Bose-Hubbard models coupled to cavity light fields

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Recent experiments on strongly coupled cavity quantum electrodynamics present new directions in "matterlight" systems. Following on from our previous work [Phys. Rev. Lett. **102**, 135301 (2009)] we investigate Bose-Hubbard models coupled to a cavity light field. We discuss the emergence of photoexcitations or "polaritons" within the Mott phase, and obtain the complete variational phase diagram. Exploiting connections to the superradiance transition in the Dicke model we discuss the nature of polariton condensation within this novel state. Incorporating the effects of carrier superfluidity, we identify a first-order transition between the super-radiant Mott phase and the single component atomic superfluid. The overall predictions of mean field theory are in excellent agreement with exact diagonalization and we provide details of superfluid fractions, density fluctuations, and finite size effects. We highlight connections to recent work on coupled cavity arrays.

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I. INTRODUCTION

Over the last few years there has been tremendous activity in studying the coherent interaction of matter and radiation in a rich variety of "matter-light" systems. Recent experiments have combined cavity quantum electrodynamics (cavity QED) with cold atomic gases, and allow access to the strongly coupled regime. This has led to pioneering work on Bose-Einstein condensates (BECs) in ultrahigh finesse optical cavities [\[1\]](#page-13-0), and with optical fibers on atom chips [\[2\]](#page-13-0). It has also stimulated advances in cavity optomechanics and condensate dynamics [\[3,4\]](#page-13-0). More recently, strong matter-light coupling has been achieved for ion crystals [\[5,6\]](#page-13-0), with potential applications in quantum information processing. These developments offer a wealth of possibilities, at the interface between quantum optics, cold atoms and condensed matter physics. The light field serves not only as a probe of the many-body system [\[7\]](#page-13-0), but may also support interesting cavity mediated phenomena and phases. It may further provide routes to simulate strongly correlated quantum systems, with proposals based on coupled cavity arrays $[8-23]$ and nonlinear optical fibers $[24]$.

Allied advances in solid state devices include cavity QED experiments with superconducting qubits in microwave resonators [\[25\]](#page-13-0). This has provided clean realizations of the paradigmatic Jaynes-Cummings [\[26\]](#page-13-0) and Dicke models [\[27\]](#page-13-0), describing two-level systems coupled to radiation. It has also led to remarkable observations of the Lamb shift [\[28\]](#page-13-0). This is complemented by the quest for polariton condensates in semiconductor microcavities [\[29–34\]](#page-13-0), where the hybridization of an exciton and a photon yields low effective mass polaritons. This offers the prospect of higher transition temperatures than for exciton BEC, and gives access to coherence properties via the cavity light field.

Motivated by this broad spectrum of activity, we examine the impact of cavity radiation on bosonic Hubbard models [\[35\]](#page-13-0). Following on from our previous work [\[36\]](#page-13-0), we focus on a two-band model in which photons induce transitions between two internal states or Bloch bands. This is a natural generalization of the much studied two-level systems coupled to radiation, and may serve as a useful paradigm in other contexts. In Ref. [\[36\]](#page-13-0) we discussed the interplay of Mott

physics, photoexcitation, and Bose condensation promoted by carrier itinerancy. In particular, we provided evidence for a novel Mott phase with photoexcitations analogous to polaritons. In this work we study this problem in more detail, with emphasis on the nature of the polariton condensate. We also highlight connections to coupled cavity arrays described by the Jaynes-Cummings-Hubbard model and its variants [\[8–23\]](#page-13-0). Additional directions in cold atoms include recent work on excitons [\[37\]](#page-13-0), generalized Dicke models [\[38\]](#page-13-0), and light propagation in atomic Mott insulators [\[39,40\]](#page-13-0).

The outline of this paper is as follows. We begin in Sec. II with an introduction to the two-band Bose-Hubbard model coupled to quantum light $[36]$. In Sec. [III](#page-1-0) we discuss the zero hopping limit of this model and anchor the phase diagram. We study the evolution with the strength of the matter-light coupling and highlight the connections to the Dicke model and the super-radiance transition $[41-44]$. In Sec. [IV](#page-4-0) we use a variational approach to obtain the overall phase diagram in the presence of hopping. We corroborate our findings in Sec. [V](#page-7-0) using numerical simulations. We discuss the relation to the bosonic BEC-BCS crossover and to other problems of current interest in Sec. [VI.](#page-9-0) We conclude in Sec. [VII](#page-10-0) and provide technical appendices.

II. MODEL

Let us consider a two-band Bose-Hubbard model coupled to the quantum light field of an optical cavity in the rotating wave approximation [\[36\]](#page-13-0):

$$
H_0 = \sum_{i\alpha} \epsilon_{\alpha} n_{i\alpha} + \omega \psi^{\dagger} \psi + \sum_{i\alpha\alpha'} \frac{U_{\alpha\alpha'}}{2} : n_{i\alpha} n_{i\alpha'} : - \sum_{\langle ij \rangle} J_{\alpha} (\alpha_i^{\dagger} \alpha_j + \text{h.c.}) + g \sum_i (b_i^{\dagger} a_i \psi + \text{H.c.}), \qquad (1)
$$

where *i* labels lattice sites, and $\alpha = a$, *b* are bosons obeying canonical commutation relations $[\alpha_i, \alpha_j] = \delta_{ij}$. These might be states of different orbital or spin angular momentum, and we assume the cavity radiation field, ψ , may induce photoexcitations between these states; see Fig. [1.](#page-1-0)

FIG. 1. (Color online) Heuristic diagram showing photoexcitations above the filled bosonic Mott state. In analogy with fermionic band insulators, the coherent superposition of a particle–hole pair and a photon will be referred to as a "polariton". Within an equilibrium framework these polaritons may Bose condense.

Here, ϵ_{α} effects the band splitting $\omega_0 \equiv \epsilon_b - \epsilon_a$, and $U_{\alpha\alpha'}$ are interactions, where :: indicates normal ordering. This yields : $n_{i\alpha}n_{i\alpha} := n_{i\alpha}(n_{i\alpha} - 1)$ for like species and : $n_{i\alpha}n_{i\alpha} :=$ $n_{i\alpha}n_{i\alpha'}$ for distinct species. J_{α} are nearest neighbor hopping parameters, and ω is the frequency of the cavity mode. For simplicity we consider just a single mode which couples uniformly to the bands. The coupling *g* is the strength of the matter-light interaction. In view of the box normalization of the photon field, the dipole coupling strength is proportional the photon field, the dipole coupling strength is proportional
to $1/\sqrt{V}$, where V is the volume of the cavity. With a fixed density of lattice sites, $\rho = N/V$, it is convenient to denote $g = \bar{g}/\sqrt{N}$, where *N* is the total number of lattice sites. We work in units where the half-band splitting $\omega_0/2 =$ $(\epsilon_b - \epsilon_a)/2 = 1.$

An important feature of the Hamiltonian [\(1\)](#page-0-0) is that the individual atom and photon numbers are *not* conserved due to the matter-light interaction. However, the total number of atomic carriers

$$
N_1 \equiv \sum_i \left(n_i^b + n_i^a \right),\tag{2}
$$

and the total number of photoexcitations

$$
N_2 \equiv \psi^{\dagger} \psi + \frac{1}{2} \sum_{i} (n_i^b - n_i^a + 1), \tag{3}
$$

are conserved and commute with H_0 . The latter counts the total number of photons plus particle-hole pairs, and we refer to these composite excitations as "polaritons"—see Fig. 1. These conservation laws reflect the global $U(1) \times U(1)$ symmetry of H_0 such that

$$
a \to e^{i\vartheta} a, \quad b \to e^{i\varphi} b, \quad \psi \to e^{-i(\vartheta - \varphi)} \psi, \tag{4}
$$

where $\vartheta, \varphi \in \mathbb{R}$. In general this symmetry involves mixing between the matter-light sectors. Moreover, it also allows for the simultaneous coexistence of Mott behavior and condensation, corresponding to an unbroken U(1) and broken U(1) symmetry, respectively. This symmetry will have a direct manifestation in the phase diagram, and will suggest implications for other multicomponent problems. We will work in the grand canonical ensemble:

$$
H = H_0 - \mu_1 N_1 - \mu_2 N_2. \tag{5}
$$

We begin by assuming that *a* are strongly interacting hardcore bosons, $U_{aa} \rightarrow \infty$, and that *b* are sufficiently dilute so that we may neglect their interactions, $U_{bb} = 0$. We will also start with $U_{ab} = 0$, before discussing departures from these conditions.

III. ZERO HOPPING LIMIT

Before embarking on a detailed examination of the model [\(1\)](#page-0-0), we investigate the zero hopping limit. As in the single-band Bose-Hubbard model [\[45,46\]](#page-13-0) this anchors the topology of the general phase diagram. In the present case this is particularly informative since the zero hopping phase diagram evolves with the matter-light coupling, *g*. In addition, the global photon mode couples *all* the sites, even in this zero hopping limit. To gain a handle on this reduced Hamiltonian, we find it convenient to develop two complementary approaches. These help illuminate different aspects of the more general itinerant problem, and provide a platform for extensions. In Sec. III A we begin with a variational approach using a coherent state ansatz for the photons. This will enable us to derive an effective single site Jaynes-Cummings model [\[47\]](#page-13-0) for the *a,b* bosons, and proceed with the minimum of technical input. In section $IIIB$ we instead map the a, b bosons on to effective spins. This yields the paradigmatic Dicke model [\[41\]](#page-13-0), describing many spins coupled to radiation. The Jaynes-Cummings and Dicke models are familiar in atomic physics and quantum optics and we provide a brief overview of these closely related Hamiltonians in Appendix [A.](#page-11-0) Both approaches yield equivalent results and indicate a novel quantum phase transition occurring within the lowest Mott lobe [\[36\]](#page-13-0). This takes place from a conventional Mott state with no photons, to a state with a nonvanishing population of photoexcitations, as the strength of the matter-light coupling is increased. This quantum phase transition coincides with the well known super-radiance transition in the Dicke model [\[41–44\]](#page-13-0), and we interpret the results in this framework. The combination of perspectives will be useful in the generalization to the itinerant problem discussed in Sec. [IV.](#page-4-0) For other proposals of Dicke models and super-radiance transitions in cold atomic gases see Refs. [\[48–50\]](#page-13-0).

