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Coherent states and the calculation of nuclear partition functions

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Coherent states are introduced as test functions to formulate the statistical mechanics of fermions and bosons interacting via schematic forces. Finite temperature solutions to the Lipkin model and to the Schütte–Da Providencia model are obtained by performing the statistical sum *à la* Hecht, e.g., by using coherent states. Comparison between present and exacts results is discussed.

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I. INTRODUCTION

The study of partition functions in the quantum many-body problem is a subject of interest, particularly in dealing with nuclear and hadronic properties at finite temperatures [1].

The main difficulty concerning the exact calculation of partition functions in realistic cases is the dimension of the configuration space associated with the Hamiltonian of the system. In consequence, one has to resort to the use of approximations. Among them we have chosen the coherent-state representation of Hecht [2], as trial test functions. In the present work we focus on the calculation of partition functions, using coherent states, for the cases of the Lipkin [3] and the Schütte and Da Providencia [4] models. Central to these calculations is the use of coherent states to express the matrix elements of the statistical density operator $\hat{\rho}=e^{-\beta H}$. We have ordered the approximations following a hierarchy, that is, starting from the integral representation of the partition function and performing different approximations to compute the matrix elements $\langle z|e^{-\beta H}|z\rangle$, where $|z\rangle$ is a coherent state. The solutions are constructed in the mean-field approximation, the random-phase approximation (RPA), and in a variational approach. The results of these approximations are compared with the exact solutions of each model, to determine their degree of validity.

The paper has been organized as follows. The essentials about the use of coherent states in statistical mechanics are presented at the beginning of Sec. II. The partition function of the Lipkin SU(2) model is presented in Sec. II A. Section II A 1 describes the approximations introduced to calculate the matrix elements of the statistical operator acting on coherent states, namely, (a) the exponential approximation and (b) the Dyson boson mapping. Next, in Sec. II A 2 and Sec. II A 3 we show how to treat the Hamiltonian and the matrix elements of the density operator in the Weiss approximation and in a variational approach, respectively. In all cases the coherent states are used as trial states to perform the statistical sum. The critical behavior of the solutions is presented at the end of Sec. II A. The solution to the Schütte and Da Providencia model is presented in Sec. II B, within the same approximations applied to discuss the Lipkin model. The exponential and the Dyson boson mapping approximations are presented in Sec. II B 1, and the variational approach is discussed in Sec. II B 2. In Sec. II C we discuss the use of the RPA approximation, in conjunction with the use of coherent states, to calculate the partition function beyond the mean-field approximation. The formalisms corresponding to the Lipkin and the Schütte and Da Providencia model are presented in Sec. II C 1 and Sec. II C 2, respectively. The results of the calculations are shown in Sec. III, together with the comparison with the exact solutions [5,6]. Conclusions are drawn in Sec. IV.

As it will become evident to the reader, particularly in going through Sec. II, we have presented all the mathematical steps that are relevant to the formalism. We have done it on purpose, in order to present the results in a form that can easily be applied to Hamiltonians others than the ones considered in this work. Also, for the benefit of the reader who may be willing to use the formalism, we are presenting the main results in the form of expressions that can straightforwardly be computed numerically.

II. FORMALISM

The mathematical foundation of the coherent-state representation can be found in the paper of Hecht [2]. This representation has shown its utility in finding the solutions of quantum mechanical systems by variational and path-integration methods. In this section we will introduce coherent states as trial states in the calculation of partition functions. We have chosen, as illustrative cases, the Lipkin [3] and the Schütte and Da Providencia models [4]. In the first part of this section, we shall briefly review the representation of partition functions, for noninteracting systems, in terms of coherent states. Next, we shall discuss the fermionic and bosonic images of these Hamiltonians, and we shall focus on the variational aspects of the problem. At the end of this section, we shall discuss the RPA approximation in the context of coherent states.

To illustrate the use of coherent states, in the calculation of the partition function in quantum statistical mechanics, let us review the case of M independent oscillators, whose Hamiltonian is written

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$$H=\sum_{k=1}^{M}\omega_k a_k^\dagger a_k. \tag{1}$$

As a trial state we introduce the coherent state

$$|z\rangle=\prod_{k=1}^{M}\sum_{i_k=0}^{\infty}\frac{|z_k|^{2i_k}}{\sqrt{i_k!}}|i_k\rangle, \tag{2}$$

hereafter we shall follow the notation $z=\rho e^{i\phi}$. The expectation value of the unnormalized statistical operator $\hat{\rho}=e^{-\beta H}$ on the trial state $|z\rangle$ reads

$$\langle z|e^{-\beta H}|z\rangle=\prod_{k=1}^{M}\sum_{i_k=0}^{\infty}\frac{|z_k|^{2i_k}}{i_k!}e^{-\beta\omega_k i_k}. \tag{3}$$

The canonical partition function is written

$$Z=\frac{1}{\pi}\int_0^{2\pi}d\phi\int_0^{\infty}d\rho\rho e^{-\rho^2}\langle z|e^{-\beta H}|z\rangle, \tag{4}$$

as an integral on the space of parameters ρ and ϕ. The coherent state $|z\rangle$ obeys the condition

$$1=\frac{1}{\pi}\int_0^{2\pi}d\phi\int_0^{\infty}d\rho\rho e^{-\rho^2}|z\rangle\langle z|, \tag{5}$$

corresponding to the metric $(1/\pi)e^{-\rho^2}$. After performing the integration in Eq. (5), the canonical partition function reads

$$Z=\prod_{k=1}^{M}\frac{1}{1-e^{-\beta\omega_k}}, \tag{6}$$

which, of course, coincides with the well-known result [7] of the Bose-Einstein statistics for a finite number of oscillators. The above results illustrate the convenience in the use of coherent states in performing the statistical sum, and they can be extended in order to describe systems with interacting particles. In the following we shall discuss the structure of the coherent states, proposed as trial states in the sense of Eq. (4), for different Hamiltonians. Generally speaking, we shall focus on the value of the ratio

$$\frac{\langle z|e^{-\beta H}|z\rangle}{\langle z|z\rangle}. \tag{7}$$

A. The Lipkin model

First let us consider the Hamiltonian of the Lipkin model [3], written in terms of the generators of the SU(2) algebra

$$H=2\epsilon S_0-\frac{V}{2}(S_+^2+S_-^2). \tag{8}$$

This Hamiltonian describes the interaction of pairs of fermions moving in two single-particle levels and the operators S_0, S_+, and S_- are written in terms of fermionic variables and their definitions can be found in Ref. [5]. The dimension of the representation is $2\Omega+1$, where Ω is half the degeneracy of the single fermion shell. The operators S_0 and $S_\pm$ obey the commutation relations

$$[S_+,S_-]=2S_0,$$
$$[S_0,S_\pm]=\pm S_\pm. \tag{9}$$

For this case we have chosen, as a trial state, the coherent state

$$|z\rangle=e^{zS_+}|0\rangle=\sum_{n=0}^{2\Omega}z^{*n}\binom{2\Omega}{n}^{1/2}|n\rangle. \tag{10}$$

