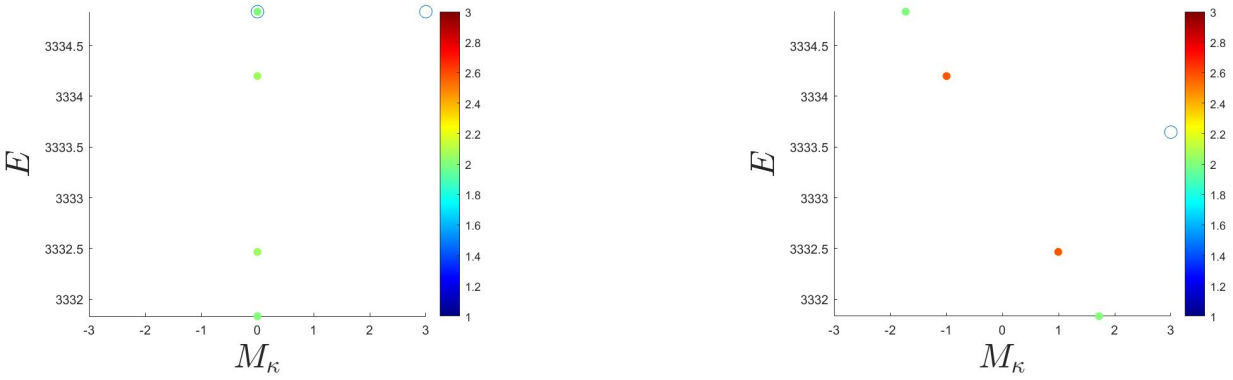


FIG. 23: States diagram for $N = 3$

Next, we examine the flux influence, when the flux changes the spectrum will rotate, see Fig.24



(a) For $\Phi = 0$

(b) For $\Phi = 1.6\pi$

FIG. 24: $M = 3, N = 3, u = 10000$

As we mention before, in the regular Fock basis there is no translation symmetry, since the phase of a jump between two states is $\tilde{\phi} = \pm\frac{\phi}{3}$ and the total flux for a cycle in the Fock space ring is $\phi_{\text{eff}} = 0$. We gauge the phase into the even states in a way that there will be a translation symmetry and the eigenstates will be the momentum states of Fock space. The gauge we use is

$$|\tilde{x}=1\rangle = |x=1\rangle = |0,2,1\rangle \qquad |\tilde{x}=4\rangle = e^{i\frac{\phi}{3}}|x=4\rangle = e^{i\frac{\phi}{3}}|2,0,1\rangle \tag{E65}$$

$$|\tilde{x}=2\rangle = e^{i\frac{\phi}{3}}|x=2\rangle = e^{i\frac{\phi}{3}}|0,1,2\rangle \qquad |\tilde{x}=5\rangle = |x=5\rangle = |2,1,0\rangle \tag{E66}$$

$$|\tilde{x}=3\rangle = |x=3\rangle = |1,0,2\rangle \qquad |\tilde{x}=6\rangle = e^{i\frac{\phi}{3}}|x=6\rangle = e^{i\frac{\phi}{3}}|1,2,0\rangle \tag{E67}$$

The effective hopping coefficient in this ring is $J_{\text{eff},1} = 2J$ and $J_{\text{eff},2} = J$. The analytical orbital occupation imbalance numbers of these $|l\rangle$ states are

$$M_\kappa = \langle n_{\kappa=1}\rangle - \langle n_{\kappa=-1}\rangle = \frac{6\sqrt{3}}{18}\left(sin(\frac{\phi-\pi l}{3}) + 2sin(\frac{\phi+\pi l}{3})\right) \tag{E68}$$

We compared the analytical calculations (black circle) the numerical diagonalization in Fig.25, we see that the M_κ are equal for the green states. Notice, the 4 orange states are degenerate states, the Matlab removes the degeneracy spontaneously, this is why the M_κ are not the same for these states.

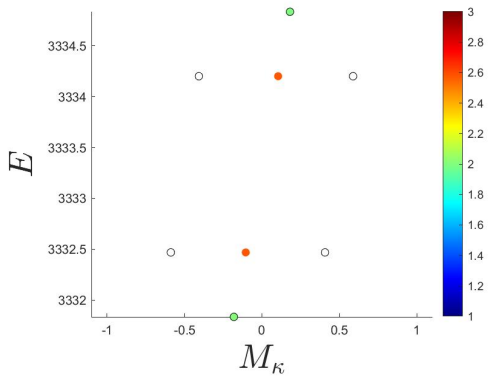


FIG. 25: The middle floor of the spectrum for $N = 3$. Black circle are the analytical calculation of Eq.27 and Eq.E60.