A. Variational approach

In the zero hopping and $U_{aa} \rightarrow \infty$ limit, the Hamiltonian (5) may be written in the form

$$
H = \tilde{\epsilon}_a \sum_i n_i^a + \tilde{\epsilon}_b \sum_i n_i^b + \tilde{\omega} \psi^\dagger \psi
$$

+
$$
g \sum_i (b_i^\dagger a_i \psi + \psi^\dagger a_i^\dagger b_i),
$$
 (6)

where the site occupancy of *a* atoms is limited to 0*,* 1. We absorb the chemical potentials in to the definitions

$$
\tilde{\epsilon}_a \equiv \epsilon_a - \mu_1 + \mu_2/2,
$$

\n
$$
\tilde{\epsilon}_b \equiv \epsilon_b - \mu_1 - \mu_2/2,
$$

\n
$$
\tilde{\omega} \equiv \omega - \mu_2.
$$
\n(7)

This bosonic Hamiltonian is analogous to the fermionic problem of localized excitons in a microcavity [\[51,52\]](#page-13-0). An instructive way to analyze the problem is to consider a coherent state for the cavity light field:

$$
|\gamma\rangle \equiv e^{-\frac{\gamma^2}{2} + \gamma \psi^{\dagger}} |0\rangle, \tag{8}
$$

where γ is a variational parameter to be determined. As usual, this is an eigenstate of the annihilation operator, ψ , with eigenvalue γ . The coherent state assumption is expected to become exact in the thermodynamic limit, and this is borne out by the complementary approach in Sec. [III B.](#page-3-0) The expectation value,

$$
\langle \gamma | H | \gamma \rangle \equiv \sum_{i} H_{\text{eff}}, \tag{9}
$$

yields an effective *single site* problem for the *a* and *b* atoms which is readily diagonalized:

$$
H_{\text{eff}} = \tilde{\epsilon}_a n^a + \tilde{\epsilon}_b n^b + \bar{\omega} \gamma^2 + g \gamma (b^\dagger a + a^\dagger b), \qquad (10)
$$

where $\bar{\omega} \equiv \tilde{\omega}/N$. This is a significant merit of the current approach, since it is directly tractable without technical input. In view of the hardcore constraint on the *a* atoms, this describes a *single* two-level system coupled to an effective "radiation field" of *b* atoms. This paradigm is described by the much studied Jaynes-Cummings model [\[47,53\]](#page-13-0), discussed in Appendix [A.](#page-11-0) The eigenstates of Eq. (10) are superpositions in the upper and lower bands. Focusing on Mott states with total occupation $n_a + n_b = n$, we consider admixtures of $|0, n\rangle$ and $|1, n-1\rangle$ in the $|n_a, n_b\rangle$ basis. The lowest eigenstate has energy

$$
E_n^- = \bar{\omega}\gamma^2 + n\tilde{\epsilon}_b - \tilde{\omega}_0/2 - \sqrt{\tilde{\omega}_0^2/4 + g^2\gamma^2 n},\qquad(11)
$$

where $\tilde{\omega}_0 \equiv \tilde{\epsilon}_b - \tilde{\epsilon}_a$ is the effective band splitting. The nonlinear dependence on \sqrt{n} is a notable feature of the Jaynes-Cummings eigenstates and has recently been seen in circuit QED experiments [\[26\]](#page-13-0). (Analogous dependence is also seen in BECs [\[1,2\]](#page-13-0) as a function of the number of atoms in the cavity.) Minimizing with respect to γ , one obtains the variational self-consistency condition

$$
\frac{\partial E_n^-}{\partial \gamma} = 2\gamma \left(\bar{\omega} - \frac{g^2 n}{\sqrt{\tilde{\omega}_0^2 + 4g^2 \gamma^2 n}} \right) = 0. \quad (12)
$$

Depending on the parameters, one may therefore obtain either the trivial solution $\gamma = 0$, corresponding to zero photon occupancy, or the nontrivial solution

$$
\gamma_{\text{var}}^2 = \frac{1}{4} \left(\frac{g^2 n}{\bar{\omega}^2} - \frac{\tilde{\omega}_0^2}{g^2 n} \right) = \langle \psi^\dagger \psi \rangle,\tag{13}
$$

corresponding to a finite photon occupancy. This latter solution is supported in the region where $\gamma_{\text{var}}^2 > 0$, or when the matterlight coupling exceeds the critical value

$$
\bar{\mathcal{G}}_c \equiv \bar{g}_c \sqrt{n} = \sqrt{\tilde{\omega}\tilde{\omega}_0},\tag{14}
$$

where for simplicity we consider $\tilde{\omega}_0 > 0$. As we shall discuss in Sec. [III B,](#page-3-0) this onset of the photon field corresponds to the well-known super-radiance transition in the Dicke model [\[41–44\]](#page-13-0). Indeed, it is readily seen from Eq. (13), that for $\mathcal{G} \geq$ $\bar{\mathcal{G}}_c$, the photon field has the characteristic variation

$$
\frac{\langle \psi^{\dagger} \psi \rangle}{N} = \frac{1}{4\tilde{\omega}^2} \left(\frac{\bar{\mathcal{G}}^4 - \bar{\mathcal{G}}_c^4}{\bar{\mathcal{G}}^2} \right),\tag{15}
$$

where $\bar{G} = \bar{g}\sqrt{n}$. See for example Table 1 of Ref. [\[54\]](#page-13-0). We shall give an alternative derivation of these results in Sec. [III B.](#page-3-0) This complementary approach becomes asymptotically exact in the thermodynamic limit and helps justify the coherent state ansatz (8) .

FIG. 2. (Color online) Zero hopping phase diagram in the $U_{aa} \rightarrow$ ∞ limit with $U_{bb} = U_{ab} = 0$. We set $\epsilon_b = -\epsilon_a = \bar{g} = 1$ and $\omega = 1$ corresponding to $\omega < \omega_0$, where $\omega_0 \equiv \epsilon_b - \epsilon_a$. The vertical line, $\bar{g} =$ \bar{g}_c , is the super-radiance transition in the Dicke model, and separates a Mott insulator (MI) with $n_a + n_b = 1$ and $\langle \psi^{\dagger} \psi \rangle = 0$, from a superradiant Mott insulator (SRMI) with $\langle \psi^{\dagger} \psi \rangle \neq 0$. Outside of these regions are the vacuum state, and the unstable region corresponding to macroscopic population of the *b* states. Whilst the total density is fixed within both Mott phases, $n_a + n_b = 1$, the individual *a* and *b* populations vary in the super-radiant phase as shown in Fig. [3.](#page-3-0) Inset: $\epsilon_b = -\epsilon_a = \bar{g} = 1$ and $\omega = 3$. For $\omega > \omega_0$ the upper and lower boundaries may cross and terminate the lobe, since for $\mu_2 > \omega_0$ the lowest stable state is the vacuum; see Appendix [D](#page-12-0) for a derivation of this.

Knowledge of the eigenvalues (11) , together with the variational consistency condition (12), enables one to construct the zero hopping phase diagram depicted in Fig. 2. The lower boundary consists of two segments. The first corresponds to the transition from the vacuum to the Mott state with no photons, and is given by the condition $E_1^-(\gamma = 0) \leq 0$ or $\mu_1 \geq \epsilon_a + \mu_2/2$. The second segment corresponds to the transition in to the photon rich Mott state and occurs when $E_1^-(\gamma_{\text{var}}) \leq 0$ where

$$
E_n^-(\gamma_{\text{var}}) = n\tilde{\epsilon}_b - \frac{\tilde{\omega}_0}{2} - \frac{n}{4\tilde{\omega}} \left(\frac{\bar{g}^4 + \bar{g}_c^4}{\bar{g}^2} \right). \tag{16}
$$

Explicitly this locus is given by

$$
\mu_1 \geqslant \frac{\epsilon_a + \epsilon_b}{2} - \frac{1}{4\tilde{\omega}} \left(\frac{\bar{g}^4 + \tilde{\omega}^2 (\omega_0 - \mu_2)^2}{\bar{g}^2} \right). \tag{17}
$$

Noting that \bar{g}_c depends on *n* according to Eq. (14) we see that $E_n^-(\gamma_{\text{var}}) \to n(\tilde{\epsilon}_b - \bar{g}^2/4\tilde{\omega})$ as $n \to \infty$. For $\tilde{\epsilon}_b - \bar{g}^2/4\tilde{\omega} \leq 0$, or chemical potentials satisfying

$$
\mu_1 \geqslant \epsilon_b - \frac{\mu_2}{2} - \frac{\bar{g}^2}{4(\omega - \mu_2)},\tag{18}
$$

it is energetically favorable to macroscopically populate the *b* levels. This corresponds to the upper boundary in Fig. 2. Indeed, in the absence of the matter-light coupling Eq. (18) yields $\tilde{\epsilon}_b \leqslant 0$ and is naturally associated with population of the *b* states; we provide the corresponding $g = 0$ phase diagram for comparison in Appendix \overline{B} . In contrast to the classical light case (where ψ is treated as a fixed *c*-number) coupling to the fluctuating quantum field, ψ , eliminates the higher Mott lobes corresponding to integer increases in the *b*-populations; the higher lobes corresponding to the *a* particles have been

FIG. 3. (Color online) Onset of magnetization $\mathcal{M} = (n_b - n_a)/2$ at the super-radiance transition, traversing a line through Fig. [2](#page-2-0) with $\mu_1 = 0$. Whilst the total density $n_a + n_b = 1$ remains pinned throughout the entire Mott region, photoexcitation promotes atoms between the bands in the super-radiant phase.

explicitly eliminated by the hardcore constraint. We confirm this reduction analytically in Appendix [D.](#page-12-0)

Accompanying the super-radiance transition is a change in the relative atomic populations or "magnetization"

$$
\mathcal{M} = \frac{1}{2}(\langle n_b \rangle - \langle n_a \rangle),\tag{19}
$$

corresponding to photoexcitation into the upper band. Indeed, the possibility of such magnetic phase transitions is a strong motivation for studying multicomponent problems, even without matter-light coupling [\[55,56\]](#page-13-0). The magnetization (19) is readily computed from the Jaynes-Cummings eigenstates [\(A6\)](#page-11-0) with $n = 1$. It also serves as an order parameter for this continuous transition:

$$
\mathcal{M} = \begin{cases}\n-\frac{1}{2}; & \tilde{\mathcal{G}} \leq \tilde{\mathcal{G}}_c, \\
-\frac{1}{2}\left(\frac{\tilde{\mathcal{G}}_c}{\tilde{\mathcal{G}}}\right)^2; & \tilde{\mathcal{G}} \geq \tilde{\mathcal{G}}_c.\n\end{cases}
$$
\n(20)

This corresponds to $\langle n_a \rangle = 1$ and $\langle n_b \rangle = 0$, for $\bar{\mathcal{G}} \leq \bar{\mathcal{G}}_c$, and a nontrivial imbalance, $\langle n_b \rangle - \langle n_a \rangle$, for $\bar{G} > \bar{G}_c$. In Fig. 3 we plot the continuous onset of population imbalance described by Eq. (20) . In Sec. III B we will see how these results emerge from the exactly solvable Dicke model.