The state with n fermion pairs is written

$$|n\rangle=N_nS_+^n|0\rangle,\quad S_-|0\rangle=0,$$
$$N_n=\sqrt{\frac{(2\Omega-n)!}{n!(2\Omega)!}}, \tag{11}$$

and the inner product of coherent states is defined by

$$\langle z|z\rangle=(1+\rho^2)^{(2\Omega)}. \tag{12}$$

The metric, in the parametric space (ρ,ϕ), is the following:

$$\frac{(2\Omega+1)}{\pi(1+\rho^2)^{(2\Omega+2)}}. \tag{13}$$

In order to calculate the grand partition function we must determine the multiplicity of the irreducible representations Γ_S for different particle numbers, namely, $0<N\leqslant 4\Omega$. The physical space is spanned by the vectors [5]

$$\{|\epsilon_1k_1,\epsilon_2k_2,\ldots,\epsilon_nk_n\rangle,$$
$$\epsilon_i\in\{1,2\},k_i\in\{1,\ldots,2\Omega+1\},\quad i\in\{1,2,\ldots,n\},$$
$$n\in\{1,2,\ldots,4\Omega\}\}, \tag{14}$$

where $|\epsilon_1k_1,\epsilon_2k_2,\ldots,\epsilon_nk_n\rangle$ represents the fermionic subspace, ϵ_i is the index corresponding to single particle levels, k represents substates, and i stands for the partition with i particles while n is the particle number of the configuration. For the fermionic subspace the number of vectors associated with a system with two levels, each of them with 2Ω substates and with a number of particles varying from 1 to 4Ω, is equal to $2^{4\Omega}$.

The fermionic subspace can be decomposed in terms of invariant and irreducible subspaces. To show this, let us consider a particular distribution of a given number of particles on two levels, with sublevels characterized by numbers ν_1 and ν_2, i.e., ν_1 is the number of sublevels that are occupied by particles in both lower and upper levels, while ν_2 is the number of sublevels that are unoccupied in the lower and upper levels. The quasispin S of the state is determined by the distribution of particles on 2τ sublevels, where $2\tau=2\Omega-\nu_1-\nu_2$. The number of particles in this configuration is $n=2(\tau+\nu_1)$. Let us call $\Gamma_{k_1,k_2,\ldots,k_{2(\tau+\nu_1)}}$ the subspace of states with ν_1 occupied and ν_2 unoccupied sublevels.

The dimension of this subspace is $2^{2\tau}$. They are $(2\Omega)!/[(2\tau)!\nu_1!\nu_2!]$ different subspaces $\Gamma_{k_1,k_2,\ldots,k_{2(\tau+\nu_1)}}$. Each of these subspaces can be decomposed into irreducible ones with multiplicity

$$g_k^\tau=\frac{(2\tau)!}{k!(2\tau-k)!}-\frac{(2\tau)!}{(k-1)!(2\tau-k+1)!}.$$

The exact grand partition function can be written [5]

$$\mathcal{Z}(\beta)=\sum_{\tau\nu_1\nu_2}\frac{2\Omega!}{(2\tau)!\nu_1!\nu_2!}\times\sum_k g_k^\tau\sum_m \exp\{-\beta[E_m^{\tau-k}-2\mu(\tau+\nu_1)]\}, \tag{15}$$

where $E_m^{\tau-k}$ is the energy of the configuration and μ is the Lagrange multiplier that fixes the average number of particles.

The grand partition function in the coherent-state representation is

$$\mathcal{Z}(\beta)=\sum_{\tau\nu_1\nu_2}\frac{2\Omega!}{(2\tau)!\nu_1!\nu_2!}e^{\beta\mu2(\tau+\nu_1)}\sum_k g_k^\tau I_{\tau-k}, \tag{16}$$

where

$$I_{\tau-k}=\frac{[2(\tau-k)+1]}{\pi}\times\int_0^{2\pi}d\phi_\tau\int_0^\infty d\rho_\tau\rho_\tau\frac{\langle z_{\tau-k}|e^{-\beta H}|z_{\tau-k}\rangle}{(1+\rho_\tau^2)^{[2(\tau-k)+2]}}. \tag{17}$$

In the above expression the integration must be performed on each partition, noticing that there is one coherent state per partition.

1. Approximations

So far, the above expressions are exact. In order to perform the integration of Eq. (17) one should, of course, calculate the expectation value of the density operator acting on the coherent state. As a first approximation we shall write the expectation value of the density operator as

$$\langle z_{\tau-k}|e^{-\beta H}|z_{\tau-k}\rangle\approx\exp\left(-\beta\frac{\langle z_{\tau-k}|H|z_{\tau-k}\rangle}{\langle z_{\tau-k}|z_{\tau-k}\rangle}\right), \tag{18}$$

which should be a good approximation for small values of $\beta\epsilon$ (and also of βV).

The exponent on the right-hand side of Eq. (18) can be calculated exactly, leading to the result

$$\frac{\langle z_{\tau-k}|H|z_{\tau-k}\rangle}{\langle z_{\tau-k}|z_{\tau-k}\rangle}=-(\tau-k)2\epsilon\times\left[\frac{1-\rho^2}{1+\rho^2}+\frac{V[2(\tau-k)-1]}{4\epsilon}\times\left(\frac{2\rho}{1+\rho^2}\right)^2\cos(2\phi)\right]. \tag{19}$$

Replacing this result in Eq. (17) and performing the integration on the angular variables one obtains

$$I_{\tau-k}\approx\int_0^\infty 2\rho d\rho\frac{[2(\tau-k)+1]}{(1+\rho^2)^{[2(\tau-k)+2]}}\times\exp\left[\beta(\tau-k)2\epsilon\left(\frac{1-\rho^2}{1+\rho^2}\right)\right]\times\mathcal{I}_0\left[2\beta V(\tau-k)[2(\tau-k)-1]\left(\frac{2\rho}{1+\rho^2}\right)^2\right], \tag{20}$$

where $\mathcal{I}_0(x)=\mathcal{J}_0(ix)$ is a Bessel function [8]. The integration of Eq. (20) can be performed numerically. By a change of variables, $x=\rho^2$ and $y=(1-x)/1+x$, the interval of integration transforms from $0\rightarrow\infty$ to $-1\rightarrow1$, and the argument becomes a product of the form $\approx e^{\alpha y}\times P(y)$, where $\alpha=2\beta\epsilon(\tau-k)$ and $P(y)$ is a polynomial in the variable y. For numerical applications it suffices to expand the Bessel function $\mathcal{I}_0$, keeping leading-order terms. High-order terms are suppressed by the exponent.

