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Interacting bosons in a three-dimensional lattice

Dian-Cheng Zhang(张典承)[1,†] and Shi-Jie Yang(杨师杰)[2]

[1] *College of Science, Hainan Tropical Ocean University, Sanya* 572022, *China*
[2] *Department of Physics, Beijing Normal University, Beijing* 100875, *China*

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We theoretically investigate the extended Bose–Hubbard model using a three-dimensional cubic lattice. In the framework of the dynamical Gutzwiller mean-field theory, we identify a checkerboard supersolid phase. By considering the repulsive interactions between next-nearest-neighbor lattice sites, we further discover an exotic type of supersolid state, whose site occupancies show a stereoscopically arrayed and staggered distribution rather than checkerboard ordering. Intriguingly, if the physical observations of two neighboring layers were superimposed, they would give rise to a checkerboard configuration. This novel structure is convincingly induced by the simultaneous existence of nearest-neighbor and next-nearest-neighbor interactions. We also identify arrayed stripes in the ground state, as well as arrayed holes in the pattern of occupancies.

Keywords: supersolid, three-dimensional (3D) optical lattice, extended Bose–Hubbard, dynamical Gutzwiller theory

PACS: 03.75.Mn, 03.75.Lm, 67.85.Fg

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1. introduction

Ultracold atoms with large magnetic moments pave the way for simulations of a wide range of nontrivial quantum phases dominated by strong dipole–dipole interactions.[1–6] One of these interesting phases is the supersolid state, which could be expected for an ensemble of soft-core bosons governed by an off-site interaction comparable to the on-site interaction.[7] Supported by significant experimental evidence in recent years,[8–13] the essential particularity of a supersolid phase lies in the simultaneous existence of superfluidity and crystalline order.[14–16] As a consequence, continuous translational invariance in a system would be destroyed and replaced by the emergence of a discrete configuration. Dramatically benefiting from its outstanding controllability, the optical lattice system has inspired effective theoretical explorations of supersolid phases in various types of lattice geometries, including one-dimensional (1D) multichains,[17–21] two-dimensional (2D) square lattices,[22–25] trigonal lattices,[26–29] kagome lattices,[30] bilayer dipolar lattices,[31] etc.

The Bose–Hubbard (BH) model provides a robust framework for investigations of the behaviors of ultracold bosons arranged in a lattice.[32–36] In the context of the BH model, off-site interactions are known as nearest-neighbor (NN) or next-nearest-neighbor (NNN) interactions, which consequently lead to the extended Bose–Hubbard (eBH) model.[37–44] By adding the NNN interaction, a striped supersolid state can be generated on the square lattice,[45] in addition to the checkerboard supersolid with phase separation.[46] Another fruitful study further discusses the direct competition between the checkerboard and striped supersolid orders.[47,48] In an earlier work, a type of collapse phase relying on the eBH model was also reported in the presence of NNN interaction.[49]

Additionally, the three-dimensional (3D) eBH model on a cubic lattice is also attractive.[50,51] It gives rise to the disordered normal liquid phase,[52] the density wave phase, and the supersolid phase at incommensurate or commensurate filling.[53,54] However, up until now, for the 3D bosonic lattice, the NNN interaction has not been considered in previous theoretical research. In this paper, we pay most attention to an eBH model on a 3D cubic lattice, whose Hamiltonian concurrently involves the NN and NNN interactions. We will engage the dynamical Gutzwiller mean-field theory (DGMFT)[55–58] to analyze the 3D eBH model. As a consequence, density-wave and supersolid phases capturing three or four sublattices are discovered. We further identify a fluctuation in the supersolid phase.

The remainder of this paper is structured as follows: in Section 2, we outline a 3D eBH model that includes the NN and NNN interactions and the numerical method used, followed by a presentation of results and discussions in Section 3. Finally, Section 4 is devoted to a brief conclusion.