B. Dicke model

As in the fermionic cases considered elsewhere [\[51,52\]](#page-13-0), an alternative way to view the zero hopping Hamiltonian (6) is as an effective spin-boson model. Within the subspace of fixed density, $n_a + n_b = n$, we introduce effective spins for *a priori* possible Mott lobes

$$
|\psi\rangle = |1, n - 1\rangle, \quad |\Uparrow\rangle = |0, n\rangle, \tag{21}
$$

where we denote bosonic states as $|n_a, n_b\rangle$. The operators

$$
S^{+} = \frac{b^{\dagger} a}{\sqrt{n}}, \quad S^{-} = \frac{a^{\dagger} b}{\sqrt{n}}, \quad S^{z} = \frac{1}{2} - n_{a}, \quad (22)
$$

form a representation of *su*(2) on this restricted Hilbert space. In the lowest Mott lobe with $n = 1$ this reduces to the usual Schwinger boson construction $[57]$. In the representation (22) the Hamiltonian [\(6\)](#page-1-0) becomes

$$
H = \tilde{\omega}_0 \sum_{i=1}^N S_i^z + \tilde{\omega} \psi^\dagger \psi + \mathcal{G} \sum_{i=1}^N (S_i^+ \psi + \text{H.c.}) + c_n, \quad (23)
$$

where $G \equiv g \sqrt{n}$ and $c_n = N(n\tilde{\epsilon}_b - \tilde{\omega}_0/2)$. This is the much studied spin-1*/*2 Dicke model [\[41\]](#page-13-0), describing *N* two-level systems coupled to radiation; see Appendix [A](#page-11-0) for a brief review. This model is integrable [\[42,44](#page-13-0)[,58\]](#page-14-0) and in the thermodynamic limit it has a quantum phase transition to a so-called super-radiant phase when [\[42–44\]](#page-13-0)

$$
\bar{\mathcal{G}}_c \equiv \mathcal{G}_c \sqrt{N} = \sqrt{\tilde{\omega}\tilde{\omega}_0},\tag{24}
$$

in agreement with our previous result [\(14\)](#page-2-0). In this context, the term super-radiance indicates the onset of many-body or cooperative effects involving the photon coupled to many atoms. This mapping not only helps justify our variational approach, but will also provide insights into polariton condensation and matter-light coherence at the super-radiance transition.

The thermodynamic limit of the Dicke model (23) may be analyzed using collective spin operators [\[59\]](#page-14-0)

$$
\mathbf{J} \equiv \sum_{i}^{N} \mathbf{S}_{i},\tag{25}
$$

where we exploit site independence of the global photon field, and $N \equiv 2S$ plays the role of a large spin. This motivates an asymptotically exact semiclassical treatment based on the Holstein-Primakoff transformation [\[59–61\]](#page-14-0)

$$
J^{+} = c^{\dagger} (2S - c^{\dagger} c)^{1/2},
$$

\n
$$
J^{-} = (2S - c^{\dagger} c)^{1/2} c,
$$

\n
$$
J^{z} = c^{\dagger} c - S,
$$
\n(26)

where c is a canonical boson. The super-radiance transition is associated with condensation of this auxiliary boson. Most crucially, this is related to condensation of *polaritons*, and *not* the a, b bosons themselves. The Dicke model (23) becomes

$$
H = \tilde{\omega}_0 (c^{\dagger} c - S) + \tilde{\omega} \psi^{\dagger} \psi + \frac{\tilde{\mathcal{G}}}{\sqrt{N}} [\psi^{\dagger} (2S - c^{\dagger} c)^{1/2} c + c^{\dagger} (2S - c^{\dagger} c)^{1/2} \psi], \quad (27)
$$

where we drop the 'constant' c_n . Within a semiclassical 1*/S* expansion around the thermodynamic limit [\[59\]](#page-14-0) we may proceed by introducing coherent states for the photon and auxiliary boson

$$
|\gamma\rangle \equiv e^{-\frac{\gamma^2}{2} + \gamma \psi^{\dagger}} |0\rangle, \quad |\zeta\rangle \equiv e^{-\frac{\zeta^2}{2} + \zeta c^{\dagger}} |0\rangle, \tag{28}
$$

where γ and ζ are classical *c*-numbers. The energy density reads

$$
\mathcal{E} \equiv \langle H \rangle / N = \tilde{\omega}_0 (\bar{\zeta}^2 - 1/2) + \tilde{\omega} \bar{\gamma}^2 + 2 \bar{\mathcal{G}} \bar{\gamma} \bar{\zeta} (1 - \bar{\zeta}^2)^{1/2},
$$
\n(29)

where $\bar{\gamma} \equiv \gamma / \sqrt{N}$, $\bar{\zeta} \equiv \zeta / \sqrt{N}$. Minimizing over $\bar{\gamma}$ gives

$$
\bar{\gamma} = -\frac{\bar{\mathcal{G}}\bar{\zeta}(1 - \bar{\zeta}^2)^{1/2}}{\tilde{\omega}}.\tag{30}
$$

Substituting back in Eq. [\(29\)](#page-3-0) yields

$$
\mathcal{E} = \frac{\bar{\mathcal{G}}^2}{\tilde{\omega}} \bar{\zeta}^4 + \left(\tilde{\omega}_0 - \frac{\bar{\mathcal{G}}^2}{\tilde{\omega}} \right) \bar{\zeta}^2 - \frac{\tilde{\omega}_0}{2},\tag{31}
$$

and we acquire an expectation value $\langle c \rangle \neq 0$ when the quadratic term becomes negative. This corresponds to the quadratic term becomes negative. This corresponds to the super-radiance quantum phase transition at $\bar{g}_c = \sqrt{\tilde{\omega}\tilde{\omega}_0}$ in agreement with the previous results. Minimizing Eq. (31) over $\overline{\zeta}^2$ and substituting into Eq. [\(30\)](#page-3-0) one obtains

$$
\bar{\zeta}^2 = \frac{\bar{\mathcal{G}}^2 - \bar{\mathcal{G}}_c^2}{2\bar{\mathcal{G}}^2}, \quad \bar{\gamma}^2 = \frac{\bar{\mathcal{G}}^4 - \bar{\mathcal{G}}_c^4}{4\tilde{\omega}^2 \bar{\mathcal{G}}^2}; \quad \bar{\mathcal{G}} \ge \bar{\mathcal{G}}_c. \tag{32}
$$

The onset of the photon field agrees with Eq. [\(15\)](#page-2-0). In addition, the expectation value $\langle J^{\dagger} \rangle = \zeta (2S - \zeta^2)^{1/2}$ tracks the condensation of the Holstein-Primakoff boson, *c*, via its coherent state parameter *ζ* :

$$
\frac{\langle J^+\rangle}{N} = \bar{\zeta} (1 - \bar{\zeta}^2)^{1/2} = -\frac{\tilde{\omega}\bar{\gamma}}{\bar{\mathcal{G}}}.
$$
 (33)

These results show that the super-radiance transition is accompanied by condensation of the Holstein-Primakoff boson, $\langle c \rangle \neq 0$. As we will discuss in Sec. [IV B,](#page-5-0) in the two-band Bose-Hubbard model coupled to light, this corresponds to condensation of the polaritonic *bilinear* $\langle b^{\dagger}a \rangle$ above the Mott background, and *not* the *a*, *b* bosons themselves. In addition to the onset of photons described by Eqs. (15) and (32) , the magnetization $\mathcal{M} \equiv \langle J^z \rangle / N$ reproduces the previous results.

The correspondence between the variational approach outlined in Sec. [III A,](#page-1-0) and the Dicke model analysis is clearly encouraging. In Sec. IV we shall extend the variational approach to include the important effects of itinerancy and carrier superfluidity.

IV. VARIATIONAL APPROACH FOR HARDCORE ATOMS

A. Phase diagram

Having confirmed a zero hopping Mott phase, with n_a + $n_b = 1$, we consider itinerancy and carrier superfluidity. Within this lowest lobe we may take *hardcore a and b* bosons. This will also be convenient for the numerical simulations in Sec. [V.](#page-7-0) While this does not affect physics *within* the lobe, the zero hopping upper boundary is modified by the restriction on the *b*-atom population. In this case we only need retain the states $|0, 0\rangle$, $|1, 1\rangle$ and the admixtures of $|0, 1\rangle$ and $|1, 0\rangle$. The zero hopping diagram shown in Fig. [2](#page-2-0) is replaced by Fig. 4. The lower boundary remains unchanged because the same eigenstates are involved, and the upper boundary becomes a mirror reflection of the lower one. This is quite natural since the *a* and *b* operators now appear on an equal footing, modulo the effects of the band splitting. More formally, this may be traced to the invariance of the hardcore Hamiltonian [\(5\)](#page-1-0) (up to a constant term) under the particle-hole transformation $a \rightarrow a^{\dagger}, b \rightarrow b^{\dagger}$, together with $\mu_1 \rightarrow \epsilon_a + \epsilon_b + U_{ab} - \mu_1$, and the interchange of the *a* and *b* operators and the hopping parameters J_a and J_b ; since hardcore bosons obey on-site *anticommutation* relations, $n \rightarrow 1 - n$, under particle-hole transformation. For $\epsilon_a = -1$, $\epsilon_b = 1$ and $U_{ab} = 0$ this involves $\mu_1 \rightarrow -\mu_1$. The particle-hole transformation also accounts for the change in the vacuum, $|0, 0\rangle \rightarrow |1, 1\rangle$.

