Models exhibiting order by projection

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We present calculations on a simple spin model which shows the phenomenon of *order by projection*. We discuss a two-level atomic system coupled to the radiation field to explore the possible relevance of order by projection in quantum optics. We point out the similarity between the effective Hamiltonian for the two-level atoms and the reduced BCS Hamiltonian used in the study of the ultrasmall metallic grains, and we present some calculations to show the transition from a nonsuperconducting to a superconducting ground state in the grains. We present a sum rule for the interacting electron systems on a lattice, exhibiting order by projection. This relates a nonextensive change in the ''kinetic energy'' due to a projection term to the extensive expectation value of the interaction in the ground state without projection.

I. INTRODUCTION

There is considerable recent interest in models exhibiting superconductivity starting from repulsion. While popular models, such as the *t-J* and Hubbard models, display superconducting phases within approximate treatments, such as slave boson mean field theories and the variational wavefunction approach, these remain somewhat unconvincing due to the uncontrolled nature of the schemes employed. One may, in fact, argue that apart from the Kohn-Luttinger[1] result for repulsive *continuum* electronic systems, there is no other compelling result for superconductivity from repulsion. In particular, electrons on a lattice have an extra property of being ''commensurate'' at certain fillings, and it is widely expected, but never quite proven, that this particular feature is of great significance, especially for high-T_c systems which are interesting near half-filling. It is therefore quite important to develop new nonperturbative methods and tools to investigate cooperative behavior of *lattice fermions*. In this context, a general idea termed *order by projection* has been introduced recently.[2,3]

The models introduced in Refs. 2 and 3 contain pairing terms, as in the BCS reduced Hamiltonian, but with large and repulsive interactions. When transformed to the Wannier basis in real space, the added term corresponds to an infinite ranged hopping of pairs of particles. Such pair hopping terms certainly occur in the lattice representation of the Coulomb interaction, but are of finite range. The theoretical models are thus in the spirit of mean-field models, the hope being that some features of the solutions are of a general nature that transcend the limitations of the starting models. In summary, it is found that the lattice Fermi system attains enhanced extended *s*-wave superconducting fluctuations A in the proximity of half-filling in reaction to the suppression of on-site *s*-wave fluctuations B (defined below). The uncertainty principle plays a crucial role in this since the *s*-wave and the extended *s*-wave ordering operators are recognized to be conjugates. Half-filling plays a special role in this enhancement, since only in its proximity can one suppress *both* $\langle B^\dagger B\rangle$ and $\langle BB^\dagger\rangle$.

The above works have used a combination of techniques, including rigorous inequalities and variational methods, on a class of models that are typified by either the Hubbard model, or the kinetic energy, to which we add a pure repulsive BCS-like interaction. The rigorous methods tell us that the extended *s*-wave correlation function is bounded from below by const/$(1-\rho)$, where ρ is the filling, and hence there is a large ''Gutzwiller''-type enhancement.

While the above work gives us an interesting and unique direction, several questions concerning the models and their behavior remain poorly understood. At precisely half-filling, the rigorous inequalities do not give us any guidance with reference to the question of whether the correlation function has actual long-ranged order (LRO), or if it is only critical, i.e., $\propto \mathcal{L}^{1+\eta}$ $(1>\eta>0)$. We discover here that the solutions do not have a true long-ranged order, and are superconducting only in the sense that the (normalized) correlations (similar to the Bragg's structure function in diffraction) $\langle A^\dagger A\rangle/L$ diverge in the thermodynamic limit. Also it is not clear if the ground-state energy density is affected at half-filling. There is also the issue of energy balance away from half-filling; we know from the inequalities that the interaction does not change the energy density, and yet one expects nonextensive energy corrections both for the potential and the kinetic energies. Can one say a little more about these?

Most of the explicit results obtained so far concern the repulsive BCS model with a large repulsive coupling constant, for which the variational calculations[3] bear out rather well the expectations arising from the general method of inequalities.[2] Barring the degeneracies of single-particle levels, the latter model actually maps on to a spin model in one-dimension, where energy plays the role of the single dimension. The model, described more fully later in this work, turns out to be difficult to solve explicitly, and was analyzed numerically in Ref. 2 by means of exact diagonalization for rather short chains, with a view to answer the above questions. In this work we extend the numerical results further to bigger systems and obtain more robust results.

In this work we introduce and solve explicitly and exactly a rather simple model that is inspired by the above spin model. This spin model consists of a large number of two-level systems; these interact via a spin-flip coupling that has the same form as in the above spin model, and the simplification consists of replacing a gradual variation of energies in the Zeeman part (representing the filled Fermi sea in the first

instance) by just a pair of energies. The model contains many elements of the more general models, but not all. The great advantage, however, is that the usual semiclassical methods, such as the Holstein-Primakoff transformation, help us solve this simplified model exactly in the thermodynamic limit, and also give an estimation of the finite size corrections. Variations of this model also arise in the study of two level systems in Quantum Optics, and we explore the connections in this work.

We find that a variant of the Feynman-Hellman coupling constant integration theorem can be utilized to formulate a rather remarkable sum rule in the models considered here. The sum rule equates an extensive expectation value to a weighted coupling constant integral of the kinetic-energy shift; the latter is not extensive, and yet adds up due to the weight factor to an extensive result. While this sum rule is true quite generally for this class of models, the above simplified model gives us an explicit example of the rule at work, and provides a ''feel'' for the nature of finite size corrections.

The organization of the paper is as follows. In Sec. II we define the general Hamiltonian with *s*-wave projection and derive the sum rule. We next present numerical results for the spin model with a linear dispersion relation at half-filling, and we discuss their implications for the behavior of correlations and energy at half-filling in the general models. In Sec. III we present the simplified spin Hamiltonian and proceed with its exact solution by semiclassical methods. We first present some calculations on the spin model with the interaction being negative and of the order of inverse system size, as in the usual BCS model. We then discuss the case of repulsion in great detail. In Sec. IV we consider the question whether the idea of order by projection can be useful for the two-level atoms interacting with the radiation field. Finally, in Sec. V we present a summary of the results.

II. THE MODELS AND A SUM RULE

We collect together in this section the various models treated in this paper. To start with, the general Hamiltonian for the interacting electrons with *s*-wave projection, as introduced in Ref. 2, is the following:

$$\mathcal{H}=\sum_{i,j}\ \sum_{\sigma}\ t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i}\ n_{i\uparrow}n_{i\downarrow}+U_sB^{\dagger}B \quad \text{(model I)}. \tag{1}$$

The first two terms in Eq. (1) with $U>0$ give the Hubbard model, and the third term is new, and represents the on site *s*-wave projection term for $U_s>0$ and of $O(1)$. Here, the operator $B=\Sigma_i c_{i\downarrow}c_{i\uparrow}$ is the on-site *s*-wave pairing operator. We refer to this as model I in the following. This added term is of particular interest for the present work, since it leads to an enhancement in the extended *s*-wave correlations. For completeness note that the extended *s*-wave pairing operator is defined as $A=-2\Sigma_{\mathbf{k}}\epsilon_{\mathbf{k}}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$, where $\epsilon_{\mathbf{k}}=-2t[\cos(k_x)+\cos(k_y)]$ on a square lattice, with $\mathbf{k}$ the momentum label and t the nearest-neighbor hopping amplitude.

