

Supersolid phase in eBHM with current

Takuya Kitagawa, Eugene Demler

Abstract

Bose-Hubbard Model with nearest neighbor interaction displays supersolid phase in the ground state as previously shown in [2],[3],[4],[5]. We explored Bose-Hubbard Model with nearest-neighbor interaction in triangular lattice in the presence of current. In particular, we identified the dynamical instability due to current in the phase diagram. We found that supersolid phase can be induced from superfluid phase by introducing current into the system.

1 introduction

Despite of the attention it attracts, realization and observation of supersolid phase have been evasive. Supersolid phase is the phase which exhibit both charge localization and superfluidity. It breaks translational and rotational symmetry due to a partial charge localization, while keeping non-zero off-diagonal elements, i.e. $\langle a \rangle \neq 0$. It has been shown that this supersolid phase occurs in Bose-Hubbard Model(BHM) with neighboring interactions (extended BHM) in works such as [2],[3],[4] and [5]. When there are repulsions among neighboring sites, the formation of a sublattice and modulation of density are preferred to distributing atoms equally at each site. This leads to the charge localization, that is not observed in ordinary Bose-Hubbard Model. A similar effect is expected from superlattice, and BEC in superlattice has been theoretically investigated and shown to have supersolid phases as well.

Recently p-wave atomic states are experimentally realized in BEC in optical lattice[1]. An atom with p-wave wavefunction spatially extends beyond one site and overlap with wavefunctions in other sites. This effect can be modeled by BHM with neighbor interactions. This is an exciting advancement that suggests the possibility of observing supersolid phase in such a system. Therefore, it is important to investigate the behavior of BHM with neighbor interactions.

In this work, we have studied extended BHM in triangular lattice with current. As a result, we obtained J vs k phase diagram, where J is the hopping strength and k is the phase twist. In particular, we have shown

this supersolid phase can be induced by introducing current into BEC in optical lattice. Below, we present the result followed by the methodology taken to obtain the result.

2 Phase Diagram for Partial Filling with Current

We numerically found the phase diagram of extended Bose-Hubbard Model in triangular lattice with current(Figure.1). We note that phase twist and current are related through $I = \frac{dE}{dk}$, where I is the current in the system. Therefore, introducing phase twist k corresponds to introducing the current I . The Hamiltonian with phase twist is given by

$$H_e = -J \left(\sum_{i,j \in O_i} a_i^\dagger a_j \right) e^{ik(r_j - r_i)} + \frac{U}{2} \left(\sum_i n_i(n_i - 1) \right) + V \left(\sum_{i,j \in O_i} n_i n_j \right) \quad (1)$$

, where O_i contains nearest-neighbor sites of i and J, V, U, k are hopping term, nearest-neighbor interaction, on-site interaction, and phase twist respectively. Here, I chose $U = 5, V = 1$. This choice of parameter corresponds to the ground states with no more than one particle per site. When V is increased relative to U , a ground state can have more than one particle per site. In addition, I chose canonical-ensemble, and set the average number of particles at one site to be $\rho = 7/12$. The motivation for this choice comes from the previous result ([5]) by Gan.et.al. In the paper, they showed that in filling $\rho < 1/3$, supersolid phase is unstable toward the phase separatoin(PS). Therefore, it is important to treat $1/3 < \rho$ when studying supersolid phase. Nonetheless, it is trivial to change these conditions in practice.

Phase diagram is plotted J against k . Superfluid(S.F.) order parameter increases as J becomes large, charge density wave (CDW) order parameter increases as J becomes small. Therefore, in the region between those, we have supersolid regime. Since we are here considering non-commesurate filling, S.F. order parameter persists down to $J = 0$, so supersolid phase also continues down to $J = 0$. We considered CDW with one-third the periodicity of the original lattice. In practice, this means we allow three inequivalent sites, A, B, C (see Figure.3).