[F] Calculation for Non-Commensurate Number of Particles

Our technique is to simulate an effective Hamiltonian that will represent the lower part of the spectrum, near the Mott state. Namely, a ring system with 3 states $|x\rangle$.

$$H_{\text{eff}} = H_{J,\text{eff}} + H_{U,\text{eff}} + E_{\text{background}} \tag{F69}$$

The effective hopping coefficient can be found:

$$\left\langle \bar{n}, \bar{n}+1, \bar{n} \middle| a_2^\dagger a_1 \middle| \bar{n}+1, \bar{n}, \bar{n} \right\rangle = (\bar{n}+1) \tag{F70}$$

Such that

$$J_{\text{eff}} = J(\bar{n}+1) \tag{F71}$$

The hopping coefficient for all transition is $c = \frac{J_{\text{eff}}}{2} e^{i\frac{\phi}{3}}$.

Moreover, we need to find the constant energy of the already existing particles in the sites (background). The constant energy for arbitrary $\bar{n}$ can be found from Interaction term,H_U, in Eq.1.Now we change notation to the one particle excitation problem, namely, $\tilde{n}_j \to \bar{n} + \tilde{n}_i$ where $\tilde{n}_i \in \{0, 1\}$.

$$\begin{aligned} H_U &= \sum_{i=1}^{3} \frac{U}{2}(\bar{n}+\tilde{n}_i)(\bar{n}+\tilde{n}_i-1) = \sum_{i=1}^{3} \frac{U}{2}\left(\bar{n}^2 + 2\bar{n}\tilde{n}_i + \tilde{n}_i^2 - \bar{n} - \tilde{n}_i\right) \\ &= \frac{U}{2} 3(\bar{n}^2 - \bar{n}) + \sum_{i=1}^{3} \frac{U}{2} 2\bar{n}\tilde{n}_i + \sum_{i=1}^{3} \frac{U}{2}\tilde{n}_i(\tilde{n}_i - 1) = \frac{U}{2}\left(3(\bar{n}^2 - \bar{n}) + 2\bar{n}\right) + \sum_{i=1}^{3} \frac{U}{2}\tilde{n}_i(\tilde{n}_i - 1) \\ H_{U,\text{eff}} &= \frac{U}{2}\left(3\bar{n}^2 - \bar{n}\right) + \sum_{i=1}^{3} \frac{U}{2}\tilde{n}_i(\tilde{n}_i - 1) = E_{\text{background}} + H_{U,\text{eff}} \end{aligned} \tag{F72}$$

Notice that $H_{U,\text{eff}} = \sum_{i=1}^{3} \frac{U}{2}\tilde{n}_i(\tilde{n}_i - 1)$ and that for all one particle excitation state the $\langle x|H_{U,\text{eff}}|x\rangle = 0$, for all possible excited states. Finally, we get,

$$E_{\text{background}} = \frac{U}{2}\left(3\bar{n}^2 - \bar{n}\right) \tag{F73}$$

There are 3 degenerate states for the one particle excitation with the same hopping coefficient connecting them, hence, the system has a translation symmetry and breaking the symmetry yields 3 momentum states $|p\rangle$ of the form:

$$|p\rangle = \frac{1}{\sqrt{3}} \sum_{x=\{1,2,3\}} e^{iPx} |x\rangle, \quad P = \frac{2\pi}{3} p, p \in \{1, 2, 3\} \tag{F74}$$

Finally the energy for these Fock-momentum states is immediate:

$$E_p = \langle p|H|p\rangle = E_{\text{background}} - J_{\text{eff}} \cdot cos\left(\frac{\phi}{3} - \frac{2\pi}{3} p\right) \tag{F75}$$

Next, we will calculate the momentum occupation number for these states:

$$\langle n_\kappa\rangle = \langle p|b_\kappa^\dagger b_\kappa|p\rangle = \frac{1}{3}\sum_{j,g=1}^{3} e^{i\frac{2\pi}{3}\kappa(j-g)}\langle p|a_j^\dagger a_g|p\rangle = \frac{1}{3}\Big(\langle p|a_1^\dagger a_1|p\rangle + e^{-i\frac{2\pi}{3}\kappa}\langle p|a_1^\dagger a_2|p\rangle + e^{-2i\frac{2\pi}{3}\kappa}\langle p|a_1^\dagger a_3|p\rangle + \\ + e^{i\frac{2\pi}{3}\kappa}\langle p|a_2^\dagger a_1|p\rangle + \langle p|a_2^\dagger a_2|p\rangle + e^{-i\frac{2\pi}{3}\kappa}\langle p|a_2^\dagger a_3|p\rangle + e^{2i\frac{2\pi}{3}\kappa}\langle p|a_3^\dagger a_1|p\rangle + e^{i\frac{2\pi}{3}\kappa}\langle p|a_3^\dagger a_2|p\rangle + \langle p|a_3^\dagger a_3|p\rangle\Big) \tag{F76}$$