FIG. 4. (Color online) Variational zero hopping diagram for *hardcore a* and *b* atoms. The symmetry about $\mu_1 = 0$ reflects the combined particle-hole and species interchange symmetry of the Hamiltonian [\(6\)](#page-1-0) in the hardcore limit; see text.

To incorporate itinerancy and superfluidity we augment the variational analysis for two component bosons in an optical lattice [\[56\]](#page-13-0) with a coherent state for light:

$$
|\mathcal{V}\rangle = |\gamma\rangle \otimes \prod_{i} [\cos \theta_{i} (\cos \chi_{i} a_{i}^{\dagger} + \sin \chi_{i} b_{i}^{\dagger})
$$

+
$$
\sin \theta_{i} (\cos \eta_{i} + \sin \eta_{i} b_{i}^{\dagger} a_{i}^{\dagger})] |0\rangle,
$$
 (34)

where $|\gamma\rangle$ is the coherent state introduced previously, and θ , χ , η , γ are to be determined. The corresponding order parameters are given by $\langle a \rangle = \frac{1}{2} \sin 2\theta \cos(\chi - \eta)$, $\langle b \rangle =$ $\frac{1}{2}$ sin 2*θ* sin(*χ* + *η*) and $\langle \psi \rangle = \gamma$. The first term in brackets in Eq. (34) describes the Mott state, and the second superfluidity. For $\theta = 0$ this coincides with the variational approach for localized excitons coupled to light [\[33\]](#page-13-0), and as we will discuss in Sec. [IV B,](#page-5-0) reproduces the previous results for $J_\alpha = 0$. More generally, Eq. (34) takes real hopping into account, involving site vacancies and interspecies double occupation. It provides a useful starting point to identify the boundaries between the Mott and superfluid regions. We consider spatially uniform phases with energy density $\mathcal{E} \equiv \langle \mathcal{V} | H | \mathcal{V} \rangle / N$:

$$
\mathcal{E} = (\tilde{\epsilon}_+ - \tilde{\epsilon}_- \cos 2\chi) \cos^2 \theta + (2\tilde{\epsilon}_+ + U_{ab}) \sin^2 \eta \sin^2 \theta
$$

$$
- \frac{z}{4} [J_a \cos^2(\chi - \eta) + J_b \sin^2(\chi + \eta)] \sin^2 2\theta
$$

$$
+ \tilde{\omega}\tilde{\gamma}^2 + \bar{g}\tilde{\gamma} \cos^2 \theta \sin 2\chi,
$$
 (35)

where *z* is the coordination and $\tilde{\epsilon}_{\pm} \equiv (\tilde{\epsilon}_b \pm \tilde{\epsilon}_a)/2$. Minimizing where *z* is the coordination and $\epsilon_{\pm} \equiv (\epsilon_b \pm \epsilon_a)/2$. Minimizing on $\bar{\gamma}$ gives $\bar{\gamma} = \langle \psi \rangle / \sqrt{N} = -\bar{g} \cos^2 \theta \sin 2\chi/2\tilde{\omega}$. This may be eliminated from Eq. (35) to yield

$$
\mathcal{E} = (\tilde{\epsilon}_+ - \tilde{\epsilon}_- \cos 2\chi) \cos^2 \theta + (2\tilde{\epsilon}_+ + U_{ab}) \sin^2 \eta \sin^2 \theta
$$

$$
- \frac{z}{4} [J_a \cos^2(\chi - \eta) + J_b \sin^2(\chi + \eta)] \sin^2 2\theta
$$

$$
- \frac{\bar{g}^2 \cos^4 \theta \sin^2 2\chi}{4\tilde{\omega}}.
$$
 (36)

The symmetries of Eq. (36) determine the domain of minimization. It is invariant under $\theta \to \theta + \pi$ and $\theta \to -\theta$, and may be minimized over $\theta \in [0, \pi/2]$. Likewise, it is invariant under $\chi \rightarrow \chi + \pi$ and $\eta \rightarrow \eta + \pi$. Since the hopping contribution favors χ and η taking the same sign, we may also minimize $\chi, \eta \in [0, \pi/2]$. To begin with we set $J_a = J_b = J$ and the

FIG. 5. (Color online) Variational phase diagram with $J_a = J_b$ *J* and $\epsilon_a = -1$, $\epsilon_b = 1$, $\omega = \bar{g} = 1$, $U_{ab} = 0$. The phases are (i) a Mott insulator (MI, dark blue), (ii) a super-radiant Mott state supporting a condensate of photoexcitations (SR-MI, light blue), (iii) a super-radiant superfluid (SR-SF, light red), and (iv) an *a*-type superfluid (a-SF, dark red). As shown by the solid line, the tetracritical line ultimately bifurcates into two bicritical points connected by a first order transition. For $\mu_1 > 0$, the a-type superfluid is replaced by a *b*-type owing to the particle-hole and species interchange symmetry of the hardcore Hamiltonian [\(5\)](#page-1-0) when $J_a = J_b$; see text.

expression may be further reduced using $J_a \cos^2(\chi - \eta)$ + $J_b \sin^2(\chi + \eta) = J(1 + \sin 2\chi \sin 2\eta)$. Minimizing over the restricted domain yields the phase diagram in Fig. 5.

For the chosen parameters, we have up to four distinct phases in the interval $\mu_1 < 0$; (i) a Mott state with $\langle a \rangle =$ $\langle b \rangle = \langle \psi^{\dagger} \psi \rangle = 0$, (ii) a super-radiant Mott state with $\langle a \rangle =$ $\langle b \rangle = 0$ and $\langle \psi^{\dagger} \psi \rangle \neq 0$, (iii) a single component superfluid with $\langle a \rangle \neq 0$ and $\langle b \rangle = \langle \psi^{\dagger} \psi \rangle = 0$, and (iv) a super-radiant superfluid $\langle a \rangle \neq 0$, $\langle b \rangle \neq 0$, $\langle \psi^{\dagger} \psi \rangle \neq 0$. Indeed, the Hamiltonian displays a $U(1) \times U(1)$ symmetry and these may be broken independently. The phase diagram reflects this pattern of symmetry breaking. In particular, the super-radiant Mott state corresponds to an unbroken $U(1)$ in the matter sector (corresponding to a pinned density and phase fluctuations) but a broken U(1) (or phase coherent condensate) for photoexcitations. As we shall discuss below, the expectation value of the *bilinear*, $\langle b^{\dagger} a \rangle \neq 0$, corresponds to the onset of coherence in the Dicke model. This novel phase may thus be regarded as a form of supersolid [\[62\]](#page-14-0) in which photoexcitations condense on the background of a Mott insulator. Although the lattice precludes *spontaneous* translational symmetry breaking (at least with this periodicity) the excitations may be thought of as mobile defects in an otherwise ordered background.

As in the zero hopping case, we may extend Fig. 5 into the region $\mu_1 > 0$ by exploiting symmetries of [\(5\)](#page-1-0). This is reflected in the variational energy by using $\sin^2 \eta = (1 -$

 $\cos 2\eta$ /2 to combine the $\tilde{\epsilon}_+$ contributions:

$$
\mathcal{E} = \frac{1}{2} (\epsilon_a + \epsilon_b) - \mu_1 - \frac{1}{2} (\epsilon_b - \epsilon_a - \mu_2) \cos 2\chi \cos^2 \theta \n+ \frac{1}{2} [U_{ab} - (\epsilon_a + \epsilon_b + U_{ab} - 2\mu_1) \cos 2\eta] \sin^2 \theta \n- \frac{zJ}{4} (1 + \sin 2\chi \sin 2\eta) \sin^2 2\theta - \frac{\bar{g}^2 \cos^4 \theta \sin^2 2\chi}{4(\omega - \mu_2)}.
$$
\n(37)

Since $J_a = J_b = J$ this is invariant (up to a constant) under $\mu_1 \rightarrow \epsilon_a + \epsilon_b + U_{ab} - \mu_1$ and $\eta \rightarrow \pi/2 - \eta$, which interchanges the superfluid order parameters $\langle a \rangle$ and $\langle b \rangle$. For the parameters used in Fig. 5, the *a*-type superfluid observed for μ_1 < 0 is replaced with a *b*-type for μ_1 > 0.

As may be seen from Fig. 5, the locus of the tetracritical line may be determined from the intersection of the superradiance transition with the Mott insulator to *a*-type superfluid phase boundary. This yields $\tilde{\epsilon}_a + zJ = 0$ as discussed in Appendix [C.](#page-12-0) This may also be seen from a Landau type expansion of $\mathcal E$. In view of the nonlinear relationship, it is convenient to expand in the angles θ , χ , η as opposed to the order parameters $\langle a \rangle$, $\langle b \rangle$, $\langle \psi \rangle$:

$$
\mathcal{E} = \tilde{\epsilon}_a - (\tilde{\epsilon}_a + zJ)\theta^2 - \left(\frac{\bar{g}^2 - \tilde{\omega}\tilde{\omega}_0}{\tilde{\omega}}\right)\chi^2 + \cdots. \tag{38}
$$

The quadratic "mass" terms vanish when $\tilde{\epsilon}_a + zJ = 0$ and the super-radiance condition $\bar{g} = \sqrt{\tilde{\omega}\tilde{\omega}_0}$ is met. In some simple cases $\mathcal E$ may be expanded directly in the order parameters. For example, throughout the entire Mott lobe where $\langle a \rangle = \langle b \rangle = 0$ we may set $\theta = 0$. Returning to Eq. [\(35\)](#page-4-0) and minimizing over *χ* yields tan $2\chi = -2\bar{g}\bar{\gamma}/\tilde{\omega}_0$. This gives $\mathcal{E} = \tilde{\epsilon}_+ + \tilde{\omega}\bar{\gamma}^2 - \tilde{\gamma}^2$ *x* yields $\tan 2\chi = -2gy/\omega_0$. This gives $\varepsilon = \epsilon_+ + \omega\gamma^2 - \sqrt{\tilde{\omega}_0^2/4 + \bar{g}^2\tilde{\gamma}^2}$, where $\bar{\gamma} = \langle \psi \rangle / \sqrt{N}$. This agrees with our variational zero hopping result (11) in the lowest lobe with $n=1$.

