Mean-field study of the Bose-Hubbard model in Penrose lattice

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We examine the Bose-Hubbard model in the Penrose lattice based on inhomogeneous mean-field theory. Since averaged coordination number in the Penrose lattice is four, mean-field phase diagram consisting of the Mott insulator (MI) and superfluid (SF) phase is similar to that of the square lattice. However, the spatial distribution of Bose condensate in the SF phase is significantly different from uniform distribution in the square lattice. We find a fractal structure in its distribution near the MI-SF phase boundary. The emergence of the fractal structure is a consequence of cooperative effect between quasiperiodicity in the Penrose lattice and criticality at the phase transition.

Introduction—Quasicrystals have aperiodic structure different from fully disordered one. Although translational symmetry is absent, the presence of sharp spots in Bragg reflection indicates long-range order [1][2]. Quasicrystals can be realized even in bilayer graphene [3] and photonic lattices [4]. In addition to various characteristics due to aperiodicity [5][6], recent new findings expand the field of quasicrystal to include superconductivity [7], quantum criticality [8], and topology [9][22]. In general, self-similarity in quasicrystals dictates fractal structure in wavefunction, phase diagram, and so on [23][24]. This characteristic is justified by the presence of the inflation and deflation rules to construct quasicrystals [25].

One of the well-known two-dimensional (2D) quasicrystals is the so-called Penrose lattice [26]. One can construct the lattice using inflation, projection, or multi-grade rules. The Penrose lattice has been studied intensively [24][27][29] and its structure dictates thermodynamically degenerate states in energy spectrum [30][31]. The presence of degeneracy is similar to the Lieb-lattice and causes a singularity in the density of state [32], being crucial for understanding antiferromagnetism at half-filling [25][33].

Ultracold gases in optical lattices provide us an ideal playground of strong correlation [34] and also quasicrystals [35][36], which allows us to investigate the interplay of strong correlation and aperiodicity. A typical strongly correlated system in optical lattice is the Bose-Hubbard model, where phase transition between Mott insulator (MI) to superfluid (SF) phase appears [39] as experimentally observed [40][41]. Recent achievements in establishing an eight-fold rotationally symmetric optical lattice attract new attention [42], in connection with theoretical investigation of an extended Bose-Hubbard with quasicrystalline confined potential [43], where spontaneous breaking of underlying eight-fold symmetry is observed. However, the effect of aperiodicity in the Bose-Hubbard model is not yet fully understood both theoretically and experimentally.

In this Letter, we investigate the phase diagram of the Bose-Hubbard model in the Penrose lattice. We use the inhomogeneous mean-field theory (IMFT) and find that the distribution of Bose condensate in the Penrose lattice exhibits a fractal structure near the MI-SF boundary. We attribute the appearance of the fractal structure to a consequence of the divergence of correlation length seen in any phase transition. Therefore, the fractal structure is a common signature of phase transition in aperiodic systems.

Model and method—The Hamiltonian of the single-band Bose-Hubbard model is defined by:

\[
H_{BH} = -J \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1),
\]

where \(\hat{b}_i\) and \(\hat{b}_j^\dagger\) are annihilation and creation of bosons at site (vertex) \(i\) and the number operator \(\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i\). The summation \(\langle i, j \rangle\) represents nearest-neighbor (NN) links in the Penrose lattice shown in Fig. 1(a). \(J\), \(\mu\), and \(U\) in Eq. (1) are the hopping energy of boson, the chemical potential, and on-site Coulomb interaction, respectively. Because of the presence of the hopping term in Eq. (1), the exact solution is inaccessible. Therefore, we use a mean-field technique and decouple the hopping term using local condensation amplitude \(\langle \hat{b}_i \rangle\). The resulting mean-field Hamiltonian is given by \(H_{MF} = \sum_i H_i + E_0\) with

\[
H_i = -J \left( \psi_i^* \hat{b}_i + H.c. \right) - \mu \hat{n}_i + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1),
\]

where \(\psi_i = \sum_{j \in NN,i} \langle \hat{b}_j \rangle\) with summation over NN links connected to the vertex \(i\) and \(E_0 = J \sum \psi_i^* \langle \hat{b}_i \rangle\).