As a second approximation we shall write the above expressions starting from a boson image of the Hamiltonian H of Eq. (8). Accordingly, we shall transform the operators $S_\pm$ and S_0 by applying the Dyson boson mapping [9]. We shall then write the Hamiltonian in the Dyson boson basis and define a suitable trial coherent state. The Dyson boson mapping of the generators $S_\pm$ and S_0 leads to

$$S_+\rightarrow b^\dagger[2(\tau-k)-b^\dagger b],$$

$$S_-\rightarrow b,$$

$$S_0\rightarrow b^\dagger b-(\tau-k). \tag{21}$$

The boson operators b and $b^\dagger$ obey the commutation rule

$$[b,b^\dagger]=1. \tag{22}$$

With the definitions of Eq. (21) the boson image of the Hamiltonian can be written

$$H_b=\epsilon[b^\dagger b-(\tau-k)] - \frac{V}{2}\left[[2(\tau-k)]^2\left(1-\frac{1}{2(\tau-k)}\right)b^{\dagger 2}+b^2\right] + V[2(\tau-k)]\left[\left(1-\frac{1}{2(\tau-k)}\right)b^{\dagger 3}b+b^{\dagger 4}b^2\right]. \quad (23)$$

We can define the coherent state

$$|z_{\tau-k}\rangle=\mathcal{N}e^{zS_+}|0\rangle\rightarrow\mathcal{N}e^{z2(\tau-k)b^\dagger}|0\rangle,$$
$$\langle z_{\tau-k}|=\langle 0|e^{z^*b}\mathcal{N}, \quad (24)$$

where $\mathcal{N}$ is a normalization. In this representation the expectation value of bilinear boson operators is written

$$\langle z_{\tau-k}|(b^\dagger)^n(b)^m|z_{\tau-k}\rangle=[2(\tau-k)]^m\rho^{n+m}\times e^{i\phi(n-m)}F_{nm}, \quad (25)$$

where

$$F_{nm}=\sum_{s=0}^{\min[2(\tau-k)-m,2(\tau-k)-n]}\frac{\rho^{2s}}{s!}[2(\tau-k)]^s. \quad (26)$$

With this definition the normalization factor $\mathcal{N}$ can be calculated and the result is

$$\mathcal{N}^{-2}=F_{00}=\sum_{s=0}^{2(\tau-k)}\frac{\rho^{2s}}{s!}[2(\tau-k)]^s = e^{2(\tau-k)\rho^2}\frac{\Gamma[2(\tau-k)+1,2(\tau-k)\rho^2]}{\Gamma[2(\tau-k)+1]}. \quad (27)$$

The expectation value of the boson image of the Hamiltonian is, therefore, written

$$\frac{\langle z_{\tau-k}|H_b|z_{\tau-k}\rangle}{\langle z_{\tau-k}|z_{\tau-k}\rangle}=f_0(\rho,\tau-k)+e^{2i\phi}f_1(\rho,\tau-k) + e^{-2i\phi}f_2(\rho,\tau-k), \quad (28)$$

where

$$f_0(\rho,\tau-k)=2(\tau-k)\epsilon\left(2\rho^2\frac{F_{11}}{F_{00}}-1\right),$$

$$f_1(\rho,\tau-k)=-[2(\tau-k)]^2\frac{V}{2}\rho^2 \times\left[\left(1-\frac{1}{2(\tau-k)}\right)\left(\frac{F_{20}}{F_{00}}-2\rho^2\frac{F_{31}}{F_{00}}\right)+\rho^4\frac{F_{42}}{F_{00}}\right],$$

$$f_2(\rho,\tau-k)=-[2(\tau-k)]^2\frac{V}{2}\rho^2\frac{F_{02}}{F_{00}}. \quad (29)$$

By replacing these results in Eq. (17) we obtain

$$I_{\tau-k}=\int_0^\infty d\rho^2 e^{-\rho^2}\exp\left[-\beta 2(\tau-k)\epsilon\left(\rho^2-\frac{1}{2}\right)\right] \times\mathcal{I}_0(2\beta\sqrt{f_1(\rho,\tau-k)f_2(\rho,\tau-k)}). \quad (30)$$

In this way, we have replaced the sum on the eigenvalues of the Hamiltonian, for all possible representations, by a sum of integrals weighted by the multiplicity of each representation. This is valid both for the fermionic, Eq. (8), and the bosonic, Eq. (23), images of the Hamiltonian.

So far, in the above approximations, we have considered the complete expression of the Hamiltonian and we have introduced coherent states to cast the statistical sum as an integration on the parametric space. We shall next discuss the results of different approximations, which are operative at the level of the Hamiltonian.

2. The Weiss approximation

The Lipkin Hamiltonian may be treated *à la* Weiss [10], by replacing pair operators by their expectation values

$$H\cong 2\epsilon S_0-\frac{V}{2}(\langle S_+\rangle S_+ + \langle S_-\rangle S_-), \quad (31)$$

where $\langle S_\pm\rangle$ is the expectation value of the operator $S_\pm$ on the coherent state $|z\rangle$. These expectation values are written

$$\langle S_+\rangle=2(\tau-k)\frac{\rho e^{-i\phi}}{1+\rho^2},$$

$$\langle S_-\rangle=2(\tau-k)\frac{\rho e^{i\phi}}{1+\rho^2}. \quad (32)$$

The density operator $e^{-\beta H}$ can be written as a product of separable exponential operators, as shown by Hecht [2]. Thus, the integral of Eq. (17) yields

$$I_{\tau-k}=\int_0^\infty 2\rho d\rho\frac{[2(\tau-k)+1]}{(1+\rho^2)^{[2(\tau-k)+2]}}f(\beta,\epsilon,V,\tau), \quad (33)$$

where

$$f(\beta,\epsilon,V,\tau)=\sum_{n=0}^{2(\tau-k)}\rho^{2n}\alpha_0^{n-(\tau-k)}\binom{2(\tau-k)}{n} \times\left[\sum_{m=0}^{2(\tau-k)-n}\binom{2(\tau-k)-m}{m}\binom{m+n}{m} \times(\alpha_-\alpha_+)^m\right]. \quad (34)$$