The second model considered here corresponds to setting $U=0$ in model I, whereby it reduces to the repulsive version of the reduced Hamiltonian of BCS, with a ''large'' coupling constant U_s (since the latter is written for attractive interactions with a coupling constant of $O(1/\mathcal{L})$ so that the energy is extensive in the ordered state). It is possible[2] to write it in spin notation using the Anderson mapping of the BCS pairing operators to pseudospins $s_i^{+}=c_{\mathbf{k}_i\uparrow}^{\dagger}c_{-\mathbf{k}_i\downarrow}^{\dagger}$ and $s_i^{z}=\frac{1}{2}(n_{\mathbf{k}_i\uparrow}+n_{-\mathbf{k}_i\downarrow}-1)$. We find the following spin-1/2 Hamiltonian:

$$\mathcal{H}=\sum_{i}^{L}\ \epsilon_i(2s_i^{z}+1)+U_s\sum_{i,j}^{L}\ s_i^{+}s_j^{-} \quad \text{(model II)}. \tag{2}$$

We refer to this as model II in the sequel. Note that index i, here, corresponds to the ith $\mathbf{k}$ mode in the momentum space, and the transformation is meaningful only in the subspace where pairs $(\mathbf{k}\uparrow,-\mathbf{k}\downarrow)$ are either absent or present. The electrons that are not parts of a Cooper pair are thus unaffected by the interaction and are ignored. In the literal mapping of the BCS model, we would find each energy level ϵ_i having a large degeneracy, corresponding to the degeneracies of the cosine bands, but in the effective model treated here, we simply consider each energy level as nondegenerate. The energies are assumed to have a linear dispersion $\epsilon_i=-\frac{1}{2}+[(i-1)/(L-1)]$, so that we have a structureless density of states. The linear ''ramp'' of energies thus represents the fermionic energy levels filled up to a certain level, and the number of electrons is given by $N=\Sigma_j(1+2s_j^{z})$, which also is twice the number of Cooper pairs. Half-filling clearly corresponds to the sector $s_{total}^{z}=0$.

We finally indicate the simplified model that is obtained by further approximating the above model II. We restrict the energies ϵ_i to be $-1(+1)$ for $i<L/2(i>L/2)$ and find

$$\mathcal{H}=-\sum_{i}^{L/2}\ 2(s_i^{z}-s_{i+L/2}^{z})+U_s\sum_{i,j}^{L}\ s_i^{+}s_j^{-} \quad \text{(model III)}. \tag{3}$$

In Sec. III, we rewrite this model in more convenient ways to bring out the solvability and we present detailed calculations in various cases.

A. Sum rule

We now present an important sum rule for the general Hamiltonian equation (1) which relates the nonextensive change in the expectation value of the Hubbard part of the Hamiltonian equation (1) due to U_s, to the expectation value of $B^{\dagger}B$ in the ground state with $U_s=0$. For convenience, let us write Eq. (1) as $\mathcal{H}=T+U_sV$, where T stands for the Hubbard part and V stands for $B^{\dagger}B$. For $U=0$, T is simply the kinetic energy of the electrons. The expectation values of operators T and V in the ground state, for a particular value of U_s, are denoted by $T(U_s)$ and $V(U_s)$, respectively.

Let $E(U_s)$ be the ground-state energy of the Hamiltonian equation (1) for a particular value of U_s. The Feynman-Hellman theorem states that $\Delta E(U_s)=E(U_s)-E(0)=\int_0^{U_s}d\lambda\,V(\lambda)$. From the general arguments of Ref. 2 we know that

$$\Delta E(U_s)=\int_0^{U_s}d\lambda\,V(\lambda)\sim o(L). \tag{4}$$

Here, L stands for the system size and $o(L)$ implies that the quantity is nonextensive, unlike $\mathcal{O}(L)$ which says that

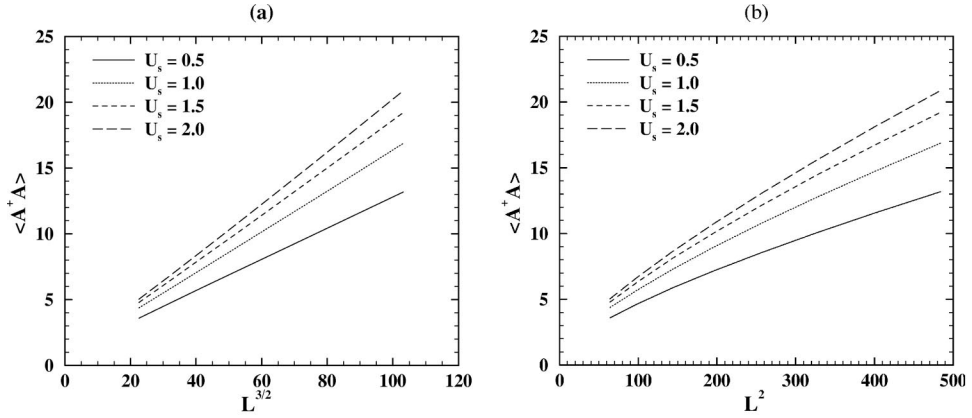

FIG. 1. The extended s-wave correlation function, $\langle A^{\dagger}A\rangle$, at half-filling is plotted against (a) $L^{3/2}$, and (b) L^2 for chains of length up to 22.

the quantity goes like L. Thus Eq. (4) implies that $\Delta E(U_s)/L\rightarrow 0$ as $L\rightarrow\infty$, i.e., the energy shift is nonextensive. Using $\lambda V(\lambda)=\Delta E(\lambda)-\Delta T(\lambda)$, and manipulating a bit, we derive[4] the following relation for the change in the ground-state energy, in the presence of the s-wave projection term:

$$\Delta E(U_s)=U_s\left(V(0)-\int_0^{U_s}\frac{d\lambda}{\lambda^2}\Delta T(\lambda)\right), \tag{5}$$

where $\Delta T(\lambda)=T(\lambda)-T(0)$. Equation (5) is true in general whereas Eq. (4), namely, is true only for the Hamiltonian equation (1). These two together imply the following sum rule:

$$V(0)=\int_0^{U_s}\frac{d\lambda}{\lambda^2}\Delta T(\lambda)+o(L). \tag{6}$$

This is quite remarkable as an extensive quantity $V(0)$ is equated by integration over an intensive quantity $\Delta T(\lambda)$ in the thermodynamic limit. In Sec. III B 3 we will see explicitly how two sides of Eq. (6) equate each other, in the thermodynamic limit [see Eqs. (29) and (30)].

