Strong-coupling perturbation theory for the extended Bose-Hubbard model

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We develop a strong-coupling perturbation theory for the extended Bose-Hubbard model with on-site and nearest-neighbor boson-boson repulsions on $(d>1)$-dimensional hypercubic lattices. Analytical expressions for the ground-state phase boundaries between the incompressible (Mott or charge-density-wave insulators) and the compressible (superfluid or supersolid) phases are derived up to third order in the hopping t. We also briefly discuss possible implications of our results in the context of ultracold dipolar Bose gases with dipole-dipole interactions loaded into optical lattices.

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I. INTRODUCTION

Ultracold atomic physics in optical lattices has created a new experimental arena where many simple model Hamiltonians can be constructed and "simulated" experimentally [1]. To date, the most successful efforts have been with bosonic atoms on optical lattices [2–5]. Here, when the single-particle bands of the optical lattice are well separated in energy, the boson-boson interaction is much smaller than that separation, and the particle filling is not too high, the system is described well by the single-band Bose-Hubbard (BH) model. This model is the bosonic generalization of the Hubbard model and was introduced originally to describe ^{4}He in porous media or disordered granular superconductors [6]. The superfluid phase of bosonic systems is well described by weak-coupling theories, but the insulating phase, where there is a gap to particle excitations with a uniform (integer) filling of the bosons on each lattice site, is a strong-coupling phenomenon that only appears when the system is on a lattice. This Mott insulator phase is incompressible and hence occupies a finite area in the parameter space of the chemical potential and the hopping. It has a transition from the incompressible phase to a compressible superfluid as the hopping or chemical potential is varied. The on-site BH model has been studied extensively, and the strong-coupling perturbation-theory approach has been shown to be quite accurate in determining this phase diagram of the system [7–9].

Recently, experimental progress has been made in constructing ultracold dipolar gases of molecules, namely, K-Rb molecules, from a mixture of fermionic ^{40}K and bosonic ^{87}Rb atoms [10,11]. In this case, the molecules are fermionic, but similar principles will allow one to also create bosonic dipolar molecules. Future experiments are likely to load these bosonic molecules into optical lattices. These systems will have a long-range boson-boson interaction mediated by their dipole moment, which can be approximated, in some circumstances, by an on-site and a nearest-neighbor repulsion. (Generically, dipole-dipole interactions will be longer ranged than just nearest neighbors and also can have directionality due to the orientations of the dipoles.) The case of an extended BH model, where the boson-boson interaction is longer ranged, has also been widely studied [12–20]. Inclusion of a nearest-neighbor repulsion can lead to the formation of a charge-density-wave (CDW) phase, where at half filling, for example, one would have a checkerboard arrangement of the density in an ordered pattern. This phase is incompressible with a finite gap to excitations. It also breaks the original translational symmetry of the lattice, forming a new crystalline phase. The CDW phase has generated significant interest, because it often can become a supersolid prior to becoming a superfluid as the interactions are reduced. A supersolid phase is a (compressible) superfluid that continues to have a density modulation (or CDW) present [21]. That is, the superfluid and crystalline orders coexist. Interest in supersolid physics has increased dramatically since the recent observation of supersolidlike behavior in low-temperature He experiments [22]. There is some numerical and theoretical evidence that the supersolid phase exists only in dimensions higher than one [15,16].

In this paper, we examine the extended BH model with on-site and nearest-neighbor boson-boson interactions via a strong-coupling perturbation theory in the hopping, plus a scaling analysis, which allows us to accurately predict the critical point and the shape of the insulating lobes in the plane of the chemical potential and the hopping. We carry out the analysis to third order in the hopping, and we perform the scaling theory using the known critical behavior at the tip of the insulating lobes [which corresponds to the $(d+1)$-dimensional XY model, and is identical for the Mott and CDW phases].

The remainder of the paper is organized as follows. After introducing the model Hamiltonian in Sec. II, we develop the strong-coupling perturbation theory in the kinetic-energy term in Sec. III, where we derive analytical expressions for the phase boundaries between the incompressible (Mott or CDW insulators) and compressible (superfluid or supersolid) phases. There we also propose a chemical-potential extrapolation technique based on scaling theory to extrapolate our third-order power-series expansion into a functional form that is appropriate for the Mott or CDW lobes, and compare these results with the mean-field ones in Sec. IV. A brief summary of our conclusions is presented in Sec. V.

II. EXTENDED BOSE-HUBBARD MODEL

We consider the following extended BH Hamiltonian with on-site and nearest-neighbor boson-boson repulsions:

$$H = -\sum_{i,j} t_{ij} b_i^\dagger b_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_{i,j} V_{ij}\hat{n}_i\hat{n}_j - \mu\sum_i \hat{n}_i, \tag{1}$$

where t_{ij} is the tunneling (or hopping) matrix elements between sites i and j, $b_i^\dagger$ (b_i) is the boson creation (annihilation) operator at site i, $\hat{n}_i = b_i^\dagger b_i$ is the boson number operator, $U > 0$ is the strength of the on-site repulsion and V_{ij} is the longer-ranged boson-boson repulsion between bosons at sites i and j, and μ is the chemical potential. In this paper, we assume t_{ij} is a real symmetric matrix with elements $t_{ij} = t$ for i and j nearest neighbors and 0 otherwise and similarly for V_{ij} (equal to $V > 0$ for i and j nearest neighbors and zero otherwise), and consider a $(d > 1)$-dimensional hypercubic lattice with M sites [23]. Note that we work on a periodic lattice with no external trap potential.

We also assume $U > zV$, where $z = 2d$ is the lattice coordination number (number of nearest neighbors). In this case, the boson occupancy of the nearest-neighbor sites in the CDW phase can only differ by 1. For instance, the first CDW phase is such that every other site is occupied by one boson and the remaining sites are left unoccupied. When $U < zV$, additional CDW phases can be present in the phase diagram. For instance, a CDW phase in which every other site is occupied by two bosons and the remaining sites are left unoccupied is energetically more favorable than a Mott phase in which every lattice site is occupied by one boson. Our results, with minor changes, can also be used to analyze these additional CDW phases if desired, but more work would be needed to examine other types of CDW order, such as columnar (stripes), which can arise from longer-range interactions.