Introduction of current to the system can lead to dynamical instability. The dynamical instability in BHM is studied by E. Altman,et.al [7] and experimentally observed by MInguscio,et.al[8]. They showed that BEC with strong uniform current decays. Similar physics applies to this system as well. However, there is a distinct difference in our dynamical instability line in Figure.1. The dynamical instability line in Figure.1 has kinks. These kinks

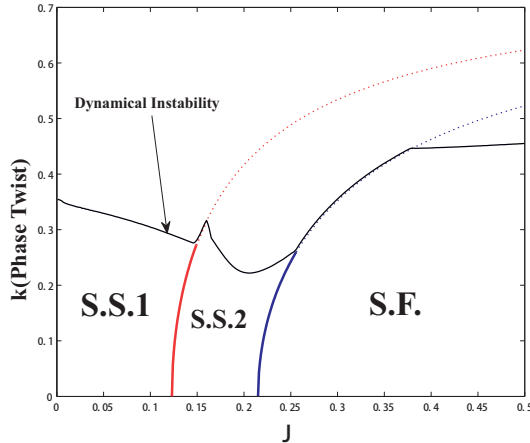


Figure 1: Phase Diagram of extended Bose-Hubbard Model, J (hopping term) vs k (phase twist) obtained within Gutzwiller approximation. Phase twist (k) is measured in units of π . To produce this phase diagram, we set $U = 5, V = 1, N = 7/12$, where U is the on-site interaction, V is neighbor-interaction, and N is the average number of particles per site. Also, phase twist k is in the direction $\theta = 0$ (See Figure.3) in real space. The black line is the dynamical instability. Red and blue lines are the continuation of parts of dynamical instability which we identify as phase transition line in Figure.5.

signify different mechanisms that can cause dynamical instabilities. One mechanism is the one investigated in the paper by E. Altman, et.al and this is simply due to overflow of phase twist. The other mechanism that we identify in this paper is the tendency of phase transition. As we describe in details below (see Figure.5), the phase of ground states depends on the phase twist k . For a given J , the system encounters phase transition point as it increases phase twist k . When this happens, dynamical instability sets in before the overflow of the twist occurs. Since these two mechanisms set in independently, there is a kink on the dynamical instability line. In particular, the instability line in Figure.1 coincides with the phase transition lines in Figure.5. This is emphasized by the red and blue lines in Figure.1

In supersolid phase 1(S.S.1), the number of particle in three inequivalent sites (A, B, C in the Figure.3) is given by $(1 - \alpha, 3/4 - \alpha, 0 + 2\alpha)$ where α is a small number, whereas in supersolid phase 2 (S.S.2), it is given by $(7/8 - \alpha, 7/8 - \alpha, 0 + \alpha)$. Superfluid phase is such that it is given by $(7/12, 7/12, 7/12)$.

These boundaries of different phases in the diagram can be understood

in the following way. As we describe in details below, the effect of current is given by the factor $e^{ik(r_j-r_i)}$ multiplied to the hopping term J . In our analysis, this term effectively changes J to $JS(k)$, where $S(k)$ is a function of phase twist. This function $S(k)$ critically depends on the geometry of the lattice. In the case of triangular lattice, the function $S(k)$ is monotonically decreasing when $0 < k < 3\pi/4$. Therefore, increasing k effectively decreases J , giving rise to the shape of the boundary in the diagram.

3 Ground State of eBHM

We first consider the phase diagram of the ground state (See Figure.3). We start from the following Hamiltonian of eBHM,

$$H_e = -J \left(\sum_{i,j \in O_i} a_i^\dagger a_j \right) + \frac{U}{2} \left(\sum_i n_i(n_i - 1) \right) + V \left(\sum_{i,j \in O_i} n_i n_j \right) - \mu \sum_i n_i$$

, where O_i contains the nearest-neighborhood of site i and J, V, U, μ are hopping term, nearest-neighbor interaction, on-site interaction, and chemical potential respectively. Note that we use grand canonical ensemble for the computation of ground state. As before, we look at the particular parameter space $U = 5, V = 1$.