B. Numerical results for model II

Here we present extended numerical results for model II. As mentioned in the Introduction, this model was studied in Ref. 2 and a preliminary numerical investigation of short chains with L up to 14 were presented for somewhat large values of U_s. In Ref. 2 the numerics was interpreted to be consistent with $\langle A^{\dagger}A\rangle\sim L^2$. However, the analytical results of Ref. 3 give $\langle A^{\dagger}A\rangle\sim L^{3/2}$. In order to resolve this issue we have computed these correlation functions for longer chains.

We computed ground-state energy E_g, $\langle A^{\dagger}A\rangle$, and $\langle B^{\dagger}B\rangle$ numerically as a function of system size L at half-filling up to $L=22$ for $U_s=0.5,1.0,1.5$, and 2.0. The results of these numerical calculations are shown below. In Fig. 1 we see that the data go fairly linearly when plotted against $L^{3/2}$ as compared to when plotted against L^2, especially for small U_s. This favors the theoretical understanding that $\langle A^{\dagger}A\rangle\sim L^{3/2}$. In Fig. 2 we have drawn a comparison between two possible behaviors for the ground state energy shift as a function of the system size L. If the system has true LRO then one expects the shift to be linear in size, whereas with critical correlations,[3] the shift should be $\propto L^{1/2}$, and hence nonextensive. We see that the data are more consistent with ΔE_g going as $L^{1/2}$. We next examine the coefficients of the leading terms of $\langle A^{\dagger}A\rangle$ and the ΔE_g, since we have variational estimates for these in Ref. 3:

$$\frac{E_g}{L}\approx e_{non}+2\frac{\sqrt{U_s\alpha(0)}}{\sqrt{|\mu_1|L}}, \tag{7}$$

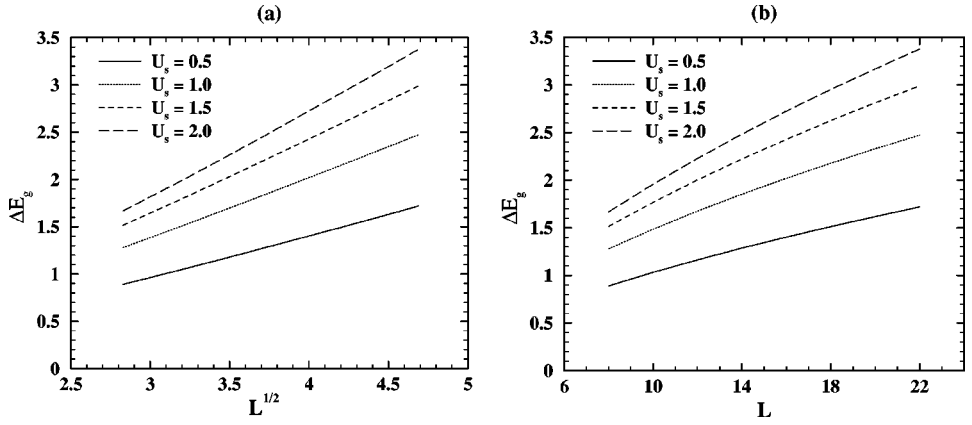

FIG. 2. The ground-state energy shift ΔE_g at half-filling is plotted against (a) $L^{1/2}$ and (b) L for chains up to $L=22$.

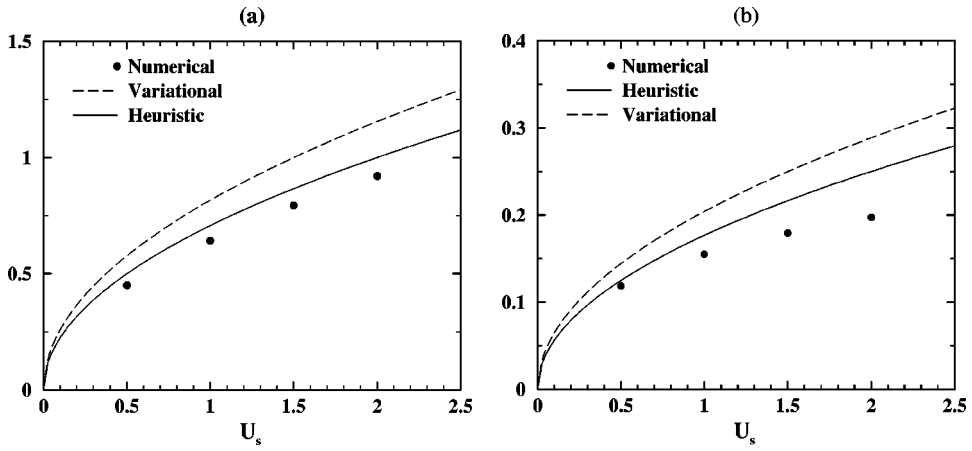

FIG. 3. Various estimates of the coefficients of the leading-order terms for (a) $\Delta E_g(\sim L^{1/2})$ and (b) $\langle A^\dagger A\rangle(\sim L^{3/2})$.

$$\alpha \approx \frac{1}{2}\sqrt{\alpha(0)|\mu_1|U_s}L^{1/2}. \tag{8}$$

Here $\alpha=\langle A^\dagger A\rangle/(4L)$ and $\mu_1=(1/L)\Sigma_{\mathbf{k}}\epsilon_{\mathbf{k}}(2f_{\mathbf{k}}-1)$. The $\alpha(0)$ is the value of α for $U_s=0$. For linear dispersion, $\alpha(0)=(L+1)/[24(L-1)]$ and $\mu_1=-L/[4(L-1)]$. Therefore, from Eqs. (7) and (8) one finds that $\langle A^\dagger A\rangle \approx \sqrt{U_s/24}L^{3/2}$ and $(E_g-E_g^0)\approx\sqrt{2U_s/3}L^{1/2}$ in the thermodynamic limit. We also have a heuristic result for $\langle A^\dagger A\rangle$ and ΔE_g in terms of $\mu_1, \Delta E_g\sim\sqrt{2U_s|\mu_1|L}$ and $\alpha=(1/2\sqrt{2})\sqrt{U_s|\mu_1|^3L}$ at half-filling, obtained from a functional integral approach. These are equivalent to replacing $\alpha(0)$ by $|\mu_1|^2/2$ in the variational results.