A. Atomic ($t = 0$) limit

To understand the zero-temperature ($T = 0$) phase diagram of the extended BH model given in Eq. (1), we start by analyzing the atomic ($t = 0$) limit. In this limit, since the kinetic energy vanishes, the boson number operator $\hat{n}_i$ commutes with all of the remaining terms of the Hamiltonian. Therefore, every lattice site is occupied by a fixed number n_i of bosons and the system is insulating.

When $V = 0$, the ground-state boson occupancy is the same for every lattice site such that $\langle \hat{n}_i \rangle = n_0$, where $\langle \cdots \rangle$ is the thermal average, and the average boson occupancy n_0 is chosen to minimize the ground-state energy for a given μ. (The symbol n_0 is an integer here and should not be confused with the condensate fraction of a superfluid.) It turns out that the ground-state energy of the n_0 state is degenerate with that of the $n_0 + 1$ state at $\mu = Un_0$. This means that the chemical-potential width of all Mott lobes is U, and that the boson occupancy increases from n_0 to $n_0 + 1$ when $\mu = Un_0 + 0^+$. For instance, the ground state is a vacuum with $n_0 = 0$ for $\mu \leq 0$; it is a Mott insulator with $n_0 = 1$ for $0 \leq \mu \leq U$; it is a Mott insulator with $n_0 = 2$ for $U \leq \mu \leq 2U$; and so on.

When $V \neq 0$, the ground state has an additional CDW phase which has crystalline order in the form of staggered boson densities, i.e., $\langle \hat{n}_i \rangle = n_A$ and $\langle \hat{n}_j \rangle = n_B$ for i and j nearest neighbors. Therefore, to describe the CDW phases, it is convenient to split the entire lattice into two sublattices A and B such that the nearest-neighbor sites belong to a different sublattice. (A lattice for which this can be done is called a bipartite lattice—we assume the number of lattice sites in each sublattice is the same here.) We assume that the boson occupancies of sublattices A and B are n_A and n_B, respectively, such that $n_A \geq n_B$. We remark that the $n_A = n_B = n_0$ states correspond to the Mott phase. It turns out that the ground-state energy of the $(n_A = n_0 + 1,\ n_B = n_0)$ state is degenerate with those of the $(n_A = n_0,\ n_B = n_0)$ and $(n_A = n_0 + 1,\ n_B = n_0 + 1)$ states at $\mu = Un_0 + zVn_0$ and $\mu = Un_0 + zV(n_0 + 1)$, respectively. This means that the chemical-potential width of all Mott and CDW lobes are U and zV, respectively, and that the ground state alternates between the CDW and Mott phases as a function of increasing μ. For instance, the ground state is a vacuum $(n_A = 0,\ n_B = 0)$ for $\mu \leq 0$; it is a CDW with $(n_A = 1,\ n_B = 0)$ for $0 \leq \mu \leq zV$; it is a Mott insulator with $(n_A = 1,\ n_B = 1)$ for $zV \leq \mu \leq U + zV$; it is a CDW with $(n_A = 2,\ n_B = 1)$ for $U + zV \leq \mu \leq U + 2zV$; it is a Mott insulator with $(n_A = 2,\ n_B = 2)$ for $U + 2zV \leq \mu \leq 2U + 2zV$; and so on.

Having discussed the $t = 0$ limit, now we are ready to analyze the competition between the kinetic- and potential-energy terms of the Hamiltonian when $t \neq 0$. As t increases, one expects that the range of μ about which the ground state is insulating (incompressible) decreases, and that the Mott and CDW phases disappear at a critical value of t, beyond which the system becomes compressible.

B. Transition from an incompressible to a compressible phase

To determine the phase boundary between the incompressible (Mott or CDW insulators) and the compressible (superfluid or supersolid) phases, we need the energies of the Mott and CDW phases and of their defect states as functions of t. The defect states are characterized by exactly one extra particle or hole which moves coherently throughout the lattice. At the point where the energy of the incompressible state becomes degenerate with its defect state, the system becomes compressible assuming that the compressibility approaches zero continuously at the phase boundary. Therefore, the phase boundary between the Mott and superfluid phases is determined by

$$E_{\mathrm{Mott}}^{\mathrm{ins}}(n_0) = E_{\mathrm{Mott}}^{\mathrm{par}}(n_0), \tag{2}$$

$$E_{\mathrm{Mott}}^{\mathrm{ins}}(n_0) = E_{\mathrm{Mott}}^{\mathrm{hol}}(n_0), \tag{3}$$

where $E_{\mathrm{Mott}}^{\mathrm{ins}}(n_0)$ is the energy of the Mott phase with n_0 bosons on every lattice site, and $E_{\mathrm{Mott}}^{\mathrm{par}}(n_0)$ and $E_{\mathrm{Mott}}^{\mathrm{hol}}(n_0)$ are the energies of the Mott-defect phases with exactly one extra particle or hole, respectively. These conditions determine the phase boundaries of the particle and hole branches of the Mott insulating lobes, $\mu_{\mathrm{Mott}}^{\mathrm{par}}$ and $\mu_{\mathrm{Mott}}^{\mathrm{hol}}$, respectively, as functions of t, U, V, and n_0. Similarly the phase boundary between the CDW and supersolid phases is determined by

$$E^{\rm ins}_{\rm CDW}(n_A,n_B) = E^{\rm par}_{\rm CDW}(n_A,n_B), \tag{4}$$

$$E^{\rm ins}_{\rm CDW}(n_A,n_B) = E^{\rm hol}_{\rm CDW}(n_A,n_B), \tag{5}$$

where $E^{\rm ins}_{\rm CDW}(n_A,n_B)$ is the energy of the CDW phase with n_A and n_B bosons on alternating lattice sites, and $E^{\rm par}_{\rm CDW}(n_A,n_B)$ and $E^{\rm hol}_{\rm CDW}(n_A,n_B)$ are the energies of the CDW-defect phases with exactly one extra particle or hole, respectively. These conditions determine the phase boundaries of the particle and hole branches of the CDW insulating lobes, $\mu^{\rm par}_{\rm CDW}$ and $\mu^{\rm hol}_{\rm CDW}$, respectively, as functions of t, U, V, n_A, and n_B. Next, we calculate the energies of the Mott and CDW phases and of their defect states as a perturbative series in the hopping t.