We look for CDW of the sublattice with one third the periodicity of the original lattice. To this end, we allow three inequivalent sites in the lattice. See Figure.3. The sublattice is shown with dotted line in the Figure.3. We define the direction $\theta = 0$ and $\theta = \pi/3$ in the real space to be the direction of two of the primitive vectors of triangular lattice (See Figure.3).

In order to find the ground state of this Hamiltonian, we use variational method. We start with generalized Gutzwiller approximation in the following form,

$$|G\rangle = \prod_i \left(\sum_n c_n |n\rangle \right)$$

where i runs over all the sites. This form of Gutzwiller approximation assumes that the ground state is separable. We further restrict the Hilbert space by including only five states ($n = 0, 1, 2, 3, 4$) at each site. We will only look at the cases in which average filling is less than 1, so this approximation should be valid in our consideration. Now under these assumptions, we minimize $\langle G | H_e | G \rangle / \langle G | G \rangle$. We present the result in Figure.3.

A similar result with different parameters is obtained by [5]. To produce the diagram above, we used Superfluid order parameter operator given by

$$SF = \frac{1}{3}(a_A + a_B + a_C)$$

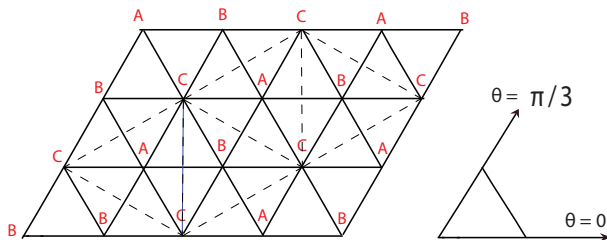


Figure 2: Triangular lattice with sublattice structure. We consider three inequivalent sites in the triangular lattice and they are denoted by A, B, C above. We look for charge localization in sublattice, which is denoted by dotted line. In the picture on the right, we defined $\theta = 0$ direction in the real space.

so that the order parameter is given by $\langle SF \rangle$. CDW order parameter operator associated with our sublattice is given by

$$CDW = \rho_k \quad (2)$$

$$= \left(\sum_i a_i^\dagger a_i e^{-i\vec{k} \cdot \vec{r}_i} \right) \quad (3)$$

where k is wave vector of sublattice, summation i running over all the lattice sites and r_i is the position of the lattice site. In the case of triangular sublattice, we take $\vec{k} = (\frac{4\pi}{3}, 0)$. CDW phase is characterized by $\langle SF \rangle = 0$ and $\langle CDW \rangle \neq 0$, whereas S.F. is characterized $\langle SF \rangle \neq 0$ and $\langle CDW \rangle = 0$. S.S. phase is defined by the region $\langle SF \rangle \neq 0$ and $\langle CDW \rangle \neq 0$. The phase diagram clearly shows the existence of supersolid phase between CDW and superfluid (S.F.) phases. Note that there could be more than one type of S.S. phase. The order parameters at $N = \frac{7}{12}$ is plotted below(Figure.4).

4 Phase Diagram with Phase Twist

4.1 Phase Diagram

First, we consider the phase diagram J vs k without the dynamical instability(See Figure.5). The consideration of this simplified phase diagram gives us an intuitive understanding of the phase diagram in Figure.1. We will consider the dynamical instability in the next section.

We introduce current into the system by going to the moving frame.