The quantities α_0, $\alpha_\pm$, γ_0, and γ are the factors entering in the separable form of the density operator

$$\exp(\gamma_0 S_0+\gamma_+S_+ + \gamma_-S_-)=e^{\alpha_-S_-}e^{\alpha_+S_+}e^{\ln(\alpha_0)}, \quad (35)$$

and their explicit expressions are the following:

$$\sqrt{\alpha_0}=\cosh(\gamma)+\frac{\gamma_0}{2\gamma}\sinh(\gamma),$$

$$\alpha_+=\frac{\beta 2(\tau-k)V}{\gamma}\frac{\rho}{1+\rho^2}\sqrt{\alpha_0},$$

$$\alpha_-=\frac{\beta 2(\tau-k)V}{\gamma}\frac{\rho}{1+\rho^2}\frac{1}{\sqrt{\alpha_0}}, \tag{36}$$

with

$$\gamma_0=-\beta\omega_f,$$

$$\gamma_+=-\beta\langle S_+\rangle,$$

$$\gamma_-=-\beta\langle S_-\rangle,$$

$$\gamma_= -\frac{\beta\omega_f}{2}\sqrt{1+\left(\frac{4(\tau-k)V}{(1+\rho^2)\omega_f}\right)^2}. \tag{37}$$

3. Variational approach

The expectation value of the Hamiltonian of Eq. (8) can also be expressed as a functional in the space of parameters of the coherent state

$$|z\rangle=e^{zS_+}|0(\beta)\rangle=\sum_{n=0}^{2\Omega}\frac{z^{*n}}{n!}S_+^n|0(\beta)\rangle. \tag{38}$$

Since

$$\langle 2S_0\rangle=n_2-n_1, \tag{39}$$

where the quantities n_j are the average occupation numbers of each single particle level, the coherent state of Eq. (38) is normalized in the sense of

$$\langle z|z\rangle=\sum_n^{2\Omega}|z|^{2n}\frac{\Gamma(-\langle 2S_0\rangle+1)}{n!\,\Gamma(-\langle 2S_0\rangle-n+1)}\approx(1+|z|^2)^{(n_1-n_2)}. \tag{40}$$

After a straightforward calculation we have obtained, for the expectation value of the Hamiltonian, the expression

$$\frac{\langle z|H-\mu N|z\rangle}{\langle z|z\rangle}=-\epsilon(n_1-n_2)\times\frac{1-\rho^2}{1+\rho^2}-V(n_1-n_2)(n_1-n_2-1)\times\frac{\rho^2}{(1+\rho^2)^2}\cos(2\phi)-\mu(n_1+n_2). \tag{41}$$

A variation of this quantity with respect to ρ and ϕ gives two solutions

$$\langle H\rangle=-\epsilon(n_1-n_2),$$

and

$$\langle H\rangle=-\frac{\Omega\epsilon}{\lambda}\frac{(n_1-n_2)}{(n_1-n_2-1)}-\frac{\epsilon\lambda}{4\Omega}(n_1-n_2)(n_1-n_2-1), \tag{42}$$

with $\lambda=V\Omega/\epsilon$. While ϕ must be equal to zero or π, the values of ρ are limited in the interval $0\leqslant\rho\leqslant\sqrt{(1-\alpha)/1+\alpha}$, with $\alpha=(2\epsilon)/V(n_1-n_2)$. In this interval we found two sets of solutions that correspond to two different phases, whose structure is determined by the occupation numbers and by the excitation energies, as will be discussed next.

The average occupation numbers n_j are determined by the variation of the grand potential

$$\Xi=\langle H-\mu N\rangle-TS, \tag{43}$$

where

$$TS=-\frac{1}{\beta}\sum_j 2\Omega_j[n_j\ln n_j+(1-n_j)\ln(1-n_j)], \tag{44}$$

such that

$$\frac{\delta\Xi}{\delta n_i}=0. \tag{45}$$

The above variation leads to two phases, namely, the normal phase, where

$$n_j=\frac{2\Omega}{1+\exp(\beta E_j)},$$

$$E_1=-\mu-\epsilon,$$

$$E_2=-\mu+\epsilon, \tag{46}$$

and the deformed one, where

$$n_j=\frac{2\Omega}{1+\exp(\beta E_j)},$$

$$E_1=-\mu-\epsilon\lambda\frac{\left(n_1-n_2-\frac{1}{2}\right)}{2\Omega}+\frac{\epsilon\Omega}{(n_1-n_2-1)^2\lambda},$$

$$E_2=-\mu+\epsilon\lambda\frac{\left(n_1-n_2-\frac{1}{2}\right)}{2\Omega}-\frac{\epsilon\Omega}{(n_1-n_2-1)^2\lambda}. \tag{47}$$

As usual, the Lagrange multiplier μ is fixed by the particle number condition

$$N=n_1+n_2. \tag{48}$$

The transition between both phases takes place at the critical temperature

$$T_c=\epsilon\left[\ln\left(\frac{2\Omega(\lambda+1)+\lambda}{2\Omega(\lambda-1)+\lambda}\right)\right]^{-1}, \tag{49}$$

for the case $N=2\Omega$.

B. The Schütte and Da Providencia model

The techniques of Sec. II A can be applied to the treatment of interactions between fermions and bosons. In this section we shall work with the Hamiltonian [4]

$$H=\omega_f(S_0+\Omega)+\omega_b b^\dagger b+G(S_+b^\dagger+S_-b), \tag{50}$$

where $S_\pm$ and S_0 are the fermion operators defined in Eq. (9) and $b^\dagger$ (b) is a boson creation (annihilation) operator.

This is the Hamiltonian introduced by Schütte and Da Providencia to describe fermion-boson interactions, and it has been applied successfully to cases of physical interest [11]. In the next two sections we shall introduce trial coherent states to calculate the matrix elements of the density operator corresponding to this Hamiltonian, in the exponential and variational approaches.