III. STRONG-COUPLING PERTURBATION THEORY

We use the many-body version of Rayleigh-Schrödinger perturbation theory in the kinetic-energy term [24] to perform the expansion (in powers of the hopping) for the different energies needed to carry out our analysis. The perturbation theory is performed with respect to the ground state of the system when the kinetic-energy term is absent. This technique was previously used to discuss the phase diagram of the on-site BH model [7,8], and its results showed excellent agreement with the quantum Monte Carlo simulations (including the most recent numerical work [25,26]). Here, we generalize this method to the extended BH model, hoping to develop an analytical approach which could also be as accurate as the numerical ones. However, we remark that our strong-coupling perturbation theory cannot be used to calculate the phase boundary between two compressible phases, e.g., the supersolid-to-superfluid transition. In addition, we cannot even tell whether the compressible phase is a supersolid or a superfluid.

A. Ground-state wave functions at zeroth order in t

For our purpose, we first need the ground-state wave functions of the Mott and CDW phases and of their particle and hole defects when $t=0$. To zeroth order in t, the Mott and CDW wave functions can be written as

$$|\Psi^{\rm ins(0)}_{\rm Mott}\rangle = \prod_{k=1}^{M} \frac{(b_k^\dagger)^{n_0}}{\sqrt{n_0!}}|0\rangle, \tag{6}$$

$$|\Psi^{\rm ins(0)}_{\rm CDW}\rangle = \prod_{i\in A, j\in B}^{M/2} \frac{(b_i^\dagger)^{n_A}}{\sqrt{n_A!}}\frac{(b_j^\dagger)^{n_B}}{\sqrt{n_B!}}|0\rangle, \tag{7}$$

where M is the number of lattice sites, and $|0\rangle$ is the vacuum state (here, we recall that the lattice is divided equally into A and B sublattices). We use here and throughout the index k to refer to all lattice sites, while the indices i and j are limited to the A and B sublattices, respectively.

On the other hand, the wave functions of the defect states are determined by degenerate perturbation theory. To zeroth order in t, the wave functions for the particle-defect states can be written as

$$|\Psi^{\rm par(0)}_{\rm Mott}\rangle = \frac{1}{\sqrt{n_0+1}}\sum_{k=1}^{M} f_k^{\rm Mott} b_k^\dagger |\Psi^{\rm ins(0)}_{\rm Mott}\rangle, \tag{8}$$

$$|\Psi^{\rm par(0)}_{\rm CDW}\rangle = \frac{1}{\sqrt{n_B+1}}\sum_{j\in B}^{M/2} f_j^{\rm CDWB} b_j^\dagger |\Psi^{\rm ins(0)}_{\rm CDW}\rangle, \tag{9}$$

where $f_k^{\rm Mott}$ is the eigenvector of the hopping matrix $t_{kk'}$ with the highest eigenvalue (which is zt) such that $\Sigma_{k'} t_{kk'} f_{k'}^{\rm Mott} = zt f_k^{\rm Mott}$, and $f_j^{\rm CDWB}$ is the eigenvector of $\Sigma_i t_{ji} t_{ij'}$ (this matrix lives solely on the B sublattice) with the highest eigenvalue (which is z^2t^2) such that $\Sigma_{ij'} t_{ji} t_{ij'} f_{j'}^{\rm CDWB} = z^2t^2 f_j^{\rm CDWB}$. Notice that we choose the highest eigenvalue of t_{ij} because the hopping matrix enters the Hamiltonian as $-t_{ij}$, and we ultimately want the lowest-energy states. Similarly for the CDW phases, the coefficient of the t^2 matrix that enters the perturbation theory is negative, so we want the highest eigenvalue again. The normalization condition requires that $\Sigma_{k=1}^{M} |f_k^{\rm Mott}|^2 = 1$ and $\Sigma_{j\in B}^{M/2} |f_j^{\rm CDWB}|^2 = 1$. Similarly, to zeroth order in t, the wave functions for the hole-defect states can be written as

$$|\Psi^{\rm hol(0)}_{\rm Mott}\rangle = \frac{1}{\sqrt{n_0}}\sum_{k=1}^{M} f_k^{\rm Mott} b_k |\Psi^{\rm ins(0)}_{\rm Mott}\rangle, \tag{10}$$

$$|\Psi^{\rm hol(0)}_{\rm CDW}\rangle = \frac{1}{\sqrt{n_A}}\sum_{i\in A}^{M/2} f_i^{\rm CDWA} b_i |\Psi^{\rm ins(0)}_{\rm CDW}\rangle, \tag{11}$$

where $f_i^{\rm CDWA}$ is the eigenvector of $\Sigma_j t_{ij} t_{ji'}$ (this matrix lives solely on the A sublattice) with the highest eigenvalue (which is z^2t^2) such that $\Sigma_{ji'} t_{ij} t_{ji'} f_{i'}^{\rm CDWA} = z^2t^2 f_i^{\rm CDWA}$. The normalization condition requires that $\Sigma_{i\in A}^{M/2} |f_i^{\rm CDWA}|^2 = 1$.

B. Ground-state energies up to third order in t

Next, we employ the many-body version of Rayleigh-Schrödinger perturbation theory in t with respect to the ground state of the system when $t=0$, and calculate the energies of the Mott and CDW phases and of their particle- and hole-defect states. To third order in t, the energy of the Mott state is obtained via nondegenerate perturbation theory and it is given by

$$\frac{E^{\rm ins}_{\rm Mott}(n_0)}{M} = U\frac{n_0(n_0-1)}{2} + zV\frac{n_0^2}{2} - \mu n_0 - n_0(n_0+1)\frac{zt^2}{U-V} + O(t^4), \tag{12}$$

which is an extensive quantity, that is, $E^{\rm ins}_{\rm Mott}(n_0)$ is proportional to the total number of lattice sites M. The odd-order terms in t vanish for the d-dimensional hypercubic lattices considered in this paper; they enter on nonbipartite lattices such as the triangular lattice. Notice that Eq. (12) recovers the known result for the on-site BH model when $V=0$ [7,8]. Similarly, to third order in t, the energy of the CDW state is also obtained via nondegenerate perturbation theory and it can be written as

$$\frac{E^{\mathrm{ins}}_{\mathrm{CDW}}(n_A,n_B)}{M} = U\frac{n_A(n_A-1)+n_B(n_B-1)}{4} + zV\frac{n_An_B}{2} - \mu\frac{n_A+n_B}{2} + \left[\frac{n_A(n_B+1)}{U(n_A-n_B-1)+V(zn_B-zn_A+1)} + \frac{n_B(n_A+1)}{U(n_B-n_A-1)+V(zn_A-zn_B+1)}\right]\frac{zt^2}{2} + O(t^4), \tag{13}$$

which is also an extensive quantity, and the odd-order terms in t also vanish. Notice that Eq. (13) reduces to Eq. (12) when $n_A=n_B=n_0$ as expected.