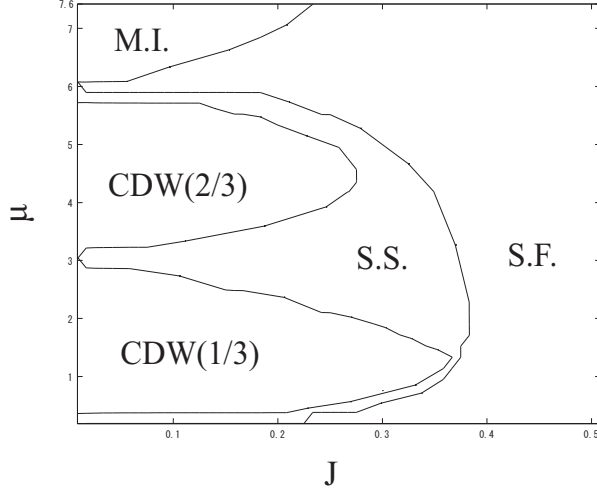


Figure 3: Phase diagram μ vs J of extended Bose-Hubbard Model within Gutzwiller approximation. Here, we set $U = 5, V = 1$. Note that in Gutzwiller approximation, we do not explicitly obtain the phase separation instability, which is argued to exist when $N < 1/3$ and possibly $N > 2/3$. The phase space denoted by S.S. includes many different supersolid phases.

Namely, we change the hopping term of the Hamiltonian such that

$$Ja_i^\dagger a_j \rightarrow Ja_i^\dagger a_j e^{ik \cdot (r(j) - r(i))}$$

where \vec{k} is the vector of the current we want to introduce. If we use the Gutzwiller approximation with real coefficients, we have $\langle a_i \rangle = \langle a_i^\dagger \rangle$. Then effective energy in moving frame is described by

$$\begin{aligned} \langle H_k \rangle &= -6S(k)J(\langle a_A \rangle \langle a_B \rangle + \langle a_B \rangle \langle a_C \rangle + \langle a_C \rangle \langle a_A \rangle) \\ &+ \frac{U}{2} \left(\sum_i n_i(n_i - 1) \right) + 3V \left(\sum_{i,j} n_i n_j \right) \end{aligned}$$

where $S(k) = (1/3)(\cos(\vec{k} \cdot \vec{a}) + \cos(\vec{k} \cdot \vec{b}) + \cos(\vec{k} \cdot \vec{c}))$ with $\vec{a} = (1, 0), \vec{b} = (1/2, \sqrt{3}/2), \vec{c} = (-1/2, \sqrt{3}/2)$. Note that we set the distance between nearest neighbor atom equal to be 1, and the vectors \vec{a}, \vec{b} correspond to the primitive vectors of triangle lattice. Therefore, introduction of current to the system is effectively the same as changing the hopping term $J \rightarrow JS(k)$. We plotted the phase diagram with phase twist k in the direction of $\theta = 0$ (Figure.3) in Figure.5.

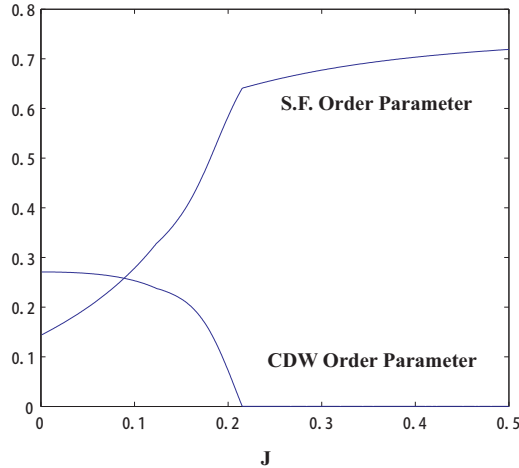


Figure 4: S.F. and CDW Order parameter in eBHM with $U = 5, V = 1, N = 7/12$. There are two phase transitions at $J \approx 0.13$ and $J \approx 0.22$.