In Fig. 3 the numerical estimates of the coefficients of the leading-order term of $\langle A^\dagger A\rangle$ and ΔE_g in L are shown together with the variational and the heuristic results. The latter is closer to the numerical value. We thus see that the theoretical estimates and the exact numerics for relatively short chains are qualitatively in consonance in suggesting critical order rather than true LRO at half-filling. Detailed examination shows that there are some discrepancies in the coefficients of the leading behavior; these seem to become larger for modestly large values of U_s, implying that the values of U_s in Ref. 2 were much too large. It seems that further finites size studies on longer systems may be needed to be completely sure of the final coefficients.

III. SIMPLIFIED SPIN MODEL

For a fairly simple choice of the dispersion relation, as mentioned earlier, model III is derived from model II. Let us label the group of spins with $\epsilon=-1$ as a and with $\epsilon=1$ as b. Then model III can be rewritten in the following convenient form:

$$\mathcal{H}=2(-S_a^z+S_b^z)+U_s(S_a^+ +S_b^+)(S_a^- +S_b^-). \tag{9}$$

Here, $\mathbf{S}_a=\Sigma_1^{L/2}\mathbf{s}_i$ and $\mathbf{S}_b=\Sigma_{L/2+1}^{L}\mathbf{s}_i$. This turns out to be a problem of two large spins $\mathbf{S}_a$ and $\mathbf{S}_b$ coupled to each other antiferromagnetically. The analog of s-wave and extended s-wave pairing operators for this spin problem are $B=S_a^- +S_b^-$ and $A=2(S_a^- -S_b^-)$.

A. Attractive case : $U_s=-\gamma/L$

Before considering the repulsive case ($U_s>0$ and $\sim\mathcal{O}(1)$) for Eq. (9), we briefly discuss the attractive case with $U_s=-\gamma/L$, where $\gamma\sim\mathcal{O}(1)$ and positive. It is clearly the case of conventional BCS-type superconductivity.

At half-filling ($\rho=1$), the spin Hamiltonian equation (9) with attractive interaction shows a first-order phase transition from the normal to superconducting ground state as γ is varied. In the thermodynamic limit, $\Delta E_g=E_g(\gamma)-E_g(0)$ is

$$\Delta E_g=\begin{cases}-2+\sqrt{2(2-\gamma)}, & \gamma<2\\ -L(\gamma/4)(1-2/\gamma)^2, & \gamma\geqslant 2.\end{cases} \tag{10}$$

We also calculate the $\langle B^\dagger B\rangle$ correlation function in the thermodynamic limit. To the leading order in L, at $\rho=1$,

$$\langle B^\dagger B\rangle=\begin{cases}L/\sqrt{2(2-\gamma)}, & \gamma<2\\ (L/2)^2[1-(2/\gamma)^2], & \gamma\geqslant 2.\end{cases} \tag{11}$$

We define an order parameter $\Omega=\sqrt{\langle B^\dagger B\rangle}/L$ (in analogy with usual mean-field theory). Here, we see that in the thermodynamic limit, there is true LRO in $\langle B^\dagger B\rangle$, and ΔE_g is extensive. Figure 4 shows the exact diagonalization and the semiclassical results for the change in the ground-state energy in Eq. (10). Figure 5 shows Ω as a function of L and γ. We see that for large enough L, the ground state is superconducting for $\gamma>2$ and normal for $\gamma<2$. Here, at $\rho=1$, $\gamma=2$ is special because the interaction can make one spin flip only if it gains an energy of amount 2 at least (which is the bandwidth). For smaller systems, Ω is significantly nonzero for $\gamma<2$, and also deviates from its thermodynamic behavior in the region $\gamma>2$.

It is worth mentioning that the reduced BCS model for studying superconductivity in the ultrasmall metal particles[5–7] can easily be mapped to the model II with $U_s=-\gamma/L$, and can further be approximated by the simpler model III studied here. The results obtained here are in the qualitative agreement with the experimental observations.[8] First, the finite size order parameter is always greater than its thermodynamic value. Second, the system is superconducting for average level spacing, $2/L$, less than interaction, γ/L. Issues such as crossover from bulk behavior to small size behavior cannot be studied rigorously here because of the

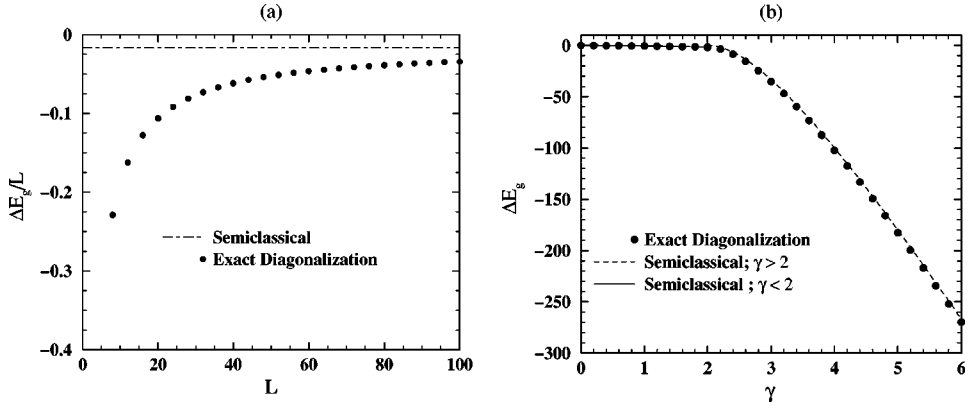

FIG. 4. Superconducting transition at $\rho=1$. (a) $\gamma=2.4$, (b) L = 400.

simple structure of the Hamiltonian, i.e., since the density of states is structureless and independent of L. As $\mathbf{S}_a$ and $\mathbf{S}_b$ are large spins, the quantum fluctuations are also insignificant.

B. Repulsive case: $U_s>0$ and $\sim\mathcal{O}(1)$

This corresponds to the projection of s-wave pairing. In the following sections we discuss this case in detail.