The calculation of the defect state energies is more involved since it requires using degenerate perturbation theory. This is because when exactly one extra particle or hole is added to the Mott phase, it could go to any of the M lattice sites and all of those states share the same energy when $t=0$. Therefore, for both Mott-defect states with exactly one extra particle or hole, the initial degeneracy is of order M and it is lifted at first order in t. A lengthy but straightforward calculation leads to the energy of the Mott particle-defect state up to third order in t as

$$E^{\mathrm{par}}_{\mathrm{Mott}}(n_0) = E^{\mathrm{ins}}_{\mathrm{Mott}}(n_0) + Un_0 + zVn_0 - \mu - (n_0+1)zt + n_0\left\{(n_0+1)\left[\frac{1-z}{U}+\frac{2(1-z)}{U-2V}+\frac{2z}{U-V}\right] - \frac{n_0+2}{2(U-V)}\right\}zt^2 - n_0(n_0+1)$$
$$\times\left\{n_0\left[\frac{z-2}{U^2}+\frac{z^2-3z+3}{(U-V)^2}\right] + (n_0+1)\left[\frac{z(1-z)}{U^2} - \frac{2z^2-6z+6}{(U-V)^2} + \frac{2z(1-z)}{(U-2V)^2} + \frac{2(z^2-3z+3)}{U(U-V)} + \frac{4(z-2)}{U(U-2V)}\right.\right.$$
$$\left.\left. + \frac{4(z^2-3z+3)}{(U-V)(U-2V)}\right] + (n_0+2)\left[\frac{z-1}{U(U-V)} - \frac{z}{4(U-V)^2}\right]\right\}zt^3 + O(t^4). \tag{14}$$

This expression is valid for all d-dimensional hypercubic lattices, and it recovers the known result for the on-site BH model when $V=0$ [7,8]. To third order in t, we obtain a similar expression for the energy of the Mott hole-defect state given by

$$E^{\mathrm{hol}}_{\mathrm{Mott}}(n_0) = E^{\mathrm{ins}}_{\mathrm{Mott}}(n_0) - U(n_0-1) - zVn_0 + \mu - n_0zt + (n_0+1)\left\{n_0\left[\frac{1-z}{U}+\frac{2(1-z)}{U-2V}+\frac{2z}{U-V}\right] - \frac{n_0-1}{2(U-V)}\right\}zt^2$$
$$- n_0(n_0+1)\left\{(n_0+1)\left[\frac{z-2}{U^2}+\frac{z^2-3z+3}{(U-V)^2}\right] + n_0\left[\frac{z(1-z)}{U^2} - \frac{2z^2-6z+6}{(U-V)^2} + \frac{2z(1-z)}{(U-2V)^2} + \frac{2(z^2-3z+3)}{U(U-V)} + \frac{4(z-2)}{U(U-2V)}\right.\right.$$
$$\left.\left. + \frac{4(z^2-3z+3)}{(U-V)(U-2V)}\right] + (n_0-1)\left[\frac{z-1}{U(U-V)} - \frac{z}{4(U-V)^2}\right]\right\}zt^3 + O(t^4), \tag{15}$$

which also is valid for all d-dimensional hypercubic lattices, and recovers the known result for the on-site BH model when $V=0$ [7,8].

On the other hand, for $d>1$ dimensions, when an extra particle or hole is added to the CDW phase, it could go to any of the $M/2$ sites in sublattice B or A, respectively. (Here, we recall that $n_A>n_B$ is assumed in this paper.) Therefore, for both CDW-defect states with an extra particle or hole in $d>1$ dimensions, the degeneracy is of order $M/2$ and it is lifted at second order in t. This is because the states occupy one of the sublattices, and they cannot be connected by one hop, but rather require two hops to be connected. Another lengthy but straightforward calculation leads to the energy of the CDW particle-defect state up to third order in t as

$$E^{\mathrm{par}}_{\mathrm{CDW}}(n_A,n_B) = E^{\mathrm{ins}}_{\mathrm{CDW}}(n_A,n_B) + Un_B + zVn_A - \mu + \left[\frac{(n_A+1)(n_B+1)z}{U(n_B-n_A)+V(zn_A-zn_B)} - \frac{n_A(n_B+1)z}{U(n_A-n_B-1)+V(zn_B-zn_A+1)}\right.$$
$$- \frac{n_B(n_A+1)z}{U(n_B-n_A-1)+V(zn_A-zn_B+1)} + \frac{n_A(n_B+2)}{U(n_A-n_B-2)+V(zn_B-zn_A+2)} + \frac{n_B(n_A+1)(z-1)}{U(n_B-n_A-1)+V(zn_A-zn_B)}$$
$$\left. + \frac{2n_A(n_B+1)(z-1)}{U(n_A-n_B-1)+V(zn_B-zn_A+2)}\right]zt^2 + O(t^4). \tag{16}$$

This expression is valid for $(d>1)$-dimensional hypercubic lattices. Notice that the odd-order terms in t vanish for these lattices. To third order in t, we obtain a similar expression for the energy of the CDW hole-defect state given by

$$E^{\mathrm{hol}}_{\mathrm{CDW}}(n_A,n_B) = E^{\mathrm{ins}}_{\mathrm{CDW}}(n_A,n_B) - U(n_A-1) - zVn_B + \mu + \Bigg[\frac{n_A n_B z}{U(n_B-n_A)+V(zn_A-zn_B)} - \frac{n_A(n_B+1)z}{U(n_A-n_B-1)+V(zn_B-zn_A+1)}$$
$$- \frac{n_B(n_A+1)z}{U(n_B-n_A-1)+V(zn_A-zn_B+1)} + \frac{(n_A-1)(n_B+1)}{U(n_A-n_B-2)+V(zn_B-zn_A+2)} + \frac{n_B(n_A+1)(z-1)}{U(n_B-n_A-1)+V(zn_A-zn_B)}$$
$$+ \frac{2n_A(n_B+1)(z-1)}{U(n_A-n_B-1)+V(zn_B-zn_A+2)} \Bigg] zt^2 + O(t^4). \tag{17}$$

This expression is also valid for $(d>1)$-dimensional hypercubic lattices where the odd-order terms in t vanish.