1. Approximations

As a convenient ansatz we have chosen the coherent state as

$$|z\rangle=e^{z_f^* S_+}e^{z_b^* b^\dagger}|0\rangle=\sum_{l=0}^{\infty}\frac{(z_b^*)^l}{\sqrt{l!}}\sum_{n=0}^{2\Omega}z_f^{*n}\binom{2\Omega}{n}^{1/2}|nl\rangle. \tag{51}$$

This form implies the use of fermionic and bosonic parameters, i.e., $z_{f(b)}=\rho_{f(b)}e^{i\phi_{f(b)}}$. The state $|0\rangle$ is the vacuum, such that $S_-|0\rangle=b|0\rangle=0$. The other elements of the definition of $|z\rangle$ are

$$|nl\rangle=N_{nl}S_+^n b^{\dagger l}|0\rangle,$$

and

$$N_{nl}=\sqrt{\frac{(2\Omega-n)!}{n!l!(2\Omega)!}}.$$

The state $|z\rangle$ is normalized

$$\langle z|z\rangle=(1+\rho_f^2)^{(2\Omega)}e^{\rho_b^2}. \tag{52}$$

In this case the metric is defined as the product of fermionic and bosonic factors

$$\frac{(2\Omega+1)}{\pi(1+\rho_f^2)^{(2\Omega+2)}}\frac{e^{-\rho_b^2}}{\pi}. \tag{53}$$

As discussed in the previous section the expectation value of the density operator on coherent states can be written as

$$\langle z_{\tau-k}|e^{-\beta H}|z_{\tau-k}\rangle\approx\exp\left(-\beta\frac{\langle z_{\tau-k}|H|z_{\tau-k}\rangle}{\langle z_{\tau-k}|z_{\tau-k}\rangle}\right), \tag{54}$$

and for the state, Eq. (51), one gets

$$\frac{\langle z_{\tau-k}|H|z_{\tau-k}\rangle}{\langle z_{\tau-k}|z_{\tau-k}\rangle}=2(\tau-k)w_f\frac{\rho^2}{1+\rho_f^2}+w_b\rho_b^2+4\Omega G\frac{\rho_b\rho_f}{1+\rho_f^2}\cos(\phi_b+\phi_f). \tag{55}$$

With this expression the integral $I_{\tau-k}$, of Eq. (17), is written as

$$I_{\tau-k}=\frac{[2(\tau-k)+1]}{1+\beta\omega_b}\int_0^\infty d\rho_f^2\frac{\exp\left(-2(\tau-k)\beta\omega_f\frac{\rho_f^2}{1+\rho_f^2}\right)\left(1-\frac{2(\tau-k)G^2\beta}{\omega_f(1+\omega_b\beta)}\frac{\rho_f^2}{1+\rho_f^2}\right)}{(1+\rho_f^2)^{(2(\tau-k)+2)}}. \tag{56}$$

The form of this integral can be simplified, by changing the integration variable, as done with the integral of Eq. (20), and the resulting integral can easily be computed numerically.

As done with the Lipkin Hamiltonian (Sec. II A 1), the Dyson boson image of the Hamiltonian of Eq. (50) is constructed by transforming pairs of fermions as

$$S_+\to b_f^\dagger[2(\tau-k)-b_f^\dagger b_f],$$
$$S_-\to b_f,$$
$$S_0\to b_f^\dagger b_f-(\tau-k), \tag{57}$$

where

$$[b_f,b_f^\dagger]=1. \tag{58}$$

The transformed Hamiltonian is, therefore, written as

$$H_b=\omega_f b_f^\dagger b_f+\omega_b b^\dagger b+G[2(\tau-k)b_f^\dagger b^\dagger+b_f b-b_f^{\dagger 2}b_f b^\dagger]. \tag{59}$$

In this representation the trial coherent state has the form

$$|z_{\tau-k}\rangle=\mathcal{N}\exp(z_f S_++z_b b^\dagger)|0\rangle\to\mathcal{N}\exp[z_f 2(\tau-k)b_f^\dagger+z_b b^\dagger]|0\rangle, \tag{60}$$

noticing that the transformation is a non-Hermitian one the coherent state is normalized as

$$\mathcal{N}^{-2}=e^{\rho_b^2}e^{2(\tau-k)\rho_f^2}\frac{\Gamma[2(\tau-k)+1,2(\tau-k)\rho_f^2]}{\Gamma[2(\tau-k)+1]}. \quad (61)$$

With these definitions, the expectation value of the Hamiltonian reads

$$\frac{\langle z_{\tau-k}|H_b|z_{\tau-k}\rangle}{\langle z_{\tau-k}|z_{\tau-k}\rangle}=2(\tau-k)\omega_f\left(\rho_f^2\frac{F_1}{F_0}-\frac{1}{2}\right)+\omega_b\rho_b^2+2(\tau-k)\times G\rho_f\rho_b e^{i(\phi_f+\phi_b)}+2(\tau-k)\times G\rho_f\rho_b e^{-i(\phi_f+\phi_b)}\left(1-\rho_f^2\frac{F_1}{F_0}\right), \quad (62)$$

with

$$F_0=\frac{e^{2(\tau-k)\rho_f^2}}{[2(\tau-k)]!}\frac{\Gamma[2(\tau-k)+1,2(\tau-k)\rho_f^2]}{\Gamma[2(\tau-k)+1]},$$

$$F_1=\frac{e^{2(\tau-k)\rho_f^2}}{[2(\tau-k)-1]!}\frac{\Gamma[2(\tau-k),2(\tau-k)\rho_f^2]}{\Gamma[2(\tau-k)+1]}. \quad (63)$$

In this case the integral $I_{\tau-k}$ is given by the following expression:

$$I_{\tau-k}=\frac{1}{1+\beta\omega_b}\int_0^\infty d\rho_f^2\exp\left[-2(\tau-k)\beta\omega_f\left(\rho_f^2\frac{F_1}{F_0}-\frac{1}{2}\right)\right]\times\exp\left[\frac{[2(\tau-k)G\beta\rho_f]^2}{1+\beta\omega_b}\left(1-\rho_f^2\frac{F_1}{F_0}\right)\right]. \quad (64)$$

2. Variational approach

The Hamiltonian of Eq. (50) can be treated in a variational approach, as described in Sec. II A 3 but with the coherent state written as a product of fermion and boson operators. We shall define the coherent state as

$$|z\rangle=e^{z_f S_+}e^{z_b b^\dagger}|0(\beta)\rangle, \quad (65)$$

and with it we shall calculate the matrix elements of the Hamiltonian. The coherent state is normalized by the inner product

$$\langle z|z\rangle=(1+\rho_f^2)^{2\Omega(n_1-n_2)}e^{\rho_b^2(1+n_b)}, \quad (66)$$

as before the occupation numbers n_j and n_b are determined from the variation of the grand potential Ξ.