In Fig. [6](#page-6-0) we present a cross section of the phase diagram (5) for $\mu_1 = -0.6$. We indicate continuous transitions by single lines and first order transitions by dotted lines. In general, the transition from the superradiant Mott state to the nonsuper-radiant *a*-type superfluid involves a discontinuous jump in the photon density. This results in a first order transition as indicated by the discontinuity in the first derivative of the energy and the order parameters as shown in Fig. [7.](#page-6-0) This first order line connects two bicritical points as indicated in Fig. [6.](#page-6-0) The length of this first order segment changes with μ_1 , and emanates from the tetracritical line as shown in Fig. 5. These overall features are also exhibited for more general hopping parameters as shown in Fig. [8,](#page-6-0) where *a*-type and *b*-type superfluids emerge for large hopping asymmetry.

B. Coherence in super-radiant Mott phase

An interesting aspect of the super-radiant Mott phase is that polariton condensation coexists with the Mott character. Within both Mott phases $\theta = 0$ and our variational wave function [\(34\)](#page-4-0) becomes

$$
|\mathcal{V}\rangle = |\gamma\rangle \otimes \prod_{i} (\cos \chi_i a_i^{\dagger} + \sin \chi_i b_i^{\dagger}) |0\rangle. \tag{39}
$$

FIG. 6. (Color online) Cross section of the phase diagram [\(5\)](#page-5-0) for $\mu_1 = -0.6$. The first order transition from the super-radiant Mott state to the *a*-type superfluid is indicated by a dashed line. The locus of this transition is determined analytically from Eq. [\(C8\)](#page-12-0). The remaining transitions are continuous.

To describe photoexcitations above the filled Mott state, we introduce a change of vacuum $|\Omega\rangle \equiv \prod_i a_i^{\dagger} |0\rangle$ so that

$$
|\mathcal{V}\rangle = |\gamma\rangle \otimes \prod_{i} \cos \chi_{i} \prod_{i} (1 + \tan \chi_{i} b_{i}^{\dagger} a_{i}) |\Omega\rangle. \tag{40}
$$

FIG. 7. Evolution of the mean field order parameters $\langle a \rangle$, $\langle b \rangle$, *γ* = $\langle \psi \rangle / \sqrt{N}$ across the transitions depicted in Fig. 6 for $\mu_2 = 0.45$. (I) First order transition from the super-radiant Mott state to the *a*-type superfluid, (II) continuous transition from the *a*-type superfluid to the super-radiant superfluid. Inset: Evolution of the variational energy (relative to the zero hopping Mott phase) across the transitions in Fig. 6 for fixed values of μ_2 . The solid line at $\mu_2 = 0.45$ has a discontinuity in the first derivative and indicates a first order transition in passing from the super-radiant Mott insulator to the *a*-type superfluid. The remaining transitions are continuous.

FIG. 8. (Color online) Variational phase diagram showing a slice through Fig. [4](#page-4-0) with $\mu_1 = -0.25$ and extended in to the (J_a, J_b) hopping plane. We use the same key as in Fig. [5](#page-5-0) and denote the *b*-type superfluid (b-SF) in orange. Single component superfluids are observed for large hopping asymmetry.

Since we are dealing with hardcore bosons this may be exponentiated, and for homogenous parameters

$$
|\mathcal{V}\rangle = |\gamma\rangle \otimes e^{N \ln \cos \chi} e^{\tan \chi \sum_i b_i^{\dagger} a_i} |\Omega\rangle.
$$
 (41)

This is already reminiscent of a coherent state for the *bilinears*, although one needs to be careful since we are dealing with hardcore bosons. Instead, we may examine condensation properties directly by computing expectation values using Eq. [\(39\)](#page-5-0). Using the Schwinger boson representation [\(22\)](#page-3-0) for the lowest lobe

$$
\mathcal{J}^+ \equiv \sum_i b_i^\dagger a_i, \quad \mathcal{J}^- \equiv \sum_i a_i^\dagger b_i, \quad \mathcal{J}^z \equiv \frac{1}{2} \sum_i \left(n_i^b - n_i^a \right), \tag{42}
$$

we may calculate the bosonic bilinear $\langle \mathcal{J}^+ \rangle$:

$$
\langle \mathcal{V} | \mathcal{J}^+ | \mathcal{V} \rangle = \sum_i \langle \mathcal{V} | b_i^\dagger a_i | \mathcal{V} \rangle = N \sin \chi \cos \chi = \frac{N}{2} \sin 2\chi. \tag{43}
$$

At $\theta = 0$ our variational analysis yields $\bar{\gamma} = -\bar{g} \sin 2\chi/2\tilde{\omega}$:

$$
\frac{\langle V|\mathcal{J}^+|\mathcal{V}\rangle}{N} \equiv \frac{\sum_i \langle b_i^\dagger a_i \rangle}{N} = -\frac{\tilde{\omega}\bar{\gamma}}{\bar{g}}.
$$
 (44)

This agrees with the result (33) obtained from the Holstein-Primakoff approach to the Dicke model [\[59\]](#page-14-0). We see that in the two-band Bose-Hubbard problem we have condensation involving *particle-hole pairs* above the Mott background with $\langle b^{\dagger} a \rangle \neq 0$. This corresponds to condensation of the Holstein-Primakoff boson $\langle c \rangle \neq 0$ in the dual formulation as evidenced by Eq. [\(33\)](#page-4-0). Crucially, condensation of $\langle b^{\dagger}a \rangle$ is *not* accompanied by condensation of the individual bosonic

carriers *a* and *b*. This follows immediately from Eq. [\(39\)](#page-5-0) where $\langle a \rangle = \langle b \rangle = 0$. Since matter-light coherence in the Dicke model translates into polariton and not carrier condensation, Mott behavior and polariton condensation may coexist.

V. NUMERICAL SIMULATIONS

We now analyze the Hamiltonian [\(1\)](#page-0-0) by exact diagonalization, imposing a maximum number of photons, $\langle \psi^\dagger \psi \rangle \leqslant M_\psi$, in addition to the hardcore a, b constraints. We consider a one-dimensional system with *N* lattice sites, with the basis of tensor product states $|\phi\rangle_a^{(v_a)} \otimes |\phi\rangle_b^{(v_b)} \otimes |\phi\rangle_\psi^{(v_\psi)}$, where $v_{a,b} = 1, \ldots, 2^N$ and $v_{\psi} = 0, 1, \ldots, M_{\psi}$. Here $|\phi\rangle_{\alpha}^{(v_{\alpha})} =$ $|n_{\alpha,1}^{(v_\alpha)}, \ldots, n_{\alpha,N}^{(v_\alpha)}\rangle$ where $n_{\alpha,i}^{(v_\alpha)} \in \{0, 1\}$, and the photon states are given by $|\phi\rangle_{\psi}^{(\nu_{\psi})} = |n_{\psi}^{(\nu_{\psi})}\rangle$ where $n_{\psi}^{(\nu_{\psi})} \in \{0, 1, ..., M_{\psi}\}\$. The total Hilbert space has dimension $D = 2^N 2^N (M_{\psi} + 1)$. In the largest case considered, with $N = 8$ sites and $M_{\psi} =$ 64 photons, this corresponds to a matrix dimension $D \approx 4E6$. Increasing M_{ψ} further has only minor influence.

Applying periodic boundary conditions in real space, we diagonalize the sparse matrix representation of *H* to obtain the ground state $|\Phi_0\rangle$ and its energy E_0 . We compute the atom and photon densities, and the density fluctuations $\sigma_{\alpha} = \sqrt{\langle \hat{n}_{\alpha}^2 \rangle - \langle \hat{n}_{\alpha} \rangle^2}$. To obtain the superfluid fraction, f_{α}^{α} , of the α $\sqrt{\hat{n}_{\alpha}^2 - \langle \hat{n}_{\alpha} \rangle^2}$. To obtain the superfluid fraction, f_s^{α} , of the α atoms, we impose a phase twist $\Theta \ll \pi$ by means of a Peierls factor $\alpha_i^{\dagger} \alpha_j \mapsto \alpha_i^{\dagger} \alpha_j e^{-i\Theta/N}$, and calculate the change in the ground state energy [\[63\]](#page-14-0):

$$
f_s^{\alpha} = \frac{N}{J_{\alpha} \langle n_{\alpha} \rangle} \frac{E_0^{(\Theta)} - E_0}{\Theta^2}.
$$
 (45)

For the single-component Bose-Hubbard model, this quantity is zero deep in the Mott insulator, and approaches unity far in the superfluid. Note that in our case, the hardcore constraint always provides an effective interaction even for large hopping, so that f_s < 1. A total superfluid density can be obtained by imposing the phases on both species *a*,*b* and calculating

$$
f_s = \frac{N}{\sum_{\alpha} J_{\alpha} \langle n_{\alpha} \rangle} \frac{E_0^{(\Theta)} - E_0}{\Theta^2}.
$$
 (46)

We supplement these superfluid diagnostics with the zero momentum occupations $n_{\alpha}(k = 0) = N^{-1} \sum_{pq} \langle \alpha_p^{\dagger} \alpha_q \rangle$.