Notice that because the Mott-defect states have corrections to first order in the hopping, while the CDW defects have corrections to second order in the hopping, the slopes of the Mott phase will be finite as $t\to 0$, but they will vanish for the CDW lobes. Hence, the shapes of the different types of insulating lobes are always different.

In one dimension $(d=1)$, however, when exactly one extra particle or hole is added to the CDW phase, the degeneracy of both of the CDW-defect states is of order $(M/2)^2$ and it is lifted at first order in t. This difference between $d>1$ and $d=1$ makes one dimension unique, and it is the reason that the supersolid phase exists in higher dimensions but not in one [15,16]. In other words, due to this large degeneracy, an extra particle or hole immediately delocalizes the bosons in $d=1$, and the crystalline order disappears. Since $d=1$ requires special attention, it will be addressed elsewhere, and we restrict the analysis here to higher dimensions.

We would like to remark in passing that the energy difference between the Mott and CDW phases with their defect states determine the phase boundary of the particle and hole branches. While all $E^{\mathrm{ins}}_{\mathrm{Mott}}(n_0)$, $E^{\mathrm{par}}_{\mathrm{Mott}}(n_0)$, and $E^{\mathrm{hol}}_{\mathrm{Mott}}(n_0)$ depend on the lattice size M, their difference does not. Therefore, the chemical potentials that determine the particle and hole branches, $\mu^{\mathrm{par}}_{\mathrm{Mott}}$ and $\mu^{\mathrm{hol}}_{\mathrm{Mott}}$, respectively, are independent of M at the phase boundaries. Similarly, while all $E^{\mathrm{ins}}_{\mathrm{CDW}}(n_A,n_B)$, $E^{\mathrm{par}}_{\mathrm{CDW}}(n_A,n_B)$, and $E^{\mathrm{hol}}_{\mathrm{CDW}}(n_A,n_B)$ depend also on the lattice size M, their difference does not. Therefore, the chemical potentials that determine the particle and hole branches, $\mu^{\mathrm{par}}_{\mathrm{CDW}}$ and $\mu^{\mathrm{hol}}_{\mathrm{CDW}}$, respectively, are also independent of M at the phase boundaries. These observations indicate that the numerical quantum Monte Carlo simulations which are based on Eqs. (2)–(5) should not have too strong a dependence on M. It also shows that exact diagonalization on finite clusters of a sufficiently large size can also yield these expressions if properly analyzed to extract the coefficients of the power series.

C. Extrapolation to infinite order via scaling theory

As a general rule, the third-order strong-coupling perturbation theory appears to be more accurate in lower dimensions. For this reason, an extrapolation technique to infinite order in t is highly desirable to determine more accurate phase diagrams. Here, we propose a chemical-potential extrapolation technique based on scaling theory to extrapolate our third-order power-series expansion into a functional form that is appropriate for the Mott and CDW lobes.

It is known that the critical point at the tip of the Mott and CDW lobes has the scaling behavior of a $(d+1)$-dimensional XY model, and therefore the lobes have Kosterlitz-Thouless shapes for $d=1$ and power-law shapes for $d>1$. For the latter case considered in this paper, we propose the following ansatz for the Mott and CDW lobes which includes the known power-law critical behavior of the tip of the lobes

$$\frac{\mu^{\mathrm{par,hol}}_{\mathrm{Mott,CDW}}}{U} = A_{\mathrm{Mott,CDW}}(x) \pm B_{\mathrm{Mott,CDW}}(x)(x^c_{\mathrm{Mott,CDW}}-x)^{z\nu}, \tag{18}$$

where $A_{\mathrm{Mott,CDW}}(x)=a_{\mathrm{Mott,CDW}}+b_{\mathrm{Mott,CDW}}x+c_{\mathrm{Mott,CDW}}x^2+d_{\mathrm{Mott,CDW}}x^3+\cdots$ and $B_{\mathrm{Mott,CDW}}(x)=\alpha_{\mathrm{Mott,CDW}}+\beta_{\mathrm{Mott,CDW}}x+\gamma_{\mathrm{Mott,CDW}}x^2+\delta_{\mathrm{Mott,CDW}}x^3+\cdots$ are regular functions of $x=dt/U$, $x^c_{\mathrm{Mott,CDW}}$ is the critical point which determines the location of the Mott and CDW lobes, and $z\nu$ is the critical exponent for the $(d+1)$-dimensional XY model which determines the shape of the Mott and CDW lobes near $x^c_{\mathrm{Mott,CDW}}$. In Eq. (18), the plus sign corresponds to the particle branch, and the minus sign corresponds to the hole branch. The parameters $a_{\mathrm{Mott,CDW}}$, $b_{\mathrm{Mott,CDW}}$, $c_{\mathrm{Mott,CDW}}$, and $d_{\mathrm{Mott,CDW}}$ depend on U, V, and n_0 or $\{n_A,n_B\}$, and they are determined by matching them with the coefficients given by our third-order expansion such that $A_{\mathrm{Mott,CDW}}(x)=(\mu^{\mathrm{par}}_{\mathrm{Mott,CDW}}+\mu^{\mathrm{hol}}_{\mathrm{Mott,CDW}})/2U$. To determine the U, V, and n_0 or $\{n_A,n_B\}$ dependence of the parameters $\alpha_{\mathrm{Mott,CDW}}$, $\beta_{\mathrm{Mott,CDW}}$, $\gamma_{\mathrm{Mott,CDW}}$, $\delta_{\mathrm{Mott,CDW}}$, $x^c_{\mathrm{Mott,CDW}}$, and $z\nu$, we first expand the left-hand side of $B_{\mathrm{Mott,CDW}}(x)(x^c_{\mathrm{Mott,CDW}}-x)^{z\nu}=(\mu^{\mathrm{par}}_{\mathrm{Mott,CDW}}-\mu^{\mathrm{hol}}_{\mathrm{Mott,CDW}})/2U$ in powers of x, and match the coefficients with the coefficients given by our third-order expansion. Then we fix $z\nu$ at its well-known values such that $z\nu\approx 2/3$ for $d=2$ and $z\nu=1/2$ for $d>2$, and set $\delta_{\mathrm{Mott,CDW}}=0$ to determine $\alpha_{\mathrm{Mott,CDW}}$, $\beta_{\mathrm{Mott,CDW}}$, $\gamma_{\mathrm{Mott,CDW}}$, and $x^c_{\mathrm{Mott,CDW}}$ self-consistently.