4.2 Diagram with Dynamical Instability

We now consider where dynamical instability occurs in the phase diagram. The dynamical instability in S.F. phase is analyzed before and well-understood [7]. In two dimension, the idea is the following. Energy E is a function of phase twist k , so that we can write it as $E(k)$. Now we consider the case in which quantum and thermal fluctuations varies the value of \vec{k} at different points in the system. For a simple case, we have $\frac{1}{2}E(k + \delta k) + \frac{1}{2}E(k - \delta k)$ as the total energy. However, this is

$$\frac{1}{2}E(k + \delta k) + \frac{1}{2}E(k - \delta k) = E(k) + \frac{1}{2} \begin{pmatrix} \delta k_x & \delta k_y \end{pmatrix} \begin{pmatrix} \frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} \\ \frac{\partial^2 E}{\partial k_y \partial k_x} & \frac{\partial^2 E}{\partial k_y^2} \end{pmatrix} \begin{pmatrix} \delta k_x \\ \delta k_y \end{pmatrix}.$$

When an eigenvalue of the hessian of $E(k)$ is negative, the system is unstable toward inhomogeneous current. In S.F. regime, the critical current obtained by this method agrees with the linear instability analysis in Gross-Pitaevskii equation in triangular lattice. See Appendix for the details. Outside of S.F. regime, we carried out numerical analysis in Gutzwiller approximation stated above. This calculation becomes significantly simpler through the relation

$$\left. \frac{\partial^2 E(k)}{\partial k_i \partial k_j} \right|_{J=J_0, \vec{k}} = J_0 \left. \frac{dE(J)}{dJ} \right|_{J=J_0 S(\vec{k})} \frac{\partial^2 S(k)}{\partial k_i \partial k_j} + J_0^2 \left. \frac{d^2 E}{dJ^2} \right|_{J=J_0 S(\vec{k})} \frac{\partial S}{\partial k_i} \frac{\partial S}{\partial k_j}$$

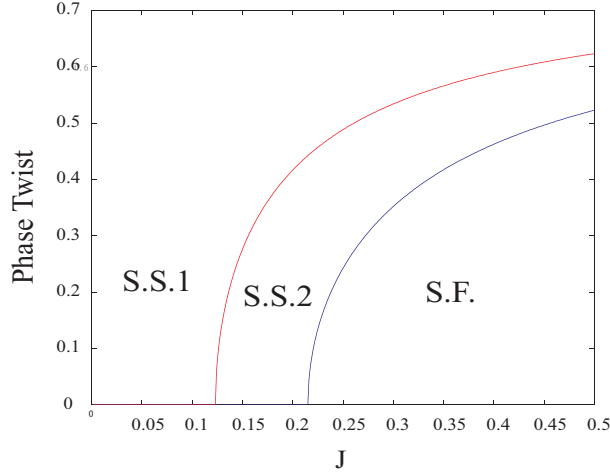


Figure 5: Phase Diagram of eBHM, J (hopping strength) against k (phase twist) within Gutzwiller approximation with $U = 5, V = 1, N = 7/12$. Again, k is taken to be in the direction of $\theta = 0$ in Figure.3.

where $E(J)$ is $\langle H_e \rangle$ and treated as a function of hopping term J . As is apparent from the expression, the first and second derivative of $E(J)$ with some weights through $S(k)$ determines the instability points. As we see below, the phase transitions from $S.F.$ to $S.S.$ as well as from $S.S.1$ to $S.S.2$ creates nonanalytical points of $\frac{d^2 E}{dJ^2}$, leading to the instability.

4.3 Dependence of the Phase Diagram on the Direction of Current

The phase diagram with current in various direction shows a similar result. This is because the dependence of $S(k)$ on the direction of k is weak.

4.4 Formation of Current Domain

The possibility of current domain is pointed out in [6] for fermion case. We can check the possibility by looking at the eigenvector of the instability. If the eigenvector has the component perpendicular to the direction of current, then our system tends toward the formation of current domain. Our numerical result shows that eigenvector is always in the direction of the current, indicating that current domain formation is not favored under the condition that $U = 5, V = 1$.