In order to obtain a self-consistent solution of Eq. (2) in the local Hilbert space containing maximally \(n_b\) bosons, we start with an initial \(\psi_i\) and then calculate \(\langle \hat{n}_i \rangle\) and \(\langle \hat{b}_i \rangle\) using the ground-state wavefunction for each vertex. We continue updating \(\psi_i\) until convergence of \(\langle \hat{n}_i \rangle\) and \(\langle \hat{b}_i \rangle\) is obtained within a certain tolerance (10^{-9} in our case). This procedure gives rise to inhomogeneous distribution of \(\langle \hat{n}_i \rangle\) and \(\langle \hat{b}_i \rangle\) on the Penrose lattice. Therefore, we call this mean-field technique the IMFT. We take \(n_b = 7\). Within IMFT, we generally find the MI and SF phases in the Bose-Hubbard model. In the MI phase, all sites have equal integer number of bosons and thus \(\langle \hat{b}_i \rangle = 0\). On the other hand, \(\langle \hat{b}_i \rangle\) is nonzero for the SF phase. We
TABLE I. Link configuration of distinct vertexes in Penrose lattice. Listed are index $\alpha$ determined in the present work, the total number of paths using $k$ links, $M_k$ ($k = 1, 2, 3$), the number of vertexes having $l$ links, to which one can access using $k$ links, $m_{k}^{(l)}$ ($l = 3, 4, 5, 6, 7$). Note that $\sum_{l} m_{k}^{(l)} = M_k$.

| $\alpha$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 |
|----------|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| $M_1$   | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  | 3  |
| $M_2$   | 15| 15| 15| 15| 15| 15| 15| 15| 15| 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 |
| $M_3$   | 11| 10| 9 | 9 | 12| 12| 11| 15| 14| 14 | 13| 6 | 5 | 5 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 5 | 10 | 20 | 10 | 2 |
| $m_{1}^{(3)}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| $m_{2}^{(4)}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 0 | 0 | 0 | 0 |
| $m_{3}^{(5)}$ | 3 | 3 | 1 | 1 | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 3 | 1 |
| $m_{4}^{(6)}$ | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $m_{5}^{(7)}$ | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $m_{6}^{(7)}$ | 7 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 4 | 0 | 2 | 4 | 0 | 2 | 4 | 4 | 4 | 2 | 0 | 0 | 0 |
| $m_{7}^{(7)}$ | 4 | 3 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 4 | 5 | 6 | 0 | 0 | 0 | 2 | 2 | 2 | 0 | 0 | 0 | 4 | 4 |

note that this self-consistent procedure gives moderately accurate results as compared with quantum Monte Carlo simulations and gives equivalent results with variational Gutzwiller method [44,52].

In the Penrose lattice, open boundary condition breaks the symmetries of Penrose tiling. On the other hand, we can construct a supercell with periodic boundary conditions (PBC), where the local symmetry of Penrose lattice remains intact throughout. Although a few defects appear in the supercell, their effect is very small. This supercell called approximant can be found by approximating golden ratio with $F(g + 1)/F(g)$, where $F(g)$ is the $g$-th sequence of Fibonacci number. Here, we set $g = 11$ and obtain a supercell with the total number of vertexes $N = 4F(2g + 1) + 3F(2g) = 167761$.

In the Penrose lattice, we can classify any vertexes in terms of their local environment. For this classification, we first find the number of NN links, $M_1$, i.e., the total number of paths using one link (the second row in Table I), which is equivalent to coordination number for each vertex in Fig. 1(a). $M_1$ changes from 3 to 7. This means that all of sites are indexed by five kinds of vertexes. Next, we count the number of NN vertexes having $l$ links, $m_{l}^{(1)}$, and make a list of them (the third-seventh rows in Table I). From the list of $m_{l}^{(1)}$ together with $M_1$, we find fourteen types of configurations, meaning that all of sites are indexed by fourteen kinds of vertexes. The total number of paths using two links from a given vertex is then expressed as $M_2 = \sum_{l=3}^{7} m_{l}^{(1)} l$, which is listed in the eighth row. We repeat this listing for the vertexes accessed by using the two links form a given vertex, which is shown in the ninth-thirteenth rows as $m_{l}^{(2)}$. In the last row of Table I, the total number of paths using three links from a given vertex ($M_3 = \sum_{l=3}^{7} m_{l}^{(1)} l$) is listed. Performing this procedure for all vertexes in our supercell, we find that there are twenty-seven kinds of vertexes, by which almost the whole system is covered. They are indexed as $\alpha$ in the first row of Table I. In this manner, we can classify all vertexes for a given $k$. We thus define the number of classes (NoC) determined by the given $k$. For example, NoC is equal to 5, 14, and 27 for $k = 1, 2$, and 3, respectively. We can increase $k$ as many as possible, but we stop $k$ up to $k = 3$ in Table I in order to make underlying physics in our model more transparent. We find NoC $\propto k^{1.93}$ in the large $k$ region (see Fig. 3(c)). We will come back to this point later.