Having discussed the strong-coupling perturbation theory, next we present the ground-state phase diagrams for $(d=2)$- and $(d=3)$-dimensional hypercubic lattices.

D. Numerical results

In Fig. 1, the results of the third-order strong-coupling perturbation theory (dotted lines) are compared to those of the extrapolation technique (circles) when $V=0.1U$. At $t=0$, the chemical-potential widths of all Mott and CDW lobes are

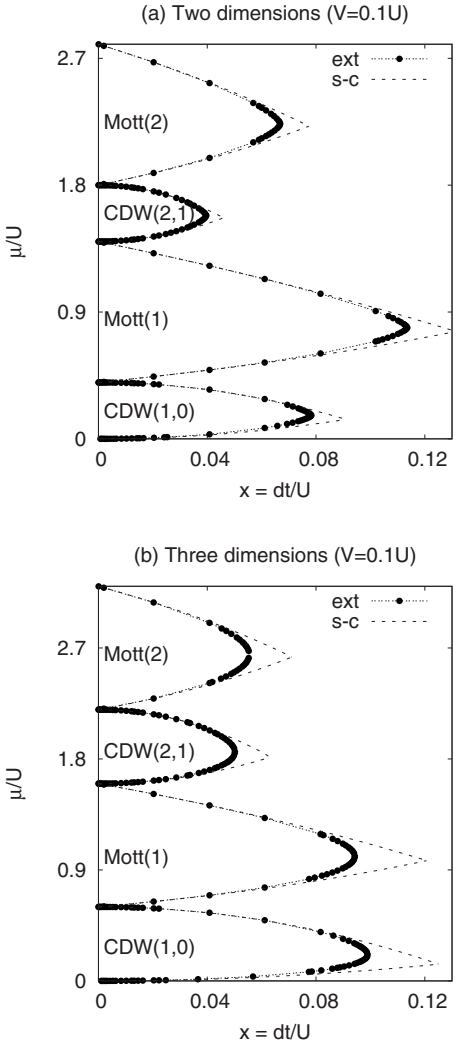

FIG. 1. Chemical potential μ (in units of U) versus $x=dt/U$ phase diagrams for (a) two-dimensional ($d=2$) and (b) three-dimensional ($d=3$) hypercubic lattices. We choose the nearest-neighbor repulsion as $V=0.1U$. The dotted lines correspond to phase boundaries for the Mott insulator to superfluid and CDW insulator to supersolid states as determined from the third-order strong-coupling perturbation theory (s-c). The circles correspond to the extrapolation fit (ext) discussed in the text.

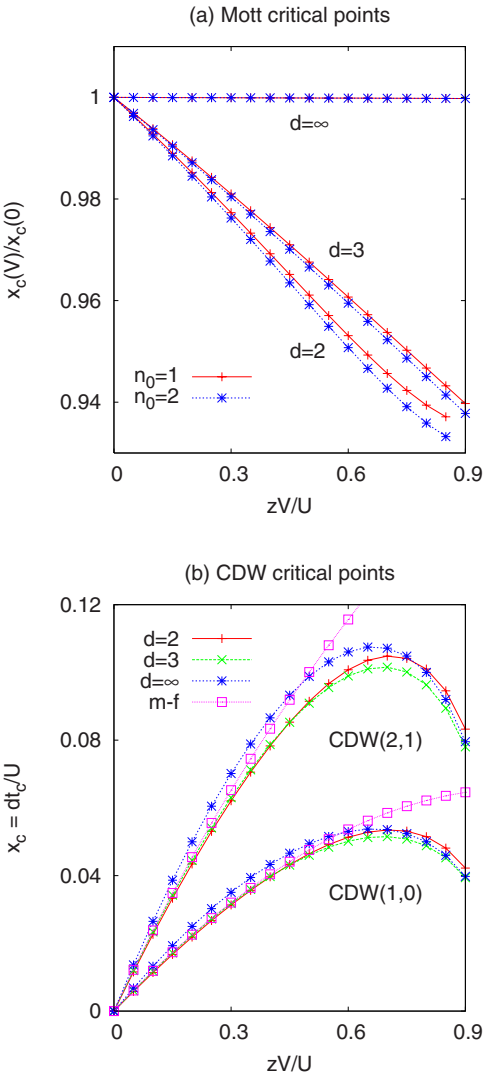

FIG. 2. (Color online) Critical points (location of the tips) $x_c=dt_c/U$ found from the chemical-potential extrapolation technique described in the text versus zV/U, where $z=2d$. In panel (a), x_c are scaled with their $V=0$ value; in infinite dimensions the exact critical hoppings for the Mott lobes are independent of V. In panel (b), comparing the extrapolated strong-coupling and exact mean-field results for the $d\to\infty$ limit shows that the critical points for the CDW lobes become less accurate as V increases. This is because the coefficient of the $O(t^4)$ term in the power series becomes very large when $zV\approx 0.7U$, which also causes an unphysical decrease in x_c for $zV\gtrsim 0.7U$ after an initial increase.

U and $0.1zU$, respectively, where $z=2d$, and that the ground state alternates between the CDW and Mott phases as a function of μ. For instance, the ground state is a vacuum ($n_0=0$) for $\mu\leq 0$; it is a CDW with ($n_A=1$, $n_B=0$) for $0\leq\mu\leq 0.1zU$; it is a Mott insulator with ($n_0=1$) for $0.1zU\leq\mu\leq(1+0.1z)U$; it is a CDW with ($n_A=2$, $n_B=1$) for $(1+0.1z)U\leq\mu\leq(1+0.2z)U$; and it is a Mott insulator with ($n_0=2$) for $(1+0.2z)U\leq\mu\leq(2+0.2z)U$.

As t increases from zero, the range of μ about which the ground state is a Mott insulator or CDW decreases, and the Mott insulator and CDW phases disappear at a critical value of t, beyond which the system becomes a superfluid near the Mott lobes or a supersolid near the CDW lobes. In addition, similar to what was found for the on-site BH model [7,8], the strong-coupling expansion overestimates the phase boundaries, and it leads to unphysical pointed tips for all Mott and CDW lobes. This is not surprising since a finite-order perturbation theory cannot describe the physics of the tricritical point correctly.