A. Small hopping and Dicke super-radiance

To verify the existence of a super-radiance transition *within* the Mott phase we begin our numerical treatment in the limit of small nonzero hopping. Figure 9 shows the Mott lobe with density $n = 1$ at $zJ = 0.1$, for two different values of M_{ψ} . For sufficiently large M_{ψ} the results are in good agreement with the variational *zero-hopping* phase diagram shown in Fig. [4,](#page-4-0) and the overall features depend only weakly on the number of sites. In order to examine the onset of super-radiance, we track the evolution of the polariton and photon densities in Fig. 10. At zero hopping, Eq. [\(24\)](#page-3-0) yields the critical coupling $\bar{g}_c^2 = \tilde{\omega}\tilde{\omega}_0 =$ $(\omega - \mu_2)(\epsilon_b - \epsilon_a - \mu_2)$. For the chosen parameters at fixed $\bar{g} = 1$, the transition occurs at a critical chemical potential, $g = 1$, the transition occurs at a critical chemical potential,
 $\mu_2^c = (3 - \sqrt{5})/2 \approx 0.382$. This onset is well reproduced at small finite hopping, as shown in Fig. 10. For $N = 1$ (where the Dicke model reduces to the Jaynes-Cummings model) we

FIG. 9. Exact diagonalization results for the phase diagram at small hopping, $zJ = 0.1$, for *hardcore a*,*b* atoms and $\epsilon_a = -1$, $\epsilon_b = 1, \omega = \bar{g} = 1, U_{ab} = 0$. The dashed (solid) lines corresponds to $N = 8$ and $M_{\psi} = 16$ ($M_{\psi} = 64$) photons, and have been obtained from spline fits to the contours at $n = 0.99$ and $n = 1.01$. The vertical line indicates the location of the super-radiance transition as determined from $\langle \psi^{\dagger} \psi \rangle/N \ge 0.01$. The results are in good qualitative agreement with the variational zero hopping results in Fig. [4,](#page-4-0) showing the continuity of this behavior into the Mott phase.

see quantized steps with fixed integer polariton density, *N*2*/N*. These form the basis of the Mott lobes observed in Jaynes-Cummings-Hubbard models [\[9,23\]](#page-13-0). Even in this extreme limit, the densities closely track the thermodynamic Dicke model

FIG. 10. Exact diagonalization results with $N = 1$, 8 sites, $J_a =$ $J_b = J$, and $zJ = 0.1$. We set $\epsilon_a = -1$, $\epsilon_b = 1$, $\omega = \bar{g} = 1$, $\mu_1 =$ $U_{ab} = 0$. The profiles show the onset of super-radiance within the Mott phase, and evolve with increasing system size toward those for the thermodynamic limit of the Dicke model. Evolution of (a) the photon density $\langle \psi^{\dagger} \psi \rangle/N$, (b) the polariton density, N_2/N . For $N = 1$ the Dicke model reduces to the Jaynes-Cummings model and exhibits quantized integer steps in the polariton density [\[9,23\]](#page-13-0). More generally these are quantized in units of 1*/N*. The value of *Mψ* is of minor importance in the range of μ_2 considered as it sets the upper limit on the number of excitations available.

results. As *N* increases, the step sizes are reduced by a factor of 1*/N* and we approach the variational thermodynamic results. This behavior in our itinerant boson model closely mirrors direct finite *N* simulations of the Dicke model; see Fig. [16.](#page-11-0) A notable difference between the Dicke and Jaynes-Cummings-Hubbard models [\[9,23\]](#page-13-0) (both with *N* sites) is reflected in their zero hopping eigenstates. In the latter, eigenstates are tensor products of superpositions of two states which differ in photon number by one, whereas in the Dicke model the global photon mode leads to a coherent photon state for large *N*. In the Dicke model the higher Mott lobes are eliminated in favor of a continuous photon onset, whereas in the Jaynes-Cummings-Hubbard models [\[9,23\]](#page-13-0) they remain in tact.

B. General phase diagram

Turning to the construction of the overall phase diagram, we first consider a fixed value $\mu_1 = 0$ and present results in the (zJ, μ_2) plane; see Figs. 11 and [12.](#page-9-0) So far we have set $U_{ab} = 0$ in order to expose the essential details. Following our original work [\[36\]](#page-13-0), we now take $U_{ab} = 1$ to help illustrate the generality of the overall results. The interspecies interaction also helps stabilize the Mott region up to larger values of the hopping.

In Fig. 11 we show density plots of atom and photon densities, and density fluctuations. In Fig. [12](#page-9-0) we plot superfluid fractions. From these data, we can identify the four different phases present in Fig. [5.](#page-5-0) The Mott-superfluid transition is visible from the deviation of the total atom density from unity in Fig. $11(a)$. The super-radiance transition corresponds to the onset of photon density in Fig. $11(b)$. Panels (c) and (d) demonstrate the existence of the single-component superfluid in the region where $n \neq 1$ and $n_a \neq 0$, while $n_b = 0$. This is also visible in the individual superfluid fractions shown in Fig. [12.](#page-9-0) We also see the onset of a nontrivial population imbalance, $n_b - n_a$, or existence of *b* bosons, accompanying the super-radiance transition. Specifically, $n_a = 1, n_b = 0$ in the left of the white region of panel (b), but $n_a < 1, n_b > 0$ above; see panels (c), (d), and (g). The nature of the two Mott phases (normal and super-radiant) is illustrated by panels (e)–(f). We observe an onset of local fluctuations σ_{α} with increasing hopping. Since the Mott state is characterized by $n = n_a + n_b = 1$, the individual atom density fluctuations σ_α in the super-radiant Mott phase are much larger than σ . In the normal Mott phase, $n_b = 0$ so that the Mott insulator consists purely of *a* atoms and hence $\sigma_a = \sigma_b = 0$. Finally, the Mott-superfluid transition is also apparent in our results for the superfluid fractions as shown in Fig. [12.](#page-9-0)

Exact diagonalization of small clusters yields an approximation to the critical value J_c for the Mott-superfluid transition by monitoring the onset of f_s , as in Fig. [12\(a\),](#page-9-0) or the local fluctuations σ of the total atom density, as in Fig. 11(e). Both *σ* and f_s are also nonzero *below* J_c for finite N [\[63\]](#page-14-0). While f_s is expected to scale to zero for $J < J_c$ as $N \to \infty$, the local density fluctuations remain nonzero in the Mott phase due to virtual hopping processes. This is illustrated in Fig. [13.](#page-9-0)

The system size *N* has a noticeable impact on the onset of correlations related to superfluidity. Since a finite size scaling analysis requires much larger system sizes, we provide approximate phase boundaries obtained from the contour

FIG. 11. Exact diagonalization results for $N = 8$ sites and $M_{\psi} =$ 16 photons. We set $\mu_1 = 0$, $J_a = J_b = J$, and $\epsilon_a = -1$, $\epsilon_b = 1$, $\omega = \bar{g} = U_{ab} = 1$. The panels show density plots of (a) total atom density, (b) photon density, (c) *a*-atom density, (d) *b*-atom density, (e) fluctuations of the total atom density, (f) fluctuations of the a-atom density, (g) fluctuations of the *b*-atom density. In particular (a) reveals the Mott-superfluid transition and (b) the super-radiance transition.

lines $\sigma(zJ, \mu_2) = 0.3$ [alternatively $f_s(zJ, \mu_2) = \text{const.}$] to indicate the onset of superfluidity, and $\langle \psi^{\dagger} \psi \rangle/N = 0.01$ to indicate super-radiance. The numerical constants for the contours have been chosen in order to obtain phase boundaries that match those suggested by the data in Figs. 11 and [12;](#page-9-0) see Fig. [13.](#page-9-0) Figure $13(c)$ shows the zero-momentum occupation $n(k = 0) = n_a(k = 0) + n_b(k = 0)$ for the atoms. The latter is expected to diverge as a function of system size in

FIG. 12. Exact diagonalization results for $N = 8$ sites and $M_{\psi} =$ 16 photons. We set $\mu_1 = 0$, $J_a = J_b = J$, and $\epsilon_a = -1$, $\epsilon_b = 1$, $\omega = \bar{g} = U_{ab} = 1$. The panels show density plots of (a) total atomic superfluid fraction, (b) *a*-atom superfluid fraction, (c) *b*-atom superfluid fraction. The Mott-superfluid transition is evident from the onset in (a), and the single component *a*-type superfluid in (b) and (c).

the SF phase, and such behavior can indeed be seen above $zJ \approx 1.1$.

Repeating the above procedure for different μ_1 values we build up a picture of the overall phase diagram as shown in Fig. [14.](#page-10-0) This may be compared to the variational analysis shown in Fig. [5.](#page-5-0) We find the same phases as in the analytical approach and the evolution of the phase boundaries is in good agreement. For the choice of $\mu_1 = 0$ these phases meet in a tetracritical point. As found analytically this extends into a tetracritical line which ultimately bifurcates into two bicritical points. The agreement between the numerical simulations and mean field theory is remarkable given the enhanced role of fluctuations in low dimensions. This mirrors the success of mean field theory in other bosonic systems and may be assisted by the long range cavity photons.

VI. RELATION TO OTHER PROBLEMS

A feature not addressed by the present mean field theory, but captured in Fig. [14,](#page-10-0) is the dispersion of the super-radiance transition with *J*; in the Mott phase, $\theta = 0$, and *J* drops out of the variational energy (35) . One way to understand this is to recast the matter contribution as

$$
|\mathcal{V}_{\mathcal{M}}\rangle = \prod_{i} (\cos \chi_i + \sin \chi_i b_i^{\dagger} a_i) |\Omega\rangle, \tag{47}
$$

where $|\Omega\rangle \equiv \prod_i a_i^{\dagger} |0\rangle$ is the filled Mott state in the absence of excitations. In the spatially uniform case

$$
|\mathcal{V}_{M}\rangle = \mathcal{N}e^{\lambda \sum_{i} b_{i}^{\dagger} a_{i}} |\Omega\rangle, \tag{48}
$$

where $\lambda \equiv \tan \chi$ and $\mathcal{N} \equiv (1 + \lambda^2)^{-N/2}$. This only accommodates *local* particle-hole pairs above the filled Mott

FIG. 13. Exact diagonalization results with $J_a = J_b = J$ and $\epsilon_a = -1, \epsilon_b = 1, \omega = \bar{g} = U_{ab} = 1$. We set $\mu_1 = 0, \mu_2 = 0.4, M_{\psi} =$ 2*N*, and show the system size dependence of (a) superfluid fraction, (b) density fluctuations, (c) zero momentum occupation. Within the Mott phase for $J < J_c$, the superfluid fraction decreases with increasing system size. This indicates a Mott-superfluid transition at approximately $zJ_c \approx 1.1$. This is compatible with the fluctuation onset criterion, $\sigma = 0.3$, that we use to determine the overall phase diagram in Fig. [14,](#page-10-0) and the divergence of $n(k = 0)$ with system size in (c) .