1. Exact diagonalization

We now proceed to solve this model explicitly and exactly. Let us note that the operators $\mathbf{S}_a^2$ and $\mathbf{S}_b^2$ commute with the operators $S_{a,b}^{\pm,z}$ and, therefore, commute with the spin-Hamiltonian equation (9). The operator $S^z=S_a^z+S_b^z$ also commutes with the same. Thus, we have three conserved quantities s_a and s_b, the quantum numbers associated with spins $\mathbf{S}_a$ and $\mathbf{S}_b$, and n, the quantum number associated with total S^z. For the exact diagonalization of the spin-Hamiltonian equation (9), we choose the basis states to be the product states of the two spins $\mathbf{S}_a$ and $\mathbf{S}_b$. We write the basis states as $|n,s_a,s_b;m\rangle=|s_a,m\rangle|s_b,n-m\rangle$. For a given filling $\rho=N/L$, where N is the number of electrons on a lattice with L number of sites, the allowed values of quantum numbers are

$$n=-\frac{L}{2}(1-\rho),\quad s_{min}\leqslant s_a\leqslant\frac{L}{4},$$
$$\max(s_{min},|n|-s_a)\leqslant s_b\leqslant\min\left(\frac{L}{2}-s_a,\frac{L}{4}\right), \tag{12}$$

where s_{min} is 0 for even $L/2$, and 1/2 for odd $L/2$. Only those values of s_a are acceptable for which the $\max(s_{min},|n|-s_a)\leqslant\min(L/2-s_a,L/4)$. Given the values of n,s_a, and s_b, the running index m in the basis states is such that $\max(n-s_b,-s_a)\leqslant m\leqslant\min(n+s_b,s_a)$. We diagonalize the Hamiltonian matrix for fixed values of n,s_a, and s_b. The minimum eigenvalue corresponds to $s_b=L/4$ and $s_a=L|2\rho-1|/4$. This we identify as the ground-state energy and the corresponding eigenvector as the ground state of the system. Fillings $\rho\leqslant1/2$ are not interesting as the operators A and B annihilates the ground state of the spin-Hamiltonian equation (9). We confine our calculations close to half-filling ($\rho=1$) as it is where one expects large enhancement in the extended s-wave pairing correlations.

2. Analytical results in the thermodynamic limit

As we noticed above, the quantum numbers s_a and s_b for the ground state are proportional to system size L. More precisely, the ground state for $\rho>1/2$ corresponds to $s_a=L(2\rho-1)/4$ and $s_b=L/4$. Therefore, in the thermodynamic limit we use the Holstein-Primakoff (HP) transforma-

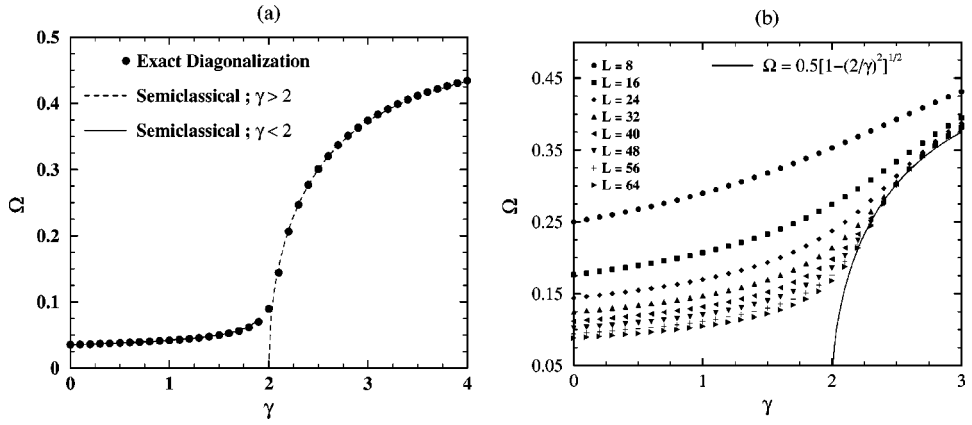

FIG. 5. Ω as a function of γ. Plot (b) shows the deviation in Ω from its thermodynamic behavior for small system size.

tion. This semiclassical approximation enables us to get analytical expressions for various quantities like $E_g, \langle A^\dagger A\rangle$, etc. to the leading order in the system size.

Let a and b be canonical bose operators, then the HP transformation states

$$S_a^+ = \sqrt{2s_a - a^\dagger a}\, a, \quad S_b^+ = b^\dagger \sqrt{2s_b - b^\dagger b},$$
$$S_a^- = a^\dagger \sqrt{2s_a - a^\dagger a}, \quad S_b^- = \sqrt{2s_b - b^\dagger b}\, b, \tag{13}$$
$$S_a^z = s_a - a^\dagger a, \quad S_b^z = -s_b + b^\dagger b.$$

For large L we expand square roots appearing in Eq. (13) only up to first order in $a^\dagger a/2s_a$ and $b^\dagger b/2s_b$. This transforms the spin-Hamiltonian equation (9) into the following bosonic Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4 + \mathcal{O}(1/L), \tag{14}$$

where

$$\mathcal{H}_0 = -2(s_a + s_b + 1) + 2U_s(s_a - s_b),$$
$$\mathcal{H}_2 = 2[(1 + s_a U_s)a^\dagger a + U_s\sqrt{s_a s_b}(ab + b^\dagger a^\dagger) + (1 + s_b U_s)bb^\dagger], \tag{15}$$
$$\mathcal{H}_4 = -U_s(a^\dagger a a a^\dagger + b^\dagger b^\dagger b b) - \frac{U_s}{2}\sqrt{s_a s_b}\left[\frac{(a^\dagger a a b + b^\dagger a^\dagger a^\dagger a)}{s_a} + \frac{(b^\dagger b b a + a^\dagger b^\dagger b^\dagger b)}{s_b}\right].$$

$\mathcal{H}_4$ is of $\mathcal{O}(1)$ [becuase $U_s \sim \mathcal{O}(1)$] and $\mathcal{H}_0 + \mathcal{H}_2$ is of order L. Therefore, $\mathcal{H}_4$ can be treated as a small perturbation to the $\mathcal{H}_0 + \mathcal{H}_2$ in the thermodynamic limit and is used to find out the higher-order corrections, and it is not important to consider $\mathcal{H}_4$ for the leading-order calculation.

The quadratic Hamiltonian $\mathcal{H}_2$ is diagonalized by the canonical transformation of (a,b) to a new set of Bose operators (η,γ) defined as $a = \cosh(\theta)\eta - \sinh(\theta)\gamma^\dagger$ and $b^\dagger = -\sinh(\theta)\eta + \cosh(\theta)\gamma^\dagger$. The quadratic Hamiltonian $\mathcal{H}_2$ is diagonal in the operators (η,γ) for the following value of θ:

$$\theta = \frac{1}{2}\ln\left[\frac{4 + U_s L\rho + U_s L\sqrt{2\rho - 1}}{\sqrt{16 + 8U_s L\rho + U_s^2 L^2(1-\rho)^2}}\right]. \tag{16}$$

It is interesting to note that θ is singular at $\rho = 1$ in the thermodynamic limit, and this singularity is carried over to other quantities of interest through θ,

$$\theta_\infty = \frac{1}{2}\ln\left(\frac{\rho + \sqrt{2\rho - 1}}{1 - \rho}\right). \tag{17}$$