In Fig. 2, we show the critical points (location of the tips) $x_c=dt_c/U$ versus zV/U. In Fig. 2(a), x_c of the Mott lobes are scaled with their $V=0$ value. The critical points are calculated with the chemical-potential extrapolation technique that is based on the scaling theory with the exponent $z\nu$ fixed to its known value. It is expected that the locations of the tips of the CDW lobes increase as a function of V, because the presence of a nonzero V is what allowed these states to form in the first place. (The Mott insulator critical points tend to

TABLE I. List of the critical points (location of the tips) $x_c=dt_c/U$ that are found from the chemical-potential extrapolation technique described in the text.

	Two dimensions				Three dimensions			
V/U	CDW(1,0)	Mott(1)	CDW(2,1)	Mott(2)	CDW(1,0)	Mott(1)	CDW(2,1)	Mott(2)
0.00		0.117		0.0691		0.0981		0.0578
0.01	0.00929	0.117	0.00465	0.0689	0.0143	0.0977	0.00717	0.0576
0.02	0.0183	0.116	0.00916	0.0687	0.0278	0.0974	0.0139	0.0574
0.03	0.0270	0.116	0.0135	0.0684	0.0405	0.0970	0.0203	0.0571
0.04	0.0354	0.116	0.0178	0.0682	0.0522	0.0966	0.0263	0.0569
0.05	0.0434	0.115	0.0219	0.0680	0.0630	0.0962	0.0317	0.0567
0.06	0.0512	0.115	0.0258	0.0678	0.0723	0.0958	0.0367	0.0564
0.07	0.0586	0.115	0.0295	0.0676	0.0814	0.0955	0.0411	0.0562
0.08	0.0656	0.114	0.0331	0.0673	0.0888	0.0951	0.0449	0.0559
0.09	0.0721	0.114	0.0365	0.0671	0.0947	0.0947	0.0480	0.0557
0.10	0.0783	0.114	0.0396	0.0669	0.0990	0.0942	0.0502	0.0555

move in as V increases.) Comparing the extrapolated strong-coupling and exact mean-field (to be discussed below) results for the $d\to\infty$ limit shows that the critical points for the CDW lobes become less accurate as V increases. It turns out that the coefficient of the $O(t^4)$ term in the power series is generally small for the Mott lobes, but it can become very large for the CDW lobes when $zV\sim U$. We recall that we assume $U>zV$ in this paper. As shown in Fig. 2(b), this also causes an unphysical decrease in x_c for $zV\gtrsim 0.7U$ after an initial increase. Therefore, inclusion of the $O(t^4)$ terms in the expansion is necessary to improve the accuracy of the phase boundaries near the tips of the CDW lobes when $zV\sim U$. In addition, we present a short list of V/U versus the critical points $x_c=dt_c/U$ in Table I for $(d=2)$- and $(d=3)$-dimensional lattices.

As a further check of the accuracy of our perturbative expansion, next we compare the $d\to\infty$ limit of our results to the mean-field one which corresponds to the exact solution on an $(d\to\infty)$-dimensional hypercubic lattice.

IV. MEAN-FIELD DECOUPLING THEORY

In the large-dimensional case, mean-field theory becomes exact. Thus examining the mean-field theory for the extended BH model provides another way to validate the strong-coupling expansion and to test to see how well the scaling result produces the correct phase diagram.

In constructing the mean-field theory, one first defines the superfluid order parameter as $\varphi_k=\langle b_k\rangle$, where $\langle\cdots\rangle$ is the thermal average, and then replaces the operator b_k with $\varphi_k+\delta b_k$ in the hopping term of Eq. (1). This approximation decouples the two-particle hopping term into single-particle ones, and the resultant mean-field Hamiltonian can be solved via exact diagonalization in a power series of φ_k. The order parameter is finite $(\varphi_k\neq 0)$ for the superfluid and supersolid ground states, and it vanishes $(\varphi_k=0)$ for the Mott and CDW phases. Therefore, $\varphi_k\to 0^+$ signals the phase boundary between an incompressible and a compressible phase. The generalized order-parameter equation to the case of $V\neq 0$ can be written as [27]

$$\varphi_k=\bar{\varphi}_k t\left[\frac{n_k+1}{Un_k+V_k^{\mathrm{dip}}-\mu}-\frac{n_k}{U(n_k-1)+V_k^{\mathrm{dip}}-\mu}\right], \quad (19)$$

where $\bar{\varphi}_k=\Sigma_{\langle k'\rangle_k}\varphi_{k'}$ is the sum of the order parameters at sites k' neighboring to site k, and $V_k^{\mathrm{dip}}=V\Sigma_{\langle k'\rangle_k}n_{k'}$ is the interaction of one atom with sites k' neighboring to the site k.

To determine the phase boundary between the Mott and superfluid phases from Eq. (19), we set $\varphi_k=\varphi_0$, $\bar{\varphi}_k=z\varphi_0$, and $V_k^{\mathrm{dip}}=zVn_0$. Since $\varphi_0\to 0^+$ near the phase boundary, Eq. (19) can be satisfied only if

$$\frac{1}{zt}=\frac{n_0+1}{Un_0+zVn_0-\mu}-\frac{n_0}{U(n_0-1)+zVn_0-\mu}, \quad (20)$$

which gives a quadratic equation for μ. Notice that this equation recovers the known result for the on-site BH model when $V=0$ [6,28], and it can be easily solved to obtain

$$\mu_{\mathrm{Mott}}^{\mathrm{par,hol}}=U(n_0-1/2)+zVn_0-zt/2\pm\sqrt{U^2/4-U(n_0+1/2)zt+z^2t^2}, \quad (21)$$

where the plus sign corresponds to the particle branch, and the minus sign corresponds to the hole branch. In the $d\to\infty$ limit, we checked that our strong-coupling perturbation results for the Mott lobes agree with this exact solution when the latter is expanded out to third order in t, providing an independent check of the algebra. (One must note that the terms V and $2V$ that appear in the denominator vanish in the limit when $d\to\infty$ because $V\propto 1/d$.) Equation (21) also shows that the Mott lobes are separated by zV, but their shapes are independent of V. In particular, the critical points for the Mott lobes are independent of V.