2. Model and method

In 3D rectangular coordinates, the size of a bosonic cubic lattice is given by $L \times L \times L$ with a unit lattice constant. From the bottom to the top of the cubic lattice, we use an integer

[†]Corresponding author. E-mail: zhangdiancheng16@mails.ucas.ac.cn

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$z \in [1, L]$ to represent the sequence of each layer, and the layer occupation is described in the x–y plane. Taking into account repulsive interactions between pairs of both NN and NNN lattice sites, the relevant Hamiltonian of an eBH model can be expressed by the following equation:

$$H = -J\sum_j (\hat{b}_j^\dagger \hat{b}_k + \text{h.c.}) - \mu \sum_j \hat{n}_j + \sum_j (V \hat{n}_j^\dagger \hat{n}_k + V_0 \hat{n}_j^\dagger \hat{n}_q) + \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1), \quad (1)$$

where the 3D coordinate of each lattice site is denoted by the subscript $j = (z, x, y)$, while k and q run over the 3D coordinates of the NN and NNN sites surrounding site j, respectively. J indicates the strength of the tunneling amplitude only between the NN sites, while $\hat{b}_j^\dagger$ ($\hat{b}_j$) can create (annihilate) a boson at one site. $\hat{n}_j$ represents the particle number operator. μ is the chemical potential, while U refers to the repulsive on-site interaction. V represents the off-site repulsive term between NN sites, and V_0 describes the strengths of both intralayer and interlayer NNN interactions. For the sake of simplicity, a constant $U = 1$ is employed in this paper. In our calculations, the periodic boundary condition is enforced.

To determine the ground states of the system, we take advantage of the DGMFT[55–57] to explore the model. The DGMFT is essentially based on the Gutzwiller variational wavefunction, which is given by

$$|\Psi\rangle = \prod_j \sum_{n=0}^{n_{\max}} f_n^j |n\rangle_j, \quad (2)$$

where $|n\rangle_j$ represents the local Fock basis at site j. An invariant $n_{\max} = 6$ is also used in the calculation as a truncation of the local maximum occupation per site. f_n^j is viewed as the complex variational amplitude, which should satisfy the normalization condition $\sum_{n=0}^{n_{\max}} |f_n^j|^2 = 1$. After employing the mean-field decoupling approximation, we gain access to the following conditions:

$$\begin{aligned} \hat{b}_j^\dagger \hat{b}_k &\simeq \varphi_j^* \hat{b}_k + \varphi_k \hat{b}_j^\dagger - \varphi_j^* \varphi_k, \\ \hat{n}_j \hat{n}_k &\simeq \rho_j \hat{n}_k + \rho_k \hat{n}_j - \rho_j \rho_k, \\ \hat{n}_j \hat{n}_q &\simeq \rho_j \hat{n}_q + \rho_q \hat{n}_j - \rho_j \rho_q. \end{aligned} \quad (3)$$

Here, the SF order parameter of a single site is defined as

$$\varphi_j = \langle \Psi | \hat{b}_j | \Psi \rangle = \sum_n \sqrt{n+1} \left(f_n^j\right)^* f_{n+1}^j. \quad (4)$$

Similarly, in the DGMFT framework, the occupancy of each lattice site reads

$$\rho_j = \langle \Psi | \hat{n}_j | \Psi \rangle = \sum_n n \left| f_n^j \right|^2. \quad (5)$$

Upon considering all these ansatzes and subsequently substituting the Gutzwiller wavefunction into the time-dependent Schrödinger equation, one can eventually obtain the evolving equation of motion for f_n^j,[56,57] which can be written as

$$\begin{aligned} i\hbar \frac{d}{dt} f_n^j = & -J(\tilde{\varphi}_j \sqrt{n} f_{n-1}^j + \tilde{\varphi}_j^* \sqrt{n+1} f_{n+1}^j) \\ & + n\left(V \sum_k \rho_k + V_0 \sum_q \rho_q\right) f_n^j \\ & + \left[\frac{U}{2} n(n-1) - \mu n\right] f_n^j, \end{aligned} \quad (6)$$

where $\tilde{\varphi}_j = \sum_k \varphi_k$. Equation (6) is a nonlinear equation that can be solved self-consistently using the two Eqs. (4) and (5), with the assistance of the standard imaginary-time-evolution technique.

3. Solutions and discussion

We now set the lattice size to $L = 10$ and pursue the ground states from $V = 0.6$, but with $V_0 = 0$. For $\mu = 1$ and $J = 0.07$, we observe a 3D checkerboard supersolid phase characterized by staggered occupancies within each layer, as well as order parameters of finite numerical values, which indicate an inherent fluidity of the system. The interlayer staggered textures are supported by discrepancies in the arrangements of occupancies between the odd and even layers, as illustrated in Fig. 1. This checkerboard structure is analogous to the results derived using the quantum Monte Carlo method[54] and an eBH model of the bosonic cubic lattice that disregards NNN interactions.