Vertexes in the Penrose lattice can be labeled with five integers, originated from cut and projection of five dimensional cubic lattice [53,59]. One can construct original Penrose lattice by mapping those labels. However, using another mapping, one finds four different 2D structures, called perpendicular space, where we assign them $Z = 1, 2, 3$, and 4 [see Figs. 1(b) and 1(c) for $Z = 1$ and 2, respectively]. We can divide perpendicular space into symmetric sections, where each section represents vertex with similar local circumstances. Therefore, one notices the index $\alpha$ in Table I mapped to different sections in the perpendicular space [see Figs. 1(b) and 1(c)]. Considering the bipartite properties of Penrose lattice, we realize that $Z = 1, 3$ and $Z = 2, 4$ are related to different subsystems, though the same $\alpha$ are shared each other.

Results—We first examine the phase diagram of the Bose-Hubbard model on the Penrose lattice. Since there are two order parameters (per vertex) $\langle \hat{n}_i \rangle$ and $\langle \hat{b}_i \rangle$ in IMFT, we expect two phases: one is MI with $\langle \hat{b}_i \rangle = 0$ and $\langle \hat{n}_i \rangle = n_0$ ($n_0 = 1, 2, \cdots$, corresponding to bosonic occupation number at each vertex), and the other is SF with $\langle \hat{b}_i \rangle \neq 0$ and $\langle \hat{n}_i \rangle = 0$ as is the case of the square lattice. Figure 2 shows the phase diagram, where we find MI phases denoted by MHI$n_0$ and SF. Since averaged coor-
The coordination number in the Penrose lattice is \( \bar{z} = 4 \), which is the same as the coordination number \( z = 4 \) in the square lattice, the phase boundary between MI and SF is expected to be similar to that of the square lattice. This is the case as shown by the dashed orange curve along MI lobes in Fig. 2 which is mean-field phase boundary for the square lattice given analytically \([60, 61]\) by

\[
zJ_c/U = \frac{-\mu - (\mu)^2 + s + 2\mu s - s^2}{1 + \frac{\mu}{U}},
\]

where \( s = \text{round}(\mu/U + 1/2) \). The similarity indicates small effect of aperiodicity on the phase boundary.

In the SF phase of square lattice, the condensation amplitude \( \langle \hat{b}_i \rangle \) is uniform, i.e., independent of \( i \), for any region in the phase diagram. On the other hand, nonuniform distribution of \( \langle \hat{b}_i \rangle \) in the Penrose lattice is easily expected from the presence of different types of vertexes as discussed in Table I. Then, an arising question is how its nonuniform distribution changes in the phase diagram. To see this, we define an \( \alpha \) dependent average of \( \langle \hat{b}_i \rangle \) as

\[
\bar{b}_\alpha = \frac{1}{N_\alpha} \sum_i \langle \hat{b}_i \rangle
\]

where \( N_\alpha \) is the number of \( \alpha \)-type vertex in the whole lattice. This quantity can distinguish the twenty-seven classes of vertexes. However, each class should have further internal structure coming from possible extension of \( M_k \) for \( k \geq 4 \). To recognize this structure, we also define a mean deviation of condensation amplitude distribution as

\[
\delta b_\alpha = \sqrt{\frac{1}{N_\alpha} \sum_i (\langle \hat{b}_i \rangle - \bar{b}_\alpha)^2}.
\]

The larger \( \delta b_\alpha / \bar{b} \) is, the deeper the internal structure is.