To determine the phase boundary between the CDW and supersolid phases from Eq. (19), we set $\varphi_i=\varphi_A$, $\bar{\varphi}_i=z\varphi_B$, and $V_i^{\mathrm{dip}}=zVn_B$ for $i\in A$ sublattice, and we set $\varphi_j=\varphi_B$, $\bar{\varphi}_j=z\varphi_A$,

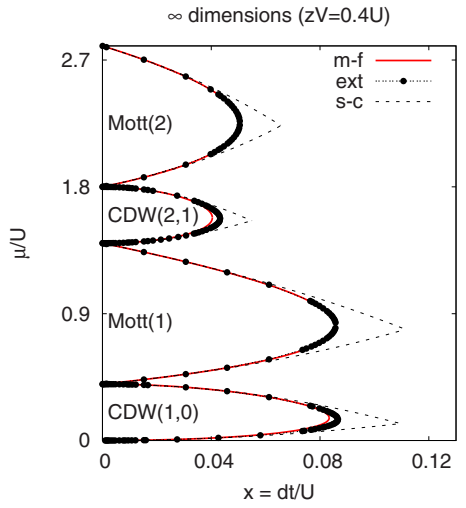

FIG. 3. (Color online) Chemical potential μ (in units of U) versus $x=dt/U$ phase diagram for a $(d\to\infty)$-dimensional hypercubic lattice. Here the nearest-neighbor repulsion scales inversely with d such that $zV=0.4U$. The dotted lines correspond to phase boundaries for the Mott insulator to superfluid and CDW insulator to supersolid states as determined from the third-order strong-coupling perturbation theory (s-c). The circles correspond to the extrapolation fit (ext) discussed in the text. The red solid lines correspond to phase boundaries for the Mott insulator to superfluid and CDW insulator to supersolid states as determined from the mean-field theory (m-f) which becomes exact for $d\to\infty$.

and $V_j^{\mathrm{dip}}=zVn_A$ for $j\in B$ sublattice. This leads to two coupled equations for φ_A and φ_B. Since $\{\varphi_A,\varphi_B\}\to 0^+$ near the phase boundary, Eq. (19) can be satisfied only if

$$\frac{1}{z^2t^2}=\left[\frac{n_A+1}{Un_A+zVn_B-\mu}-\frac{n_A}{U(n_A-1)+zVn_B-\mu}\right]\times\left[\frac{n_B+1}{Un_B+zVn_A-\mu}-\frac{n_B}{U(n_B-1)+zVn_A-\mu}\right], \tag{22}$$

which gives a quartic equation for μ. Since a simple closed-form analytic solution for μ is not possible, we solve Eq. (22) with MATHEMATICA for each of the CDW lobes separately. In the $d\to\infty$ limit, we also checked that our strong-coupling perturbation results for the CDW lobes agree with this exact solution when the latter is expanded out to third order in t, providing again an independent check of the algebra.

In Fig. 3, the results of the third-order strong-coupling perturbation theory (dotted lines) is compared to those of the exact mean-field theory (red solid lines) and of the extrapolation technique (circles) for an infinite $(d\to\infty)$-dimensional hypercubic lattice when $zV=0.4U$. Notice that in infinite dimensions, both t and V must scale inversely with d such that dt and dV are finite. The extrapolated solutions are indistinguishable from the exact ones for the Mott lobes, and they are within 5% of each other for the tips of the CDW lobes. It turns out that this minor disagreement around the tips of the CDW lobes is due to the large coefficient of the $O(t^4)$ term in the power-series expansion. Therefore, we conclude that, even in infinite dimensions, the agreement of the third-order strong-coupling perturbation theory with the exact mean-field theory is quite good.

V. CONCLUSIONS

We analyzed the zero-temperature phase diagram of the extended BH model with on-site and nearest-neighbor boson-boson repulsions in $(d>1)$-dimensional hypercubic lattices. We used the many-body version of Rayleigh-Schrödinger perturbation theory in the kinetic-energy term with respect to the ground state of the system when the kinetic-energy term is absent. This technique was previously used to discuss the phase diagram of the on-site BH model [7,8], and its extrapolated results showed excellent agreement with the recent quantum Monte Carlo simulations [25,26]. Here, we generalized this method to the extended BH model, hoping to develop an analytical approach which could be as accurate as the numerical ones.

We derived analytical expressions for the phase boundaries between the incompressible (Mott or CDW insulators) and compressible (superfluid or supersolid) phases up to third order in the hopping t. However, we remark that the strong-coupling perturbation theory developed here cannot be used to calculate the phase boundary between two compressible phases, e.g., the supersolid-to-superfluid transition. We also proposed a chemical-potential extrapolation technique based on the scaling theory to extrapolate our third-order power-series expansion into a functional form that is appropriate for the Mott or CDW lobes.

We believe some of our results could potentially be observed with ultracold dipolar Bose gases loaded into optical lattices [27,29]. This is motivated by the recent success in observing superfluid–to–Mott insulator transition with ultracold pointlike Bose gases loaded into optical lattices. Such lattices are created by the intersection of laser fields, and they are nondissipative periodic potential-energy surfaces for the atoms. An ultracold dipolar Bose gas can be realized in many ways with optical lattices. For instance, heteronuclear molecules which have permanent electric dipole moments, Rydberg atoms which have very large induced electric dipole moment, or chromiumlike atoms which have large intrinsic magnetic moment can be used to generate sufficiently strong long-ranged dipole-dipole interactions.

This work can be extended in several ways if desired. For instance, our current results for the CDW phase are not directly applicable to the one-dimensional case. We are currently working on this problem and will report our results elsewhere. In addition, it turns out that the coefficient of the $O(t^4)$ term in the power series is generally small for the Mott lobes, but it can become very large for the CDW lobes when $zV\sim U$. Therefore, inclusion of the $O(t^4)$ is necessary to improve the accuracy of the phase boundaries near the tips of the CDW lobes when $zV\sim U$. One can also examine frustration effects by performing these calculations on nonbipartite lattices. In addition, one can include the next-nearest-neighbor repulsion term to the current model, which would lead to additional striped CDW phases. Lastly, one can also

examine how the momentum distribution changes with the hopping in the CDW phase or in the Mott phase when there is a nearest-neighbor repulsion. This last calculation could have direct relevance for experiments on these systems and would generalize recent results for the $V=0$ case [30].

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