This leads us to expect that $\rho = 1$ is a special filling where the system undergoes some kind of a transition. Let E_g be the ground-state energy and we define two other quantities, α and β, related to the operators A and B, respectively, such that

$$\alpha = \frac{\langle A^\dagger A\rangle_{U_s}}{4L}, \quad \beta = \frac{\langle B^\dagger B\rangle_{U_s}}{L}. \tag{18}$$

In the limit of large L and ρ close to 1,

$$\frac{E_g}{L} \approx -\rho + \frac{2}{L}\left(\frac{2\rho - 1}{1 - \rho}\right) + \mathcal{O}\left(\frac{1}{L^2}\right), \tag{19}$$

$$\alpha \approx \frac{2\rho - 1}{(1 - \rho)} + \mathcal{O}\left(\frac{1}{L}\right), \tag{20}$$

$$\beta \approx 0. \tag{21}$$

At $\rho = 1$,

$$\frac{E_g}{L} = -1 + \frac{\sqrt{2U_s}}{L^{1/2}} - \frac{4 + U_s}{2L} + \mathcal{O}\left(\frac{1}{L^{3/2}}\right), \tag{22}$$

$$\alpha = \frac{1}{2}\left(\sqrt{\frac{U_s}{2}} - \frac{U_s}{2\sqrt{L}} + \frac{(1 + 2U_s)}{\sqrt{2U_s}L}\right)L^{1/2} + \mathcal{O}\left(\frac{1}{L}\right), \tag{23}$$

$$\beta = \frac{1}{\sqrt{2U_s L}} - \frac{1}{2L} + \mathcal{O}\left(\frac{1}{L^2}\right). \tag{24}$$

Equation (20) is consistent with enhancement inequality as mentioned in Ref. 2. Equation (23) implies that the correlation function $\langle A^\dagger A\rangle$ goes as $L^{3/2}$ and thus affirms that there exists a quasi-long-range order in the pairing correlation of an extended s-wave type at commensurate filling. Another important point to notice is that both at and away from half-filling, the ground-state energy density is the same as for the case without the projection term; that is, $\lim_{L\to\infty}(E_g/L) = \langle T\rangle_{U_s=0}/L = -\rho$. However, the leading-order finite size correction to the energy per site changes from $1/L$ in Eq. (19) with a coefficient that diverges near $\rho = 1$, to $1/\sqrt{L}$ at $\rho = 1$ as in Eq. (22).

Let us compare the above results with that of variational calculation on model I with $U = 0$, as given in Ref. 3. There, at $\rho = 1, E_g/L \approx e_{non} + 2\sqrt{\alpha(0)U_s/|\mu_1|L}$ and $\langle A^\dagger A\rangle/L \approx 2\sqrt{U_s\alpha(0)|\mu_1|L}$, where $\alpha = \langle A^\dagger A\rangle/4L$ and $\mu_n = \Sigma_k \epsilon_{\mathbf{k}}^n(2f_k - 1)/L$. Here, e_{non} is the noninteracting energy density, and $\alpha(0)$ is the value of α at $U_s = 0$. For the present choice of dispersion relation, that is $\epsilon_i = -1(+1)$ for $i \leqslant L/2(> L/2), \alpha(0) = \rho/2$, and $\mu_1 = -\rho$. At $\rho = 1$, we obtain $2\alpha \approx \sqrt{U_s/2L^{1/2}}$ and $E_g/L \approx -1 + \sqrt{2U_s/L}$ which is the same as given above. The heuristic results are also the same in this case. In terms of μ_1, away from half-filling, the lower bound on $\langle A^\dagger A\rangle$ given by the enhancement inequality[2] is $\sim 2\mu_1^2 L/(1-\rho)$. We find that the exact result is twice the value of the lower bound. Thus close to half-filling, $\alpha \sim 1/(1-\rho)$, which is consistent with Eq. (20).

Figure 6 compares the results of exact diagonalization with the semiclassical analytical calculations. One can see a good agreement between the equations of the best-fit curves for the exact diagonalization data and the semiclassical leading-order expressions for E_g and $\langle A^\dagger A\rangle$.

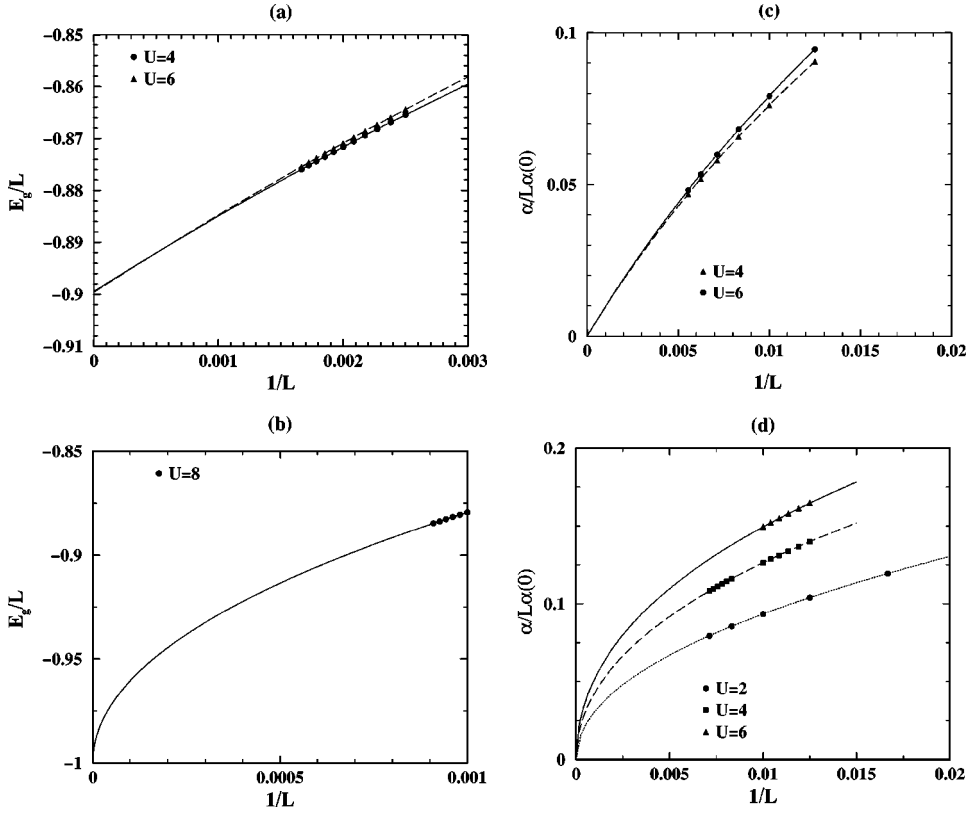

FIG. 6. Continuous lines are the best-fit lines and the points are the exact diagonalization results. (b) and (d) are at half-filling whereas (a) and (c) are at $\rho=0.9$ and 0.8, respectively.