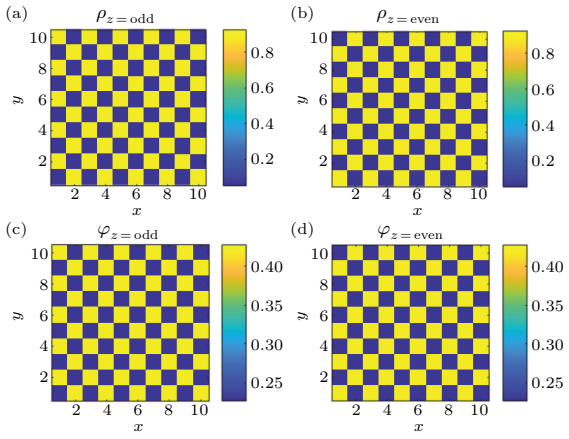


Fig. 1. The ground state corresponding to $U = 1$, $V = 0.6$, $V_0 = 0$, $\mu = 1$, and $J = 0.07$. The upper panel illustrates the occupancy distributions, and the lower panel depicts order parameters. The left column relates to the layer of an odd σ, and the right column relates to the layer of an even σ.

We now turn to the case where NNN interaction is present. For $V = V_0 = 0.6$, while keeping the other physical parameters as shown in Fig. 1, the system has a layer-dependent and alternating configuration, as displayed in Fig. 2. For each layer, the lattice sites featuring nonzero occupancies are displayed, as well as the order parameters. From top to bottom, layers with odd values of z exhibit spatially consistent occupancy distributions, while the other layers with even z values share another distinct arrangement of occupancies. This

modulated structure turns out to be a stereoscopically arrayed supersolid phase. Interestingly, as observed in the right column of Fig. 2, the superposition of the densities of an odd layer and an even layer, readily exemplified by any two neighboring layers of the cubic lattice, would give rise to a checkerboard pattern, which is traditionally generated by eBH models that disregard terms corresponding to NNN interactions.[46,54]

We now introduce the average occupancy defined by $\bar{\rho} = \sum_j \rho_j / L^3$. The checkerboard supersolid phase of Fig. 1 obviously features $\bar{\rho} = 1/2$. However, the structure of the arrayed supersolid state shown in Fig. 2 presents $\bar{\rho} = 1/4$. In our numerical simulation, it appears that the arrayed supersolid state can also be observed for a stronger chemical potential, while the spatially arrayed assignment necessarily conforms to an integer multiple of quarter filling. Its formation is triggered by the introduction of the NNN interaction into a 3D eBH model, as it is not accessible in the absence of NNN interactions, according to our results.

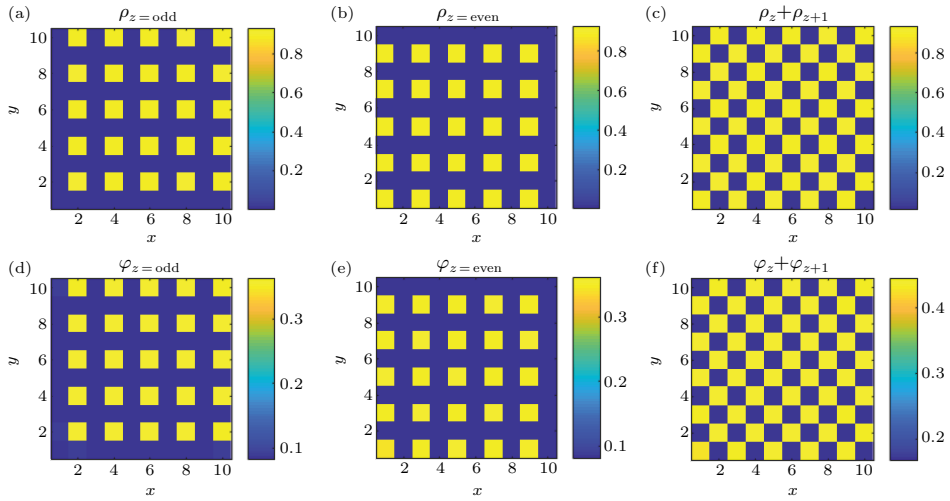


Fig. 2. The ground state corresponds to $U = 1$, $V = V_0 = 0.6$, $\mu = 1$, and $J = 0.07$. The upper panel describes the distributions of occupancies, and the lower panel depicts order parameters. The left column is connected with the layer of an odd σ, while the middle column corresponds to the even layer. The right column describes the superposition of densities on an odd and an even layer.