Lets find each contribution:

$$\langle p|a_1^\dagger a_1|p\rangle = \frac{1}{3}\Big(\langle x=1|a_1^\dagger a_1|x=1\rangle + \langle x=2|a_1^\dagger a_1|x=2\rangle + \langle x=3|a_1^\dagger a_1|x=3\rangle\Big) = \frac{\bar{n}+1+\bar{n}+\bar{n}}{3} = \frac{3\bar{n}+1}{3} \tag{F77}$$

$$\langle p|a_1^\dagger a_2|p\rangle = \frac{1}{3}e^{iP(2-1)}\langle x=1|a_1^\dagger a_2|x=2\rangle = \frac{1}{3}e^{iP}(\bar{n}+1) \tag{F78}$$

$$\langle p|a_1^\dagger a_3|p\rangle = \frac{1}{3}e^{iP(3-1)}\langle x=1|a_1^\dagger a_3|x=3\rangle = \frac{1}{3}e^{2iP}(\bar{n}+1) \tag{F79}$$

$$\langle p|a_2^\dagger a_1|p\rangle = \frac{1}{3}e^{iP(1-2)}\langle x=2|a_2^\dagger a_1|x=1\rangle = \frac{1}{3}e^{-iP}(\bar{n}+1) \tag{F80}$$

$$\langle p|a_2^\dagger a_2|p\rangle = \frac{1}{3}\Big(\langle x=1|a_2^\dagger a_2|x=1\rangle + \langle x=2|a_2^\dagger a_2|x=2\rangle + \langle x=3|a_2^\dagger a_2|x=3\rangle\Big) = \frac{\bar{n}+\bar{n}+1+\bar{n}}{3} = \frac{3\bar{n}+1}{3} \tag{F81}$$

$$\langle p|a_2^\dagger a_3|p\rangle = \frac{1}{3}e^{iP(3-2)}\langle x=2|a_2^\dagger a_3|x=3\rangle = \frac{1}{3}e^{iP}(\bar{n}+1) \tag{F82}$$

$$\langle p|a_3^\dagger a_1|p\rangle = \frac{1}{3}e^{iP(1-3)}\langle x=3|a_3^\dagger a_1|x=1\rangle = \frac{1}{3}e^{-2iP}(\bar{n}+1) \tag{F83}$$

$$\langle p|a_3^\dagger a_2|p\rangle = \frac{1}{3}e^{iP(2-3)}\langle x=3|a_3^\dagger a_2|x=2\rangle = \frac{1}{3}e^{-iP}(\bar{n}+1) \tag{F84}$$

$$\langle p|a_3^\dagger a_3|p\rangle = \frac{1}{3}\Big(\langle x=1|a_3^\dagger a_3|x=1\rangle + \langle x=2|a_3^\dagger a_3|x=2\rangle + \langle x=3|a_3^\dagger a_3|x=3\rangle\Big) = \frac{\bar{n}+\bar{n}+\bar{n}+1}{3} = \frac{3\bar{n}+1}{3} \tag{F85}$$

So Eq.F76 reduces to

$$\langle n_\kappa\rangle = \frac{1}{3}\Big(\frac{3\bar{n}+1}{3} + e^{-i\frac{2\pi}{3}\kappa}\frac{1}{3}e^{iP}(\bar{n}+1) + e^{-2i\frac{2\pi}{3}\kappa}\frac{1}{3}e^{2iP}(\bar{n}+1) + \\ + e^{i\frac{2\pi}{3}\kappa}\frac{1}{3}e^{-iP}(\bar{n}+1) + \frac{3\bar{n}+1}{3} + e^{-i\frac{2\pi}{3}\kappa}\frac{1}{3}e^{iP}(\bar{n}+1) + e^{2i\frac{2\pi}{3}\kappa}\frac{1}{3}e^{-2iP}(\bar{n}+1) + e^{i\frac{2\pi}{3}\kappa}\frac{1}{3}e^{-iP}(\bar{n}+1) + \frac{3\bar{n}+1}{3}\Big) \\ = \frac{1}{9}\Big(3(3\bar{n}+1) + 2e^{-i\frac{2\pi}{3}\kappa}e^{iP}(\bar{n}+1) + 2e^{i\frac{2\pi}{3}\kappa}e^{-iP}(\bar{n}+1) + e^{2i\frac{2\pi}{3}\kappa}e^{-2iP}(\bar{n}+1) + e^{-2i\frac{2\pi}{3}\kappa}e^{2iP}(\bar{n}+1)\Big)$$