background, and may thus be regarded as the BEC limit of the BEC-BCS crossover problem. By analogy with the fermionic BCS approach to exciton insulators [\[64,65\]](#page-14-0), and the crossover problem in 40 K [\[66\]](#page-14-0), one expects that excitons may lower their energy by spreading out in real space and pairing in momentum space. In this regard, the "BCS" pairing phenomenon in Bose gases has a long history, with the Valatin-Butler wave function [\[67\]](#page-14-0) playing the role of the BCS state. This has been developed in a series of early works motivated by liquid 4 He $[68–73]$ and biexciton formation [\[74–76\]](#page-14-0). This later emerged in studies of high-*Tc* superconductivity [\[77\]](#page-14-0) and two-component Bose gases [\[78,79\]](#page-14-0). The interesting possibility of bound states of three or four particles has also been explored [\[80,81\]](#page-14-0). Central to these studies is the requirement to stabilize attractive Bose gases against collapse, with the aid of short-range repulsion or internal structure. When this condition is met, and at sufficiently low densities where exciton overlap is negligible, it has been argued that such pairing states may exist [\[73\]](#page-14-0). In the present context, stabilization of the paired state and the absence of carrier condensation is brought about by the interplay of Mott physics and photoexcitation. It would be

FIG. 14. (Color online) Overall phase diagram obtained by exact diagonalization with $N = 8$ sites and $M_{\psi} = 16$ photons. We set $J_a = J_b = J$, $\epsilon_a = -1$, $\epsilon_b = 1$, $\omega = \bar{g} = 1$, and $U_{ab} = 1$, and use the same key as in Fig. [5.](#page-5-0) We extract the Mott-superfluid boundaries from the onset of density fluctuations, $\sigma \geq 0.3$, and the super-radiance transition from the onset of photons, $\langle \psi^{\dagger} \psi \rangle/N \geq 0.01$; see text. The simulations show the distinct phases and the bifurcation of the tetracritical line suggested by mean field theory. The bifurcation is indicated by the regions where the two boundaries overlap along a line rather than a single tetracritical point.

interesting to explore this problem in more detail, and we leave these refinements to future studies.

As noted in our previous work, the connection to the BEC-BCS crossover for bosons is reinforced by the Feshbach resonance problem studied in the continuum [\[82–86\]](#page-14-0) and on the lattice [\[87–89\]](#page-14-0). Performing a particle-hole transformation, the matter-light coupling reads $\psi^{\dagger} a_i b_i$. Aside from the global nature of the photon, this converts *a* and *b* into a "molecule" ψ . At the outset there are eight possible phases corresponding to separate condensation of $\langle a \rangle$, $\langle b \rangle$, $\langle \psi \rangle$. At the mean field level, only five of these may survive; condensation of two variables provides an effective field (as dictated by the coupling) which induces condensation of the other. In Figs. [5](#page-5-0) and 14 the band asymmetry, $\epsilon_a < \epsilon_b$, in conjunction with the chosen parameters, reduces this to four or less. Nonetheless, the additional *b*-type superfluid is stabilized for larger values of μ_1 owing to the particle-hole and species interchange symmetry involving $\mu_1 \rightarrow \epsilon_a + \epsilon_b + U_{ab} - \mu_1$. In contrast to the single species mean field theory [\[82–84\]](#page-14-0), this two species case supports an atomic superfluid, since condensation of one carrier no longer induces an effective field. Moreover, condensation may leave a U(1) symmetry intact, which allows the coexistence of Mott and phase coherent behavior.

In deriving Eq. (35) and the phase diagram, we are primarily concerned with the matter-light coupling. As such we incorporate U_{ab} as in Ref. [\[56\]](#page-13-0). Within this variational approach,

FIG. 15. (Color online) The classical light limit of Eq. [\(1\)](#page-0-0) (where *ψ* is a replaced by a *c*-number), may be simulated in optical superlattices [\[92\]](#page-14-0) where the coupling *g* represents tunneling between different wells, *a* and *b*.

this interaction has no impact on the Mott states with $\theta = 0$, as evident from the energy density [\(35\)](#page-4-0). Nonetheless, the presence of the matter-light coupling stabilizes the nontrivial phases in Fig. [5](#page-5-0) and provides good agreement with the numerical simulations. However, as noted by Söyler et al. [\[90\]](#page-14-0) and previous works [\[78–81\]](#page-14-0), analogous pairing phases may be supported in the two-component Bose-Hubbard model, *without* matter-light coupling, through a more sophisticated treatment of *Uab* itself. Indeed, on-site repulsive interactions, $U_{ab}n_a n_b$, favor a particle of one species and a hole of the other on the same site. Treating this pairing in a BCS approach, one may replace $n_i^a n_i^b$ by $|\Delta_i|^2 + (\Delta_i b_i^{\dagger} a_i + \text{H.c.})$, where $\Delta_i \equiv$ $\langle a_i^{\dagger} b_i \rangle$, is to be determined self-consistently. This field acts as a *local* "photon", and a similar mean field phenomenology may ensue. Such pairing also occurs in fermionic models [\[37\]](#page-13-0). Although our discussion has focused on a single *global* photon, the symmetry analysis is more general. This is supported by studies of the two-band Bose-Hubbard model for equal fillings and commensurate densities [\[91\]](#page-14-0).

In closing we note that the classical light limit of Eq. [\(1\)](#page-0-0) (where ψ is replaced by a *c*-number) may be simu-lated in optical superlattices [\[92\]](#page-14-0) where $g_i a_i b_i^{\dagger}$ represents tunneling between different wells; see Fig. 15. In the case of hardcore *a*-atoms and soft core *b*-atoms this provides an analog of the Jaynes-Cummings-Hubbard models considered in Refs. [\[9,23\]](#page-13-0). This geometry may also be useful in realizing other "matter-bath" systems.

VII. CONCLUSIONS

We have investigated the two-band Bose-Hubbard model coupled to a single mode of a cavity light field. We combine analytical and numerical techniques and find good agreement between the approaches. The model displays a novel phase in which "polaritons" condense on the platform of a bosonic Mott insulator. We extend our previous work [\[36\]](#page-13-0) in several directions including an investigation of the overall phase diagram, and the nature of polariton condensation. In particular, we use the framework of the Dicke model to discuss how polariton condensation emerges in the absence of carrier condensation. In terms of numerical results, we have presented superfluid fractions, atom density fluctuations and zero-momentum occupation, and analyzed the phase diagram under variation of μ_1 . In addition, we have addressed the effects of finite cluster size

and the photon cutoff. This helps illustrate connections to work on Jaynes-Cummings-Hubbard models and coupled cavity arrays. This topic has broad connections to other problems of current interest including atom-molecule mixtures and the BEC-BCS crossover in bosonic systems.

There are many avenues for further research including nonequilibrium aspects and collective excitations [\[93,94\]](#page-14-0). It would be interesting to develop numerical techniques to explore finite temperature polariton condensation and the onset of phase coherence in the Mott phase. It would also be worthwhile to examine the phase diagram with soft core bosons with finite U_{aa} and U_{bb} .

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APPENDIX A: DICKE MODELS

Throughout this manuscript we make use of the Dicke model [\[41\]](#page-13-0) and its reductions. In the literature this appears in various guises and with different names so we present a brief guide. The Dicke model describes *N* two-level systems or "spins" coupled to radiation

$$
H = \omega_0 \sum_{i}^{N} S_i^z + \omega \psi^{\dagger} \psi + \frac{\bar{g}}{\sqrt{N}} \sum_{i}^{N} (\psi^{\dagger} S_i^- + S_i^+ \psi), \quad (A1)
$$

where S_i is a spin-1/2 operator and ψ is a canonical boson. Here ω_0 is the level-splitting between the two-level systems, ω is the frequency of the cavity mode, and \bar{g} is the strength of the matter-light coupling. In quantum optics the Dicke model is also known as the Tavis-Cummings model [\[95\]](#page-14-0). In the special case of a single spin, $N = 1$, the Dicke model is often referred to as the Jaynes-Cummings model [\[47\]](#page-13-0). The Hamiltonian $(A1)$ is written in the so-called rotating wave approximation in which terms of the form $S_i^{\pm} \psi^{\pm}$ are excluded. In the absence of these terms, the model is integrable [\[42,44](#page-13-0)[,58\]](#page-14-0) and exhibits a super-radiance quantum phase transition when $\bar{g} = \sqrt{\omega \omega_0}$ [\[41–44\]](#page-13-0); for a discussion of the model including counterrotating terms see Ref. [\[54\]](#page-13-0). Depending on the application these models are often recast in different representations and we gather a few results below.

1. Jaynes-Cummings

The simplest case is the Dicke model with $N = 1$, or the Jaynes-Cummings model, describing a single two-level system coupled to radiation. It plays a central role in the variational analysis presented in Sec. [III A,](#page-1-0) and recent problems in matterlight systems, e.g., [\[9,23\]](#page-13-0). A convenient representation is the single site Hamiltonian

$$
H = \epsilon_a n_a + \epsilon_b n_b + g(b^\dagger a + a^\dagger b), \tag{A2}
$$

where *a* is a hardcore boson (restricted to occupancy zero or one) and *b* may take arbitrary occupancy. We may construct exact eigenstates of total integer occupation, $n = n^a + n^b \ge 1$, as superpositions

where the first and second entries of the states are the occupations of the *a* and *b* particles, respectively. In matrix form this yields the eigenvalue problem

$$
\begin{pmatrix} \epsilon_a + (n-1)\epsilon_b & g\sqrt{n} \\ g\sqrt{n} & n\epsilon_b \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E_n \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (A4)
$$

where we recall that $b|n\rangle = \sqrt{n}|n-1\rangle$ and $b^{\dagger}|n\rangle =$ $\sqrt{n+1}|n+1\rangle$ for bosons. The eigenvalues are given by

$$
E_n^{\pm} = n\epsilon_b - \omega_0/2 \pm \sqrt{\omega_0^2/4 + g^2 n},\tag{A5}
$$

where $\omega_0 \equiv \epsilon_b - \epsilon_a$. This agrees with the spectrum of the Jaynes-Cummings model given by Greentree *et al.* [\[9\]](#page-13-0), where we identify ϵ_a , ϵ_b , and *g* with their parameters ϵ , ω , and β . The coefficients in the corresponding normalized eigenvectors $|n\rangle_{\pm}$ may be written

$$
\alpha_{\pm} = \frac{-\omega_0/2 \pm \chi(n)}{\sqrt{2\chi^2(n) \mp \omega_0 \chi(n)}},
$$

\n
$$
\beta_{\pm} = \frac{g\sqrt{n}}{\sqrt{2\chi^2(n) \mp \omega_0 \chi(n)}},
$$
\n(A6)

where $\chi(n) \equiv \sqrt{\omega_0^2/4 + g^2 n}$. We note that there is a minor typing error in the eigenstates given in the methods section of Ref. [\[9\]](#page-13-0), where the basis states $|1, n-1\rangle$ and $|0, n\rangle$ are erroneously reversed. Equivalently, one may reverse the sign of $\Delta \equiv \omega_0$ in their expression.