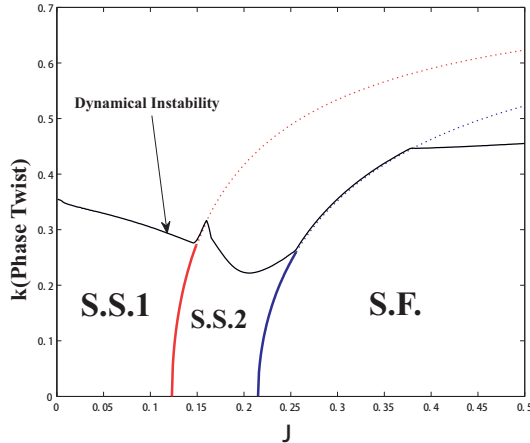


Figure 6: Phase Diagram of extended Bose-Hubbard Model, J (hopping term) vs k (phase twist) obtained by Gutzwiller approximation. Here, we have $U = 5, V = 1, N = 7/12$, where U is the on-site interaction, V is neighbor-interaction, and N is the average number of particles per site. Also, phase twist k is in the direction $\theta = 0$ (See Figure.3) in real space. The purple line is the dynamical instability. Red and blue lines are the continuation of parts of dynamical instability which we identify as phase transition line in Figure.5.

5 Limit and Problems

I would like to discuss the limit of my method.

First, since Gutzwiller approximation is a kind of mean-field theory, it can give us unphysical result, though from previous results, we assume that this approximation gives us a good starting point to understand Bose-Hubbard Model. In my calculation for $N = 2/3$, I observed a discontinuity in order parameter at the phase transition from S.F. to S.S. Since at different N , we only observe the second phase transition, so we believe this first order phase transition is artifact of mean-field theory. However, this indicates the limit of Gutzwiller approximation.

Acknowledgement

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A Appendix

A.1 Linear Instability Analysis

In this section, we present the result of linear instability analysis in triangular lattice in superfluid regime. Linear instability analysis is developed in works such as [9] and [10].

We start from the Gross-Pitaevskii equation for extended Bose-Hubbard Model. Hamiltonian for extended Bose-Hubbard Model is given by

$$H_e = -J \left(\sum_{i,j} a_i^\dagger a_j \right) + \frac{U}{2} \left(\sum_i n_i(n_i - 1) \right) + V \left(\sum_{i,j} n_i n_j \right). \quad (4)$$

(Discrete) Gross-Pitaevskii equation corresponding to this Hamiltonian is given by

$$i \frac{\partial \psi_i}{\partial t} = -J \sum_{k \in O} \psi_k + U |\psi_i|^2 \psi_i + V \psi_i \sum_{k \in O} \psi_k. \quad (5)$$

where O is the nearest-neighbor sites in triangular lattice.

We can find the steady-state solution to this equation of the form $\psi_i(t, x) = \psi_0 \exp(i(\vec{k} \cdot \vec{x} - \nu t))$ where ψ_0 is independent of t and x . Then, ν given by

$$\nu = -JS(k) + U |\psi_0|^2 + 6V |\psi_0|^2$$

with $S(k) = 2(\cos(\vec{k} \cdot \vec{a}) + \cos(\vec{k} \cdot \vec{b}) + \cos(\vec{k} \cdot \vec{c}))$ with $\vec{a} = (1, 0)$, $\vec{b} = (1/2, \sqrt{3}/2)$, $\vec{c} = (-1/2, \sqrt{3}/2)$.

Now the idea is the following. We introduce a perturbation to the phase twist \vec{k} . Since Gross-Pitaevskii equation is linear, only phase twists with opposite sign couple through complex conjugation, so without loss of generality, we consider the perturbed wave function of the form $\psi_i(\vec{q}) = (\psi_0 + u(t)e^{i\vec{q} \cdot \vec{x}} + v^*(t)e^{-i\vec{q} \cdot \vec{x}})e^{i(\vec{k} \cdot \vec{x} - \nu t)}$. We suppose that the coefficient of the perturbation $u(t)$ and $v(t)$ are small and time dependent. To the linear order of u and v , we expand the right-hand side of Gross-Pitaevskii equation and analyze the time dependence of u and v . If either of them grows in time, that is, if the eigenvalue of the matrix on the right hand side is imaginary, then the system is unstable toward the development of such perturbation. We identify this as the onset of dynamical instability.