So finally we get

$$\langle n_\kappa\rangle = \frac{1}{9}\Big(3(3\bar{n}+1) + (\bar{n}+1)\Big[4cos(\frac{2\pi(p-\kappa)}{3}) + 2cos(\frac{4\pi(p-\kappa)}{3})\Big]\Big) \tag{F86}$$

And the orbital occupation imbalance is

$$M_\kappa = \langle n_{\kappa=1}\rangle - \langle n_{\kappa=-1}\rangle = \frac{\bar{n}+1}{9}\Big(4cos(\frac{2\pi(p-1)}{3}) + 2cos(\frac{4\pi(p-1)}{3}) - 4cos(\frac{2\pi(p+1)}{3}) - 2cos(\frac{4\pi(p+1)}{3})\Big)$$

$$M_\kappa = \frac{2\sqrt{3}(\bar{n}+1)}{9}\Big(2sin(\frac{4\pi p}{6}) - sin(\frac{8\pi p}{6})\Big) \tag{F87}$$

As an example see the case of $N = 4$ particles, namey, $\bar{n} = 1$. For $u = 10000$ we get $E_{\text{background}} = 2500$.
The full spectrum of the regular BHH in Fig.26. Now we add the analytical calculation for the effective system

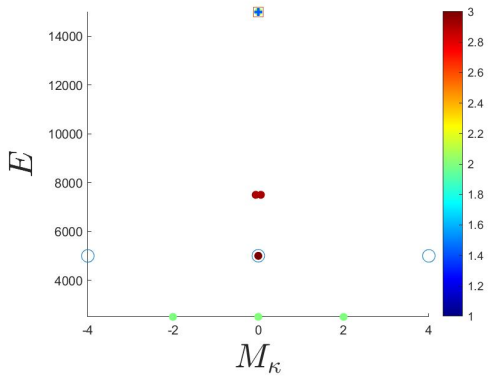


FIG. 26: E(M_κ) for M=3 N=4 $\Phi = 3.1\pi$

with black circles and focus on the lower part of Fig.26, namely we zoom to a region near $E_{\text{background}}$, see Fig.27.

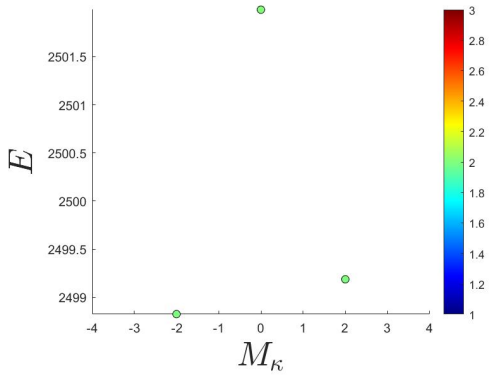
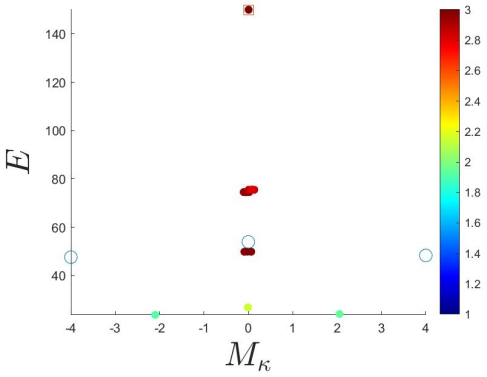
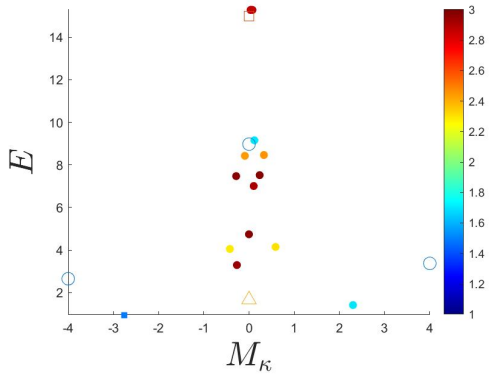


FIG. 27: E(M_κ) as in Fig.26 with the analytical calculation for the effective system

Next we will demonstrate how the level of excitation get closer as u get smaller, see Fig.28 We see that for $u = 100$



(a) $u = 100$



(b) $u = 10$

FIG. 28: Smaller u for $N = 4$

the two lower levels are still separated although the purity of the lower states changed. For $u = 10$ the two levels are mixed together, pertubation theory doesn't work.

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