2. Dicke model

The generic Dicke model $(A1)$ is integrable for arbitrary *N* [\[42,44,](#page-13-0)[58\]](#page-14-0), but is most conveniently analyzed in the thermodynamic limit, $N \rightarrow \infty$ [\[59\]](#page-14-0). However, in numerical simulations we must deal with the effects of finite *N* and truncations of the photon Hilbert space. In Fig. 16 we show the evolution of the polariton density, N_2/N , where $N_2 =$ $\psi^{\dagger}\psi + \sum_{i} (S_i^z + 1/2)$, and the photon density as a function of

FIG. 16. Evolution of the polariton density, N_2/N , in the Dicke model for $N = 1, 2$ sites and comparison to the $N \to \infty$ thermodynamic limit. For $N = 1$ the Dicke model reduces to the Jaynes-Cummings model and the quantized polariton steps correspond to the Mott lobes discussed in Ref. [\[9\]](#page-13-0). In the Dicke model these steps are quantized in units of $1/N$ and as $N \to \infty$ we approach the variational results. Inset: Evolution of the photon density. The magnetization (or population imbalance) may be obtained by subtraction. All figures population imbalance) may be obtained by subtraction. All figures
show the onset of super-radiance at $\mu_2 = (3 - \sqrt{5})/2 \approx 0.382$, for $\omega \rightarrow \tilde{\omega} = 1 - \mu_2, \omega_0 \rightarrow \tilde{\omega}_0 = 2 - \mu_2$, and $\bar{g} = 1$.

FIG. 17. Zero hopping phase diagram for the Hamiltonian [\(6\)](#page-1-0) in the absence of matter-light interaction, with $\epsilon_a = -1, \epsilon_b = 1, \omega = 1$, $g = 0$. The loci $\tilde{\epsilon}_a = 0$, $\tilde{\epsilon}_b = 0$, $\tilde{\omega} = 0$, indicated by the lower, upper, and vertical lines, respectively, delineate the regions of population onset for a, b, ψ in the grand canonical ensemble. When g is switched on the horizontal boundaries bend downward and evolve into those shown in Fig. [2.](#page-2-0)

N. This is obtained by solution of the finite dimensional matrix problem. Both plots exhibit discrete jumps which track the thermodynamic results. For $N = 1$ the Dicke model reduces to the Jaynes-Cummings model and the quantized polariton steps correspond to the Mott lobes discussed in Ref. [\[9\]](#page-13-0).

APPENDIX B: ZERO HOPPING PHASE DIAGRAM WITH $g = 0$

An instructive way to think about the topology of the zero hopping phase diagram in Fig. [2,](#page-2-0) is in the absence of the matterlight coupling. In Fig. 17 we plot the loci $\tilde{\epsilon}_a = 0$, $\tilde{\epsilon}_b = 0$, $\tilde{\omega} =$ 0, corresponding to population transitions in the Hamiltonian [\(6\)](#page-1-0) for $g = 0$. When g is switched on, the horizontal boundaries bend downward and continuously evolve into those shown in Fig. [2.](#page-2-0)

APPENDIX C: VARIATIONAL PHASE BOUNDARIES

The variational energy for the finite hopping problem allows some analytic progress with the phase boundaries, and highlights connections to the Dicke model. In the absence of competition from other phases, the transition between the non-super-radiant insulator ($\theta = \chi = \bar{\gamma} = 0$) and the *a*-type superfluid ($\theta \neq 0$, $\chi = \eta = \bar{\gamma} = 0$) for example occurs when $\tilde{\epsilon}_a + zJ = 0$. This may be seen by explicit computation of the energies of each phase. The energy density in the generic Mott phase is

$$
\mathcal{E}_{\theta=0} = (\tilde{\epsilon}_+ - \tilde{\epsilon}_-\cos 2\chi) - \frac{\bar{g}^2 \sin^2 2\chi}{4\tilde{\omega}}.
$$
 (C1)

Minimizing on χ yields either $\chi = 0$, corresponding to an ordinary Mott insulator, with $\mathcal{E}_{\text{MI}} = \tilde{\epsilon}_{+} - \tilde{\epsilon}_{-}$, or

$$
\cos 2\chi = \frac{2\tilde{\omega}\tilde{\epsilon}_{-}}{\bar{g}^2} \equiv \frac{\tilde{\omega}\tilde{\omega}_0}{\bar{g}^2},\tag{C2}
$$

corresponding to the super-radiant Mott insulator. At this nontrivial stationary point

$$
\frac{\partial^2 \mathcal{E}}{\partial \chi^2} = \frac{2 \left(\bar{g}^4 - \tilde{\omega}^2 \tilde{\omega}_0^2 \right)}{\tilde{\omega} \bar{g}^2}.
$$
 (C3)

This corresponds to a minimum (with $\tilde{\omega} > 0$) provided $\bar{g} > \sqrt{\tilde{g}}$ $\sqrt{\tilde{\omega}\tilde{\omega}_0}$. This coincides with the super-radiance transition in the Dicke model [\[41–44\]](#page-13-0). The energy density in the super-radiant Mott phase is

$$
\mathcal{E}_{\text{SRMI}} = \mathcal{E}_{\text{MI}} - \frac{(\bar{g}^2 - \tilde{\omega}\tilde{\omega}_0)^2}{4\bar{g}^2\tilde{\omega}}.
$$
 (C4)

Similarly, in the *a*-type superfluid

$$
\mathcal{E}_{\text{aSF}} = (\tilde{\epsilon}_{+} - \tilde{\epsilon}_{-})\cos^2\theta - \frac{zJ}{4}\sin^2 2\theta. \tag{C5}
$$

Minimizing on θ yields either $\theta = 0$ or $\cos 2\theta = -\frac{(\tilde{\epsilon}_+ - \tilde{\epsilon}_-)}{zJ}$. The latter yields

$$
\mathcal{E}_{\text{aSF}} = -\frac{(\tilde{\epsilon}_+ - \tilde{\epsilon}_- - zJ)^2}{4zJ}.
$$
 (C6)

The condition $\mathcal{E}_{\text{MI}} = \mathcal{E}_{\text{aSF}}$ yields the MI-aSF boundary $\tilde{\epsilon}_{+}$ – $\tilde{\epsilon}_- + zJ = 0$ or equivalently $\tilde{\epsilon}_a + zJ = 0$. This meets the super-radiance onset $\bar{g}^2 = \tilde{\omega}\tilde{\omega}_0$ at $\bar{g}^2 = \tilde{\omega}(\tilde{\epsilon}_b + zJ)$ or

$$
\mu_1 = \epsilon^b - \frac{\mu_2}{2} - \frac{\bar{g}^2}{\omega - \mu_2} + zJ.
$$
 (C7)

In a similar fashion, the transition between the super-radiant Mott state and the *a*-type superfluid occurs when \mathcal{E}_{SRMI} = $\mathcal{E}_{\rm aSF}$ or

$$
zJ(\bar{g}^2 - \tilde{\omega}\tilde{\omega}_0)^2 = \bar{g}^2\tilde{\omega}(\tilde{\epsilon}_a + zJ)^2.
$$
 (C8)

APPENDIX D: ABSENCE OF HIGHER LOBES IN COUPLING TO QUANTUM LIGHT

In Fig. [2](#page-2-0) we see that only the Mott lobe with atomic density, $n = 1$, is supported due to the coupling to the quantum light field. To prove that only this lobe survives we compare the energies of the higher states to those depicted in Fig. [2.](#page-2-0) Without loss of generality we may focus on the stable region defined by $\tilde{\epsilon}_b - \bar{g}^2/4\tilde{\omega} > 0$. Within this domain $E_n^-(\gamma_{var})$ and $E_n^{-}(\gamma = 0)$ are both smoothly increasing functions of *n*. Furthermore, while the super-radiance condition [\(14\)](#page-2-0) holds, $E_n^{-}(0) \ge E_n^{-}(\gamma_{var})$. We immediately conclude that whenever the *n* = 1 super-radiance condition is met ($\bar{g}^4 > \tilde{\omega}^2 \tilde{\omega}_0^2$), the ground state energy is either $E_1^-(\gamma_{\text{var}})$ or 0, the vacuum energy. However, outside of this region we must examine whether the lowest energy super-radiant state is lower in energy than either $E_1^-(0)$ or the vacuum.

To address this let us consider super-radiant states with *n >* 1. These are candidates for the ground state within the region, $\bar{g}^4 < \tilde{\omega}^2 \tilde{\omega}_0^2 < n^2 \bar{g}^4$, where the upper bound follows from the super-radiance condition and the lower bound precludes the region in which $E_1^-(\gamma_{\text{var}})$ is supported. If $\tilde{\omega}_0 > 0$, taking roots of the inequality yields $\tilde{\omega}_0 > \tilde{\omega} \tilde{\omega}_0^2 / n \bar{g}^2$ and $\tilde{\omega}_0 > g^2 / \tilde{\omega}$. In conjunction with the condition for stability, we see that $E_n^{-}(\gamma_{\text{var}}) > \tilde{\epsilon}_a = E_1^{-}(0)$. That is to say, the ground state never has $n > 1$.

If $\tilde{\omega}_0 \leq 0$ a stronger statement can be made. Invoking the super-radiance condition, $\tilde{\omega}_0 < -\tilde{\omega}\tilde{\omega}_0^2/n\bar{g}^2$, it follows that $E_n^{-}(\gamma_{var}) > 0$ for *all n*. Hence the vacuum must be the ground state when $\tilde{\omega}_0 \le 0$. [The latter implies $E_1^-(0) = \tilde{\epsilon}_a \ge \tilde{\epsilon}_b > 0$, where the last inequality has followed from the stability requirement.] We see that a sufficient condition for termination of the Mott lobe is $\mu_2 > \omega_0$. However, since $\mu_2 < \omega$ in general, such regimes are only stable for $\omega_0 < \omega$; see Fig. [2.](#page-2-0)

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