3. Variational approach

We next perform a variational calculation for the bosonized Hamiltonian equation (14). The motivation for this digression is that the variational approach, while yielding finally the same result as in the above exact diagonalization, gives additionally a picture of the competing energies. It also gives a useful hint in the cases where exact diagonalization is not possible.[3] In the thermodynamic limit, we neglect $\mathcal{H}_4$ and all higher terms. As we are interested in the ground state, we put $s_a=L(2\rho-1)/4$ and $s_b=L/4$. Then the kinetic-energy part of the spin-Hamiltonian equation (9), viz., $\mathcal{T}=2(-S_a^z+S_b^z)$, becomes $\mathcal{T}=-L\rho+2(a^\dagger a+b^\dagger b)$, under the HP transformation and the potential-energy term, $U_s(S_a^+ + S_b^+)(S_a^- + S_b^-)$, becomes $\mathcal{V}=(U_sL/2)(\sqrt{2\rho-1}a + b^\dagger)(\sqrt{2\rho-1}a^\dagger + b)$. We use $|\psi_v\rangle=\exp[-\theta(b^\dagger a^\dagger - ab)]|0\rangle$ as the variational ansatz for the ground-state wave function. Here $|0\rangle$ is the vacuum of operators a and b. A more general variational wave function, viz., $|\psi_v\rangle = \exp(-(\theta/2L)[\mathcal{T},B^\dagger B]|\phi\rangle$ has been discussed for models exhibiting order by projection in Ref. 3 where $|\phi\rangle$ is the ground state of the Hamiltonian without projection. The variational wave function used in the present work is a special form of the more general one. The prefactor in the variational wave function generates several Cooper particles and Cooper hole pairs in the ground state $|0\rangle$. The expectation values of operators $\mathcal{T}$ and $\mathcal{V}$ in this variational wave function are

$$T_v(\theta)=-L\rho+4\sinh^2\theta, \tag{25}$$

$$V_v(\theta)=\frac{U_sL}{2}(\sqrt{2\rho-1}\cosh\theta-\sinh\theta)^2. \tag{26}$$

Minimizing the variational energy, $E_v(\theta)=T_v(\theta)+V_v(\theta)$, with respect to θ gives us the same value of parameter θ as given in Eq. (16). We see that as long as θ is of $\mathcal{O}(1)$, the kinetic-energy shift $\sinh^2\theta$ is nonextensive. Away from $\rho=1$, we can thus make $V_v(\theta)$ vanish by choosing $\theta=\ln[(1+\sqrt{2\rho-1})/\sqrt{2(1-\rho)}]$. At $\rho=1$, we are pushed to a diverging $\theta\sim\mathcal{O}(\ln L)$, since $V_v(\theta)=U_sLe^{-\theta}/2$. This necessarily costs more kinetic-energy shift, but fortunately $\sinh^2\theta \sim\mathcal{O}(\sqrt{L})$ so the shift is not extensive. One can see that in the thermodynamic limit, for $\rho<1$:

$$E_g=-L\rho+\frac{2(2\rho-1)}{1-\rho},\quad \alpha=\frac{2\rho-1}{1-\rho},\quad \beta=0. \tag{27}$$

Similarly, for $\rho=1$, minimizing $E_v(\theta)$ we get $\theta=\frac{1}{4}\ln(U_sL/2)$ and so

$$E_g=-L+\sqrt{2U_sL},\qquad \alpha=\frac{1}{2}\sqrt{U_sL/2},\quad \beta=1/\sqrt{2U_sL}. \tag{28}$$

It is nice to see that this simple spin model explicitly verifies the assertions, based on general physical arguments made in Ref. 2, namely, in the thermodynamic limit (i) the presence of the *s*-wave projection term makes no difference to the ground-state energy per site, (ii) it leads to the enhancement in the extended *s*-wave pairing correlation func-

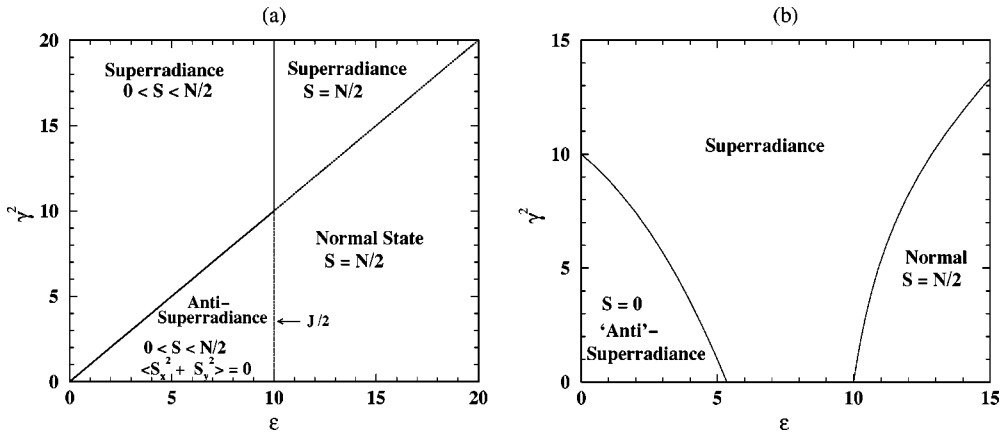

FIG. 7. $J=20$. (a) $\epsilon_1=\epsilon_2$, (b) $\epsilon_2 \gg \epsilon_1$. The figure with $\epsilon_1 \neq \epsilon_2$ gives rise to an antisuperradiant phase with total $S_z=0$.

tion near half-filling, and (iii) there is quasi-long-range order in the extended *s*-wave pairing correlation at half-filling.

As we have explicit expressions for $T(U_s)$ and $V(U_s)$ in this simple model, we take this opportunity to see how the sum rule stated in the beginning [Eq. (6)] is satisfied in the thermodynamic limit. Setting θ as given in Eq. (16) into Eq. (26) (and writing U_s as λ), we get

$$T(\lambda)=-L\rho-2+\frac{2(4+\lambda L\rho)}{\sqrt{16+8\lambda L\rho+\lambda^2L^2(1-\rho)^2}}, \quad (29)$$

$$V(\lambda)=\frac{L}{2}\left[\frac{4\rho+\lambda L(1-\rho)^2}{\sqrt{16+8\lambda L\rho+\lambda^2L^2(1-\rho)^2}}-(1-\rho)\right]. \quad (30)$$

Integrating $\Delta T(\lambda)/\lambda^2$ from $\lambda=0$ to U_s, and taking limit $L\to\infty$ gives $V(0)$ both for $\rho<1$ and $\rho=1$. The reason why the integral of a nonextensive quantity $\Delta T(\lambda)$ equals the extensive quantity V(0) in the thermodynamic limit is that a very large contribution arises for $\lambda\sim\mathcal{O}(1/L)$ where the weight factor $1/\lambda^2$ becomes large. This becomes very clear when one rescales λ as λ/L in the integral $\int_0^{U_s}d\lambda[\Delta T(\lambda)/\lambda^2]$ to bring out a factor of L outside the integral. The remaining integral is a number in the thermodynamic limit which is precisely $V(0)$. Thus, we see that the sum rule is saturated for the $\lambda\sim\mathcal{O}(1/L)$.