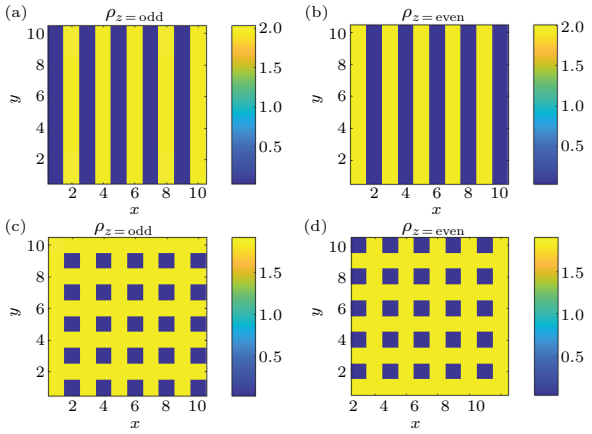


Fig. 3. The ground states at $U = 1$, and $V = V_0 = 0.6$. Panel (a) corresponds to $\mu = 6.5$, and $J = 0.07$; (b) is relatd to $\mu = 10$, and $J = 0.06$.

When the chemical potential is increased, more intriguing quantum behaviors are enabled. In Fig. 3(a), we consider $\mu = 6.5$ and $J = 0.07$. As shown, every layer of the 3D lattice is filled with a series of stripes, whose assignments to the even and odd layers visibly alternate in the horizontal plane. The ground state of Fig. 3(a) possesses $\bar{\rho} = 1$. Also, the stripes are stereoscopically arrayed in the 3D space. For $\mu = 10$ and $J = 0.06$, there is a range of holes conspicuously arrayed in Fig. 3(b), rather than arrayed particles. This conforms to $\bar{\rho} = 0.75$. However, these arrayed holes would not be observed for $\mu < 8$. Additionally, the relevant order parameters have completely consistent modulations, so they have not been displayed in Fig. 3.

In the presence of NNN interactions, arrayed occupancies or stripes have previously been reported in a 2D eBH model.[46–48] Contrasting the 3D model with its 2D counterpart, at quarter filling, intralayer arrayed occupancies can not only be observed in the x–y plane but also in the y–z and z–x planes. Similarly, in the x or y direction, the lattice sites are also alternately occupied in an interlayer arrangement. As a dimensional effect, the destruction of translational invariance takes place in 3D space. With respect to the structure shown in Fig. 3(a), its stripes are visible in the x–y as well as the y–z plane, but from the perspective of a z–y cross section, its occupancies display a checkerboard pattern. Moreover, the arrayed holes characterized by lattice sites of vanishing densities are not accessible in the 2D system, according to earlier studies.

Experimentally, atoms with significant magnetic dipole moments can develop dipole–dipole interactions, which appropriately function as off-site interactions in the eBH model. For instance, the 3D eBH model can be applied to an erbium ensemble,[4] and an erbium quantum gas in a 3D trap also exhibits the supersolid phase.[60] Therefore, an erbium gas prepared on a cubic lattice may be a promising platform on which to realistically implement our model. A strong challenge is the activation of the NNN interaction, which demands skillful

and delicate tuning of a type of polarizing magnetic field to achieve dipole excitation.[4]

4. Summary

We theoretically investigated quantum phases of ultracold bosons on a 3D cubic lattice using the eBH model, which incorporates repulsive interactions between NN or NNN pairs of lattice sites. With the assistance of the DGMFT, we reproduced the checkerboard supersolid state in the absence of NNN interactions. Additionally, the introduction of the NNN interaction contributed to novel physics inaccessible to conventional eBH models. For example, the ground states of the system adopted an arrayed supersolid phase, which heavily depended on an integer multiple of quarter filling. We also discovered arrayed stripes and arrayed holes, which represent stronger chemical potentials.

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