Expansion of the Gross-Pitaevskii equation to the leading order gives

$$\frac{d}{dt} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} A + C|\psi_0|^2 & C(\psi_0)^2 \\ -C(\psi_0^*)^2 & B - C|\psi_0|^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \quad (6)$$

where $A = -J(S(k+q) - S(k))$, $B = J(S(k-q) - S(k))$, and $C = (U + VS(q))$. Now note that $S(q) = S(-q)$. Schematically, we obtain the

eigenvalue of the form $\alpha \pm c\sqrt{\beta}$. Since we are only interested in whether the eigenvalue is imaginary or not, we can only look at the inside of the square root of the eigenvalues, β . This value is given by

$$\beta = J(2S(k) - S(k+q) - S(k-q)) \left(4|\psi_0|^2 (U + VS(q)) + J(2S(k) - S(k+q) - S(k-q)) \right)$$

When this expression becomes negative, the eigenvalue becomes imaginary, so that u or v blows up as $t \rightarrow \infty$. In the superfluid regime, we assume that the second factor of this expression is positive. This is true when the first factor is close to zero (the instability point). Also this is true when $4UN \gg J$, where $N = |\psi_0|^2$ is the average number of particles per site.

Then the sign of the expression is dictated by $(2S(k) - S(k+q) - S(k-q))$. For a given \vec{k} , we can minimize this expression over \vec{q} and if the minimum is negative, dynamical instability sets in at this phase twist \vec{k} . We can check this for various \vec{k} .

We checked that the dynamical instability analysis through mass matrix in the article agrees with linear instability analysis in superfluid regime. The result is shown below. Figure.7 is the minimum value of the function $(2S(k) - S(k+q) - S(k-q))$ for phase twist in $\theta = 0$ direction in Figure.3 at various magnitude k . We note that this function becomes negative at $|k| \approx 0.59$.

Figure.8 is the extension of instability line in Figure.1 from $J = 1$ to $J = 6$. In the Figure, we denoted the dynamical instability line expected from linear instability analysis above. As one can see, the instability from mass matrix indeed approaches $|k| \approx 0.59$ as $J \rightarrow \infty$.

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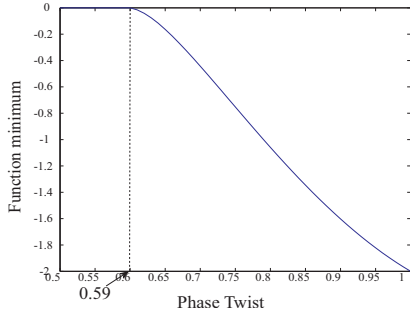


Figure 7: The result of Linear Instability Analysis. Plotted is the minimum of function $(2S(k) - S(k+q) - S(k-q))$ with phase twist k in the direction of $\theta = 0$. At $|k| \approx 0.59$, the function minimum takes negative value, indicating the dynamical instability

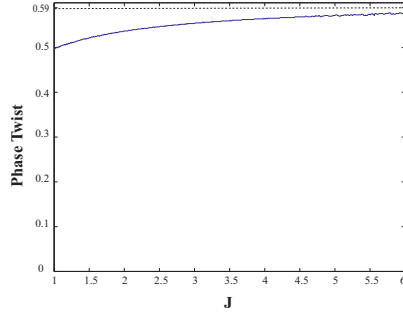


Figure 8: Extension of the dynamical instability line in Figure.1 in the superfluid regime, between $J = 1$ and $J = 6$ where J is the hopping strength. The instability line asymptotically approaches a value close to $|k| \approx 0.59$, which is the dynamical instability point expected from linear instability analysis. This point is indicated above as the dotted line.

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