IV. ORDER BY PROJECTION AND ANTISUPERRADIANCE

In this section we study a system of two-level atoms coupled to a single-mode radiation field, and interacting among themselves via an ''exchange'' interaction. The motive is to discuss the relationship of order by projection in quantum optics. The model Hamiltonian that we study here is given as

$$\mathcal{H}_{DJ}=a^\dagger a+\epsilon_1S_1^z+\epsilon_2S_2^z+\frac{\gamma}{\sqrt{L}}[(S_1^++S_2^+)a + a^\dagger(S_1^-+S_2^-)]+\frac{J}{L}\mathbf{S}_1\cdot\mathbf{S}_2, \quad (31)$$

where $J\sim\mathcal{O}(1)$ and positive. Here energy is measured in the units of photon energy, ϵ_1 and ϵ_2 are the transition energies of the two species of the two-level atoms and L is the total number of atoms (of both types). The coupling of the atoms of different types to the field is assumed to be the same, i.e., γ which is an intensive number proportional to the $\sqrt{L/V}$, where V is the volume of the cavity. The operators $S_{1,2}^z$ are known as the population inversion operators in quantum optics. The operators $S_{1,2}^+$ and $S_{1,2}^-$ are such that the total electric dipole operator of the atomic subsystems is proportional to $(S^++S^-)_{1,2}$ where the magnitude of the atomic dipole matrix element is the proportionality constant (phase factor included in the definition of $S^\pm$). In terms of the Pauli matrices, $S_1^+=\Sigma_i\sigma_i^+$ and $S_1^z=\Sigma_i\sigma_i^z/2$, where the index i runs over the atoms of type 1. The operator σ_i^+ causes the transition of ith atom from its ground state to its excited state. Similarly, one can write corresponding operators for atoms of type 2. These operators follow the angular-momentum algebra and therefore, are treated like the spin operators.

The inclusion of exchange interaction, $(J/L)\mathbf{S}_1\cdot\mathbf{S}_2$, in the Hamiltonian is purely mathematical with no clear idea of how such an interaction can be realized in real experiments. For $J=0$, this is the Dicke model of superradiance[9,10] for two species of atoms. It has a superradiant ground state with $\langle a\rangle\sim\sqrt{L}$ and $\langle S_x^2+S_y^2\rangle\sim L^2$. Here, $S_{x,y}$ are the x,y components of the total ''spin'' $\mathbf{S}_1+\mathbf{S}_2$. Thus, ''superradiant phase'' is a thermodynamic phase with large number of atoms in their excited states, in cooperation with the photons unlike a ''normal'' phase where all atoms are in their ground states. It is a phase where photons condense and two atomic subsystems develop in-phase macroscopic dipoles. Superradiance is attained below a certain temperature T_c for $\gamma^2>\epsilon$, where $\epsilon^{-1}=(\epsilon_1^{-1}+\epsilon_2^{-1})/2$. For $\gamma^2<\epsilon$, the system is normal. For $J>0$, the exchange term tends to break the cooperation between the field and atoms. For suitable strength of J, it drives the systems to a new ground state where two atomic subsystems develop out of phase dipoles and photons do not condense. Thus, $\langle S_x^2+S_y^2\rangle=0$ and $\langle a\rangle=0$. We identify it as the antisuperradiant state (this term is borrowed from Mandel and Wolf[11]). This is in analogy with the states identified with extremely weak decay which have been observed experimentally[12] for a system of low-density excited molecules enclosed between metallic mirrors. The model equa-

tion (31) is studied by mean-field methods and by using the Holstein-Primakoff transformation. The phase diagram obtained is shown in Fig. 7.

The coupling of atoms to the radiation can be viewed as an effective interaction, $-(\gamma^2/L)(S_1^+ + S_2^+)(S_1^- + S_2^-)$, among atoms. This is the same as what we studied for the case of superconductivity in the metallic grains in Sec. III A. Extending this analogy further, projecting out *s*-wave Cooper pairing can be taken as projecting out superradiance in the atom-field system. Under this projection, ordering occurs in the operator, $A = \epsilon_1 S_1^+ + \epsilon_2 S_2^+$, due to antiparallel transverse fluctuations for $\epsilon_1 \neq \epsilon_2$ and total $S^z = 0$. Adding an exchange term to the Dicke model has a similar effect of suppressing superradiance, though it does not project out superradiance. Thus, it is clear that antisuperradiance does not necessarily imply order in *A*, but the antisuperradiant phase in Fig. 7(b) is a region where one can look for order by projection.

V. SUMMARY AND CONCLUSION

In this paper we have explored the phenomenon of ''order by projection'' within a simple and solvable model in detail. We derived a sum rule for the lattice Fermi systems with *s*-wave projection which relates the intensive change in the kinetic energy to the extensive interaction energy. We solved the simple spin model both exactly and semiclassically. It is shown explicitly that away from half-filling $\langle A^\dagger A \rangle \sim 1/(1-\rho)$ and that the energy shift ΔE_g is intensive. At $\rho = 1$, $\langle A^\dagger A \rangle \sim L^{3/2}$ and $\Delta E_g \sim L^{1/2}$. Thus the energy density is unchanged and there is quasi-LRO in *A* at half-filling. The numerical results for $\langle A^\dagger A \rangle$ and ΔE_g are presented for model II with linear dispersion. They are in agreement with the above behavior of the correlation function and the ground-state energy. We briefly discuss the attractive case of model III which is equivalent to the reduced BCS model of superconductivity. Finally, we discussed the possible relevance of order by projection in quantum optics. We discussed antisuperradiance and found that it does not necessarily imply order by projection, though it may be a region of phase diagram to look for order by projection.

In conclusion, we explicitly showed that the extended *s*-wave pairing correlations are enhanced in the close proximity of half-filling by suppressing *s*-wave pairing, and the system attains critical superconducting order in the extended *s*-wave channel at half-filling. Thus, these results support the possibility of the superconductivity arising from pure repulsion with no explicit attractive interaction. We have also pointed out the similarity of models studied in the case of superconductivity in metallic grains and the atom-field system and the spin model exhibiting order by projection.

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