The expectation value of the Hamiltonian on these coherent states is given by

$$\frac{\langle z|H-\mu N|z\rangle}{\langle z|z\rangle}=-\omega_f\Omega(n_1-n_2)\times\frac{1-\rho_f^2}{1+\rho_f^2}+\omega_b[n_b+\rho_b^2(1+n_b)^2]+G4\Omega(n_1-n_2)(1+n_b)\times\frac{\rho_f\rho_b}{(1+\rho_f^2)^2}\cos(\phi_f+\phi_b). \quad (67)$$

The variation of the above ratio with respect to ρ_f, ρ_f, ϕ_f, and ϕ_b gives

$$-\omega_f\Omega(n_1-n_2-1)+\omega_b n_b, \quad (68)$$

for the normal phase, and

$$\omega_b n_b-\Omega\omega_f\left(\frac{\chi^2}{2}(n_1-n_2)^2+\frac{1}{2\chi^2}-1\right), \quad (69)$$

for the deformed phase with $\chi=G\sqrt{2\Omega/(\omega_f\omega_b)}$. As shown in Sec. II A 3 the occupation numbers are determined from the minimization of the grand potential Ξ. The corresponding results are

$$n_j=\frac{1}{1+\exp(\beta E_j)},$$

$$E_1=-\mu-\frac{\omega_f}{2},$$

$$E_2=-\mu+\frac{\omega_f}{2}, \quad (70)$$

for the normal phase, and

$$n_j=\frac{1}{1+\exp(\beta E_j)},$$

$$E_1=-\mu-\frac{\omega_f}{2}\chi^2(n_1-n_2),$$

$$E_2=-\mu+\frac{\omega_f}{2}\chi^2(n_1-n_2), \quad (71)$$

for the deformed phase.

The Lagrange multiplier μ is fixed by the number equation

$$N=n_1+n_2. \quad (72)$$

C. Coherent states and the RPA

The Hamiltonian of Eq. (1) describes free bosons and also the linear (RPA) version of a Hamiltonian with interactions, regardless of the fermionic or bosonic nature of the elementary degrees of freedom. In this linear form

$$H_{RPA}=H_0+\omega\Gamma^\dagger\Gamma. \tag{73}$$

The phonon operators $\Gamma^\dagger$ and Γ obey boson commutation rules, and they are written as superposition of pairs of fermions or bosons [12]. Therefore, we can think of a coherent state of the form $|z\rangle=e^{z\Gamma^\dagger}|0\rangle$ and proceed to calculate the partition function as done at the beginning of Sec. II. In this fashion Eq. (6) yields the result

$$Z_{RPA}=e^{-\beta H_0}\frac{1}{1-e^{-\beta\omega}}. \tag{74}$$

This shows again the convenience in the use of coherent states in performing the statistical sum. Next we shall show how this procedure applies for the cases of the Lipkin's and the Schütte and Da Providencia's models.

1. The Lipkin model

The Hamiltonian of Eq. (8) has two solutions: (i) the normal solution, which is valid at temperatures $T>T_c$, and (ii) the deformed one, which is valid for $T<T_c$. The critical temperature T_c is determined by the condition

$$\chi\tanh\left(\frac{\epsilon}{2T}\right)\bigg|_{T=T_c}=1. \tag{75}$$

In the normal phase the constant H_0 of Eq. (73) has the form

$$H_0=-\omega_f\Omega\tanh\left(\frac{\epsilon}{2T}\right)-\frac{1}{2}(2\epsilon-\omega),$$

with the RPA eigenvalue

$$\omega=\omega_f\sqrt{1-\left[\frac{2\Omega}{2\Omega-1}\chi\tanh\left(\frac{\epsilon}{2T}\right)\right]^2}. \tag{76}$$

In the deformed phase the corresponding values are

$$H_0=-\omega_f\Omega\left[\frac{1}{2\chi}+\frac{\chi}{2}\tanh\left(\frac{E}{2T}\right)^2\right]-\frac{1}{2}(2E-\omega), \tag{77}$$

which is the constant appearing in Eq. (73), and

$$\omega=2E\sqrt{1-\left(\frac{\Omega}{2\Omega-1}\right)^2\left(1+\frac{1}{\left[\chi\tanh\left[\left(\frac{E}{2T}\right)\right]^2\right]}\right)^2}, \tag{78}$$

which is the RPA eigenvalue, and

$$E=\frac{\omega_f}{2}\chi\tanh\left(\frac{\epsilon}{2T}\right), \tag{79}$$

which is the fermion excitation energy.

These expressions, for the RPA eigenvalue ω and for the ground-state energy H_0, determine the value of Z_{RPA}, Eq. (74), in an unique way in spite of the normal or deformed character of the solution.

2. The Schütte and Da Providencia model

The Schütte and Da Providencia model, when treated in the same way, has a solution that exhibits a phase transition at the critical temperature T_c, such that

$$\chi^2\tanh\left(\frac{\omega_f}{4T}\right)\bigg|_{T=T_c}=1, \tag{80}$$

where ω_f is the energy of a pair of fermions. The constant H_0, for this model, has the form

$$H_0=-\omega_f\Omega\tanh\left(\frac{\omega_f}{4T}\right)+\omega_f\Omega+\omega_b n_b-\frac{1}{2}(2\epsilon-\omega). \tag{81}$$