In Fig. 3(a), we plot \( \bar{b}_\alpha / \bar{b} \) and \( \delta b_\alpha / \bar{b} \) as a function of \( \bar{z}J/U \) along the horizontal dotted line in Fig. 2 where \( \bar{b} = \sum_i \langle \hat{b}_i \rangle / N \) with \( N = \sum_\alpha N_\alpha \). We note that \( \delta b_\alpha / \bar{b} \) is denoted by the length of bars for each \( \bar{b}_\alpha / \bar{b} \). At large \( \bar{z}J/U \) far from the phase boundary, \( \bar{b}_\alpha / \bar{b} \) is tend to be
duce a new quantity that can characterize distinct number of vertexes more than 27 listed in Table I. We use $\langle \tilde{b}_i \rangle$ for this purpose. We i) make shifting and scaling for $\langle \tilde{b}_i \rangle$ to be located within [0,1], ii) sort the scaled $\langle \tilde{b}_i \rangle$ from 0 to 1, iii) calculate the difference of $\langle \tilde{b}_i \rangle$ between $i$ and $i+1$ from $i = 1$ to $i = N - 1$, and iv) count the number of the difference (gap) whose magnitude is more than a given small threshold value. We call this number the number of gap (NoG). For example, NoG is zero for the square lattice because $\langle \tilde{b}_i \rangle$ is independent of $i$. In the Penrose lattice, we have four NoG in the large limit of $\varepsilon J/U$ since there are five distinct values of $\langle \tilde{b}_i \rangle$. We show log-log plot of NoG in Fig. 3(b) along the horizontal dotted line in Fig. 2 where four different threshold values, $10^{-5}$, $5 \times 10^{-6}$, $10^{-6}$, and $5 \times 10^{-7}$ are used. With approaching to the phase boundary at $\varepsilon J/U = 0.084$, NoG increases, indicating the increase of distinct vertexes. Interesting is that, with decreasing the threshold value, NoG rapidly increases near the boundary and shows a diverging behavior with an approximate exponent around $-0.9$, i.e., NoG $\propto (J - J_c)^{-0.9}$. This resembles to a critical behavior toward continuous phase transition as suggested from the vanishing of averaged order parameter $\tilde{b}$ [see inset of Fig. 3(a)].

In order to understand this diverging behavior more, we focus on the fact that the increase of NoG corresponds to the increase of distinct vertexes. The latter is measured by NoC, whose large region is proportional to $k^{-1.93}$ as shown in Fig. 3(c). Therefore, diverging behavior in NoG is directly connected to diverging behavior in NoC at large $k$. Since $k$ represents the number of links from a given vertex, we may regard $k$ as a measure of correlation length $\xi$ from a given vertex. Based on this reasoning, we have NoG $\propto$ NoC $\propto k^{-1.93} \propto \xi^{-1.93}$. Since $\xi \propto (J - J_c)^{-0.5}$ for the mean-field phase transition, we finally expect that NoG $\propto (J - J_c)^{-0.96}$, whose exponent is not far from the calculated one in NoG, $-0.9$. This indicates that diverging behavior in NoG is a consequence of criticality in the mean-field phase transition. We note that this critical behavior does not appear if $\mu/U = n_0$ and $J/U \to 0$.

Usefulness of perpendicular space presentation has already been found in considering magnetism on the Penrose lattice [27, 33]. Therefore, we show the perpendicular space representation of $\langle \tilde{b}_i \rangle$ in Fig. 4 for two sets of parameters at the end of the red dashed line in Fig. 2. We recognize notable differences in the two cases. For the parameter far from the phase boundary, we find fourteen distinct sections in Figs. 4(c) and 4(d). The number corresponds to the number of distinct vertexes obtained by taking into account $M_I$ and $m_{10}^I$ as discussed above. On the other hand, for the parameter close to the phase boundary, we can see a fractal structure in Figs. 4(a) and 4(b). For example, we find a various size of star structure inside stars. We can understand the emergence of...
the fractal structure near the phase transition as follows. Because of diverging behavior in NoG near the MI-SF phase boundary, all distances become relevant. We have found from the previous discussion that tracing far distant links by increasing $k$ enhances NoC dramatically. Therefore we can expect further distinguishable sections in the perpendicular space, resulting in fractal nature. In other words, a combination of criticality leading to phase transition and aperiodicity is a key for emergence of fractal structure.

**Conclusion**—We have obtained mean-field phase diagram in the Penrose-Bose-Hubbard model. We have found that the Penrose lattice does not change the MI-SF boundary drastically in comparison with square lattice, because of the same averaged coordination number. However, the spatial distribution of Bose condensate is unequal, and indeed fractal structure appears in the perpendicular representation of condensation amplitude near the MI-SF phase transition. This is a consequence of the cooperative effect of criticality leading to phase transition and quasiperiodicity, which is expected to be a common feature in aperiodic strongly correlated systems.

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