The RPA eigenvalue is given by

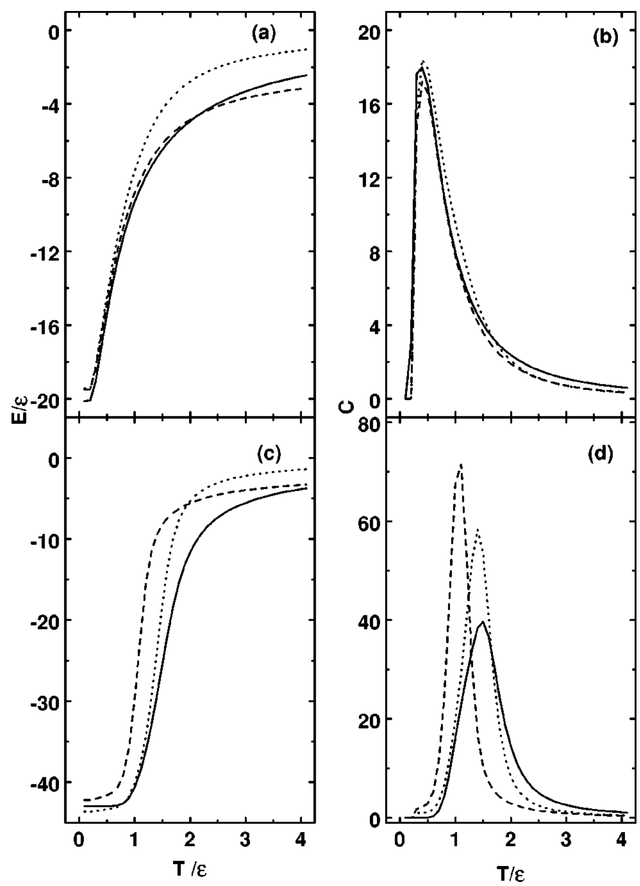

FIG. 1. Results for the Lipkin model. The mean value of the energy E/ϵ scaled by the single particle energy ϵ and the specific heat C as functions of the scaled temperature T/ϵ. The upper boxes, (a) and (b), are the results corresponding to the normal phase. Cases (c) and (d) correspond to the deformed phase. The exact solution of the model is shown with solid lines. Dashed and dotted lines correspond to the exponential solution of Eq. (18) and to the Dyson boson expansion of Eq. (21), respectively. The parameters of the model are $\Omega=10$, $N=20$, and $\epsilon=0.5$ MeV. The coupling constant $\chi=V(2\Omega-1)/2\epsilon$, was fixed at the value $\chi=0.5$ (normal solution, upper boxes), and $\chi=4$ (deformed solution, lower boxes).

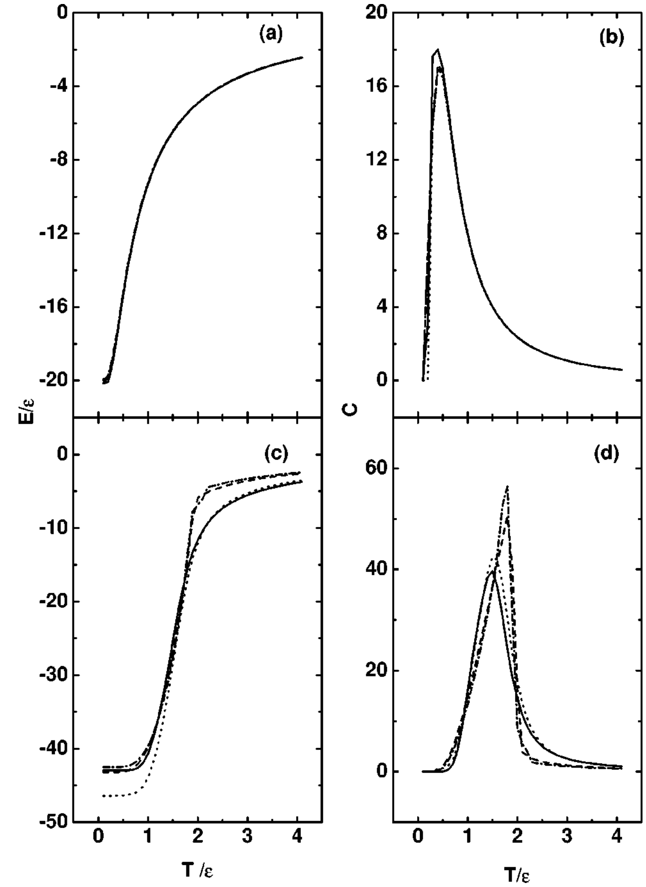

FIG. 2. Results for the Lipkin model. The mean value of the energy, E/ϵ, scaled by the single particle energy ϵ and the specific heat C as functions of the scaled temperature T/ϵ. The upper boxes, (a) and (b), are the results corresponding to the normal phase. Cases (c) and (d) correspond to the deformed phase. The exact results are shown with solid lines. Dashed lines are the results of the RPA approximation, dotted-lines correspond to the Weiss approximation, and dashed-dotted lines shows the results of the variational approach, respectively. The parameters of the model are given in the caption of Fig. 1.

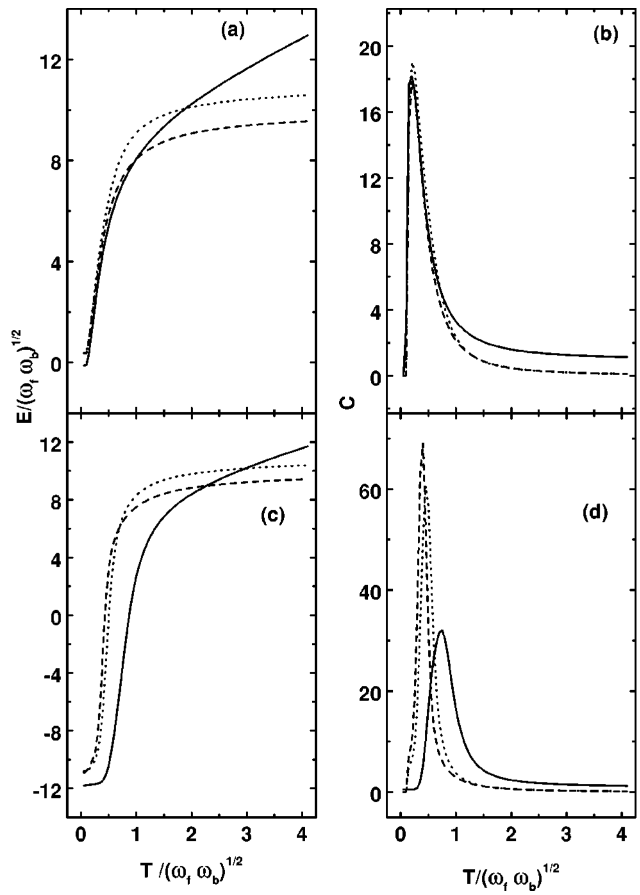

FIG. 3. Results for the Schütte and Da Providencia model. The mean value of the energy $E/(\omega_f\omega_b)^{(1/2)}$ scaled by the product of the fermion and boson energies, and the specific heat C as functions of the scaled temperature $T/(\omega_f\omega_b)^{(1/2)}$. The upper boxes, (a) and (b), are the results corresponding to the normal phase. Cases (c) and (d) correspond to the deformed phase. The exact solution of the model is shown with solid lines. Dashed and dotted lines correspond to the exponential solution of Eq. (56) and to the Dyson boson expansion of Eq. (64), respectively. The parameters of the model are $\Omega=10$, $N=20$, $\omega_f=1$ MeV, and $\omega_b=1$ MeV. The coupling constant $\chi=G\sqrt{(2\Omega)/\omega_f\omega_b}$ was fixed at the value $\chi=0.5$ (normal solution, upper boxes) and $\chi=2$ (deformed solution, lower boxes).

$$\omega=\frac{1}{2}|\omega_f-\omega_b|+\frac{1}{2}\sqrt{(\omega_f+\omega_b)^2-4\omega_f\omega_b\chi^2\tanh\left(\frac{\omega_f}{4T}\right)} \tag{82}$$

in the normal phase. The corresponding expressions for the deformed regime are given by

$$H_0=-\omega_f\Omega\left[\frac{1}{\chi^2}+\chi^2\tanh\left(\frac{E}{2T}\right)\right]+\omega_f\Omega+\omega_b n_b-\frac{1}{2}(2E-\omega),$$

$$\omega=\frac{1}{2}\sqrt{E^2+\omega_b^2-2\omega_f\omega_b},$$

and

$$E=\frac{\omega_f}{2}\chi^2\tanh\left(\frac{E}{2T}\right), \tag{83}$$

which are the constant term, the eigenvalue, and the fermion excitation energy, respectively. The boson occupation number is defined as

$$n_b=\frac{1}{e^{(\omega_b/T)}-1}. \tag{84}$$

With these elements the partition function is written in the form of Eq. (74).

In the next section we shall apply the results presented in this section, to illustrate the convenience of the method.

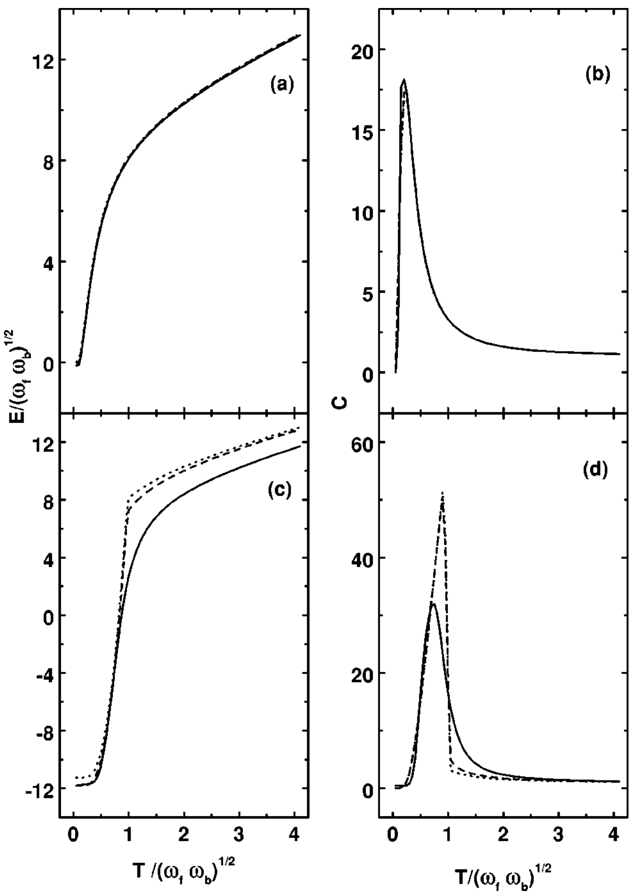

FIG. 4. Results for the Schütte and Da Providencia model. The mean value of the energy $E/(\omega_f\omega_b)^{(1/2)}$ scaled by the product of the fermion and boson energies, and the specific heat C as functions of the scaled temperature $T/(\omega_f\omega_b)^{(1/2)}$. The upper boxes, (a) and (b), are the results corresponding to the normal phase. Cases (c) and (d) correspond to the deformed phase. The exact solution of the model is shown with solid lines. Dashed lines represent the results of the RPA treatment and with dotted lines we have represented the results of the variational approach. The parameters of the model are given in the caption of Fig. 2.

III. RESULTS AND DISCUSSION

We have applied the expressions obtained in the previous section to calculate the partition function for the considered Hamiltonians. For the case of the Lipkin model, the parameters have been fixed at the values $2\epsilon=1$ MeV, $\Omega=10$, and $N=20$ particles. We have defined $\chi=V(2\Omega-1)/2\epsilon$ as the dimensionless strength of the interaction. We have chosen the values $\chi=0.5$ and $\chi=4$ to represent solutions in the normal and deformed phases, respectively. Figure 1 shows the results corresponding to the energy and the specific heat, calculated with the partition function obtained by using the various approximations discussed in the text. Figures 1(a) and 1(b) correspond to the normal phase ($\chi=0.5$) and Fig. 1(c) and Fig. 1(d) correspond to the deformed phase ($\chi=4$). The exact solution, both for the energy and for the specific heat, is shown together with the results obtained by using the exponential approximation and the Dyson boson mapping approximation. The results of these approximations agree rather well in the normal phase, although the exponential approximation of Eq. (20) is closer to the exact result. The Dyson boson mapping approximation seems to agree with the exact result better than the exponential approach in the deformed phase. Notice that in all cases the use of the coherent states facilitates the otherwise cumbersome summation on the eigenstates of the Hamiltonian. Concerning the other approximations introduced in the text, the results are displayed in Fig. 2. One can see that the approximations that go beyond the mean field yield a better agreement, both in the normal and in the deformed phases. For the case of the normal phase the results nearly coincide with the exact ones. Concerning the deformed phase the Weiss approximation gives better results at higher values of the scaled temperature. These features are also exhibited by the results corresponding to the model of Schütte and Da Providencia. Figure 3 shows the results corresponding to the mean-field-type of approximations, while Fig. 4 shows the results corresponding to the approximations which go beyond the mean field. Again, for these cases the exact solutions are nearly reproduced by some of the approximations. Notice that in all cases the use of coherent states, as trial states, has shown its power in spite of the complications posed by the statistical sum. Also, a very characteristic feature of the statistical mechanics of systems with discrete spectrum, e.g., the Schottky effect [13,14], present in both the Lipkin and the Schütte and Da Providencia model, becomes manifest when coherent states are used to calculate partition functions. This is clearly shown by the calculated specific heat, for both models, as depicted in the figures.

IV. CONCLUSIONS

In this work we have introduced coherent states to calculate the partition function and related derivatives, like the mean value of the energy and the specific heat, associated to fermion and boson Hamiltonians. We have taken the Hamiltonians of the Lipkin and the Schütte and Da Providencia models, which have been studied intensively in the literature.

In addition to the use of coherent states we have also performed mean field and RPA-like approximations. For the case of the mean-field approaches the Dyson boson mapping appears to be a rather good approximation, while in the case of approximations that go beyond the mean field, the variational approach did show its power in reproducing exact values. Because in realistic situations, one does not have exact solutions at hand, one should necessarily rely upon approximations. From the comparison shown in the present work we strongly support the use of coherent states in the statistical treatment of realistic Hamiltonians, since for them exact solutions are not always available.

ACKNOWLEDGMENTS

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