Generalized statistical self-consistent approach

R. Rossignoli and A. Plastino
Physics Department, National University, 1900 La Plata, Argentina
(Received 20 January 1988)

A general self-consistent approximation for statistical operators is introduced. The scheme reduces to a statistical mean-field description when applied to the case of single-particle observables. The present, quite general context allows, however, the examination of the approach from a different perspective, and enables the straightforward construction of higher order self-consistent approximations.

I. INTRODUCTION

The mean-field approximation constitutes one of the most important tools for dealing with complex many-body systems, and it certainly offers a quite favorable starting point for more accurate (and usually rather involved) treatments. In this paper we wish to carefully examine some interesting details connected with the statistic mean-field approach (i.e., thermal Hartree-Fock[1] and, in general, thermal Hartree-Fock-Bogoliubov[2,3]) that allow for a natural extension to more elaborate frameworks.[4–6]

The basic idea is to base the description of a system on a particular set of operators, chosen by the observer, in order to deal with a tractable density operator. In this way, observables considered relevant for the phenomenon being studied are expressed in terms of a given subset of variables, simplifying the description. The approach proposed in this work constitutes the extension of thermal mean-field treatments to general off equilibrium situations, and to arbitrary density operators.

The most general mean-field approach is obtained in that case in which the chosen set of observables is formed by one-body operators. In particular, we shall be able to build mean-field descriptions from the sole knowledge of an arbitrary set of appropriate expectation values, and to find the corresponding effective temperatures and Lagrange multipliers.

The paper is organized as follows: In Sec. II we review the general statistical description of a quantum system, based on information theory.[4–6] In Sec. III we derive, as the *leit-motiv* of this effort, a general self-consistent approach for statistical operators. The formalism is applied in Sec. IV to single-particle fermion operators, as a special example, and is illustrated in Sec. V with reference to a nontrivial, exactly solvable many fermion model. Finally, some conclusions are drawn in Sec. VI.

II. STATISTICAL DESCRIPTION OF A QUANTUM SYSTEM

Let us consider a quantum system about which the observer possesses as sole information the expectation values O_i of m arbitrary observables $\hat{O}_i$ (linearly independent). The appropriate density or statistical operator $\hat{\rho}$ is obtained by maximizing the information entropy[4–6] (we assume $k_\beta=1$)

$$S=-\mathrm{Tr}(\hat{\rho}\ln(\hat{\rho}))\ , \tag{2.1}$$

subject to the m constraints

$$\langle \hat{O}_i\rangle=\mathrm{Tr}(\hat{\rho}\hat{O}_i)=O_i,\quad i=1,\ldots,m\ . \tag{2.2}$$

The result can be attained by maximizing the magnitude

$$S'=S+\sum_{i=1}^{m}\lambda_i O_i\ , \tag{2.3}$$

where λ_i are Lagrange multipliers which must be appropriately determined in order to comply with (2.2). The well-known result is[4–6]

$$\hat{\rho}=\exp\left[\lambda_0+\sum_{i=1}^{m}\lambda_i\hat{O}_i\right]\ , \tag{2.4}$$

where λ_0 is a normalization constant,

$$\lambda_0=-\ln\left\{\mathrm{Tr}\left[\exp\left[\sum_{i=1}^{m}\lambda_i\hat{O}_i\right]\right]\right\}\ . \tag{2.5}$$

Using (2.4), S and S' acquire the expressions

$$S=-\lambda_0-\sum_{i=1}^{m}\lambda_i O_i\ , \tag{2.6a}$$

$$S'=-\lambda_0\ . \tag{2.6b}$$

The following important properties can be shown to be satisfied:[4–6]

$$\frac{\partial S}{\partial O_i}=-\lambda_i\ , \tag{2.7a}$$

$$\frac{\partial S'}{\partial \lambda_i}=O_i\ , \tag{2.7b}$$

where S' is considered a function of the m parameters λ_i, while S of the m expectation values O_i.

Equations (2.7a) or (2.7b) can be employed in order to connect Lagrange multipliers with expectation values. Equation (2.7a) can be utilized to verify the stationary character of the density operator (2.4). Expanding $\ln(\hat{\rho})$ in a complete basis of observables,

$$\hat{\rho}=\exp\left[\lambda_0+\sum_{i=1}^{n}\lambda_i\hat{O}_i\right], \tag{2.8}$$

where $\{\hat{O}_i,\ i=m+1,\ldots,n\}$ denote a complementary set of operators needed to span the complete space, the maximization of S subject to the constraints (2.2) can be accomplished by taking as variational parameters the unknown mean values O_i, $i>m$. By virtue of (2.7a), we attain $\lambda_i=0$, for $i>m$.

If the expectation values O_i, $i=1,\ldots,m$, are linearly independent and physically meaningful (i.e., feasible values in quantum mechanics), the solution (2.4) can be proved to be unique. Pure states correspond to $\hat{\rho}^2=\hat{\rho}$, and can be accommodated as the limit when the parameters λ_i tend to $\pm\infty$. We should remark that the observables $\hat{O}_i$ are completely arbitrary in this formalism, so that the operator (2.4) is not necessarily stationary. For more detailed discussions and interesting elaborations concerning the above outlined approach, the reader is referred to the comprehensive monograph of Ref. 6, and also to Refs. 7–11.

III. A GENERAL SELF-CONSISTENT APPROACH

We present now the main results of the present effort. In general, the exact statistical operator $\hat{\rho}$ (2.4) may be intractable. The connection between the λ_i's and the O_i's is not quite simple, and often requires the diagonalization of $\ln(\hat{\rho})$, which amounts to a very heavy numerical task, if the number of accessible states over which the traces are taken is large. Besides, inferred mean values of arbitrary operators are not easily dealt with, when using (2.4). Therefore, we will consider, as the essential ingredient to be dealt with in this work, an approximate solution for $\hat{\rho}$ in which we restrict it to the form

$$\hat{\rho}_{\text{app}}=\exp\left[\lambda_0+\sum_{j=1}^{k}\lambda_j\hat{P}_j\right], \tag{3.1}$$

where $\{\hat{P}_j,\ j=1,\ldots,k,k\geq m\}$, is a chosen set of operators picked up by the observer, in order to build up a tractable $\hat{\rho}$. However, let us assume that the avaliable experimental data still consist of the expectation values (2.2). Our idea is now to choose, as the best $\hat{P}_{\text{app}}$, that which maximizes the (approximate) entropy

$$S_{\text{app}}=-\text{Tr}[\hat{\rho}_{\text{app}}\ln(\hat{\rho}_{\text{app}})]=-\lambda_0-\sum_{j=1}^{k}\lambda_jP_j, \tag{3.2}$$

subject to the constraints

$$\text{Tr}(\hat{\rho}_{\text{app}}\hat{O}_i)=O_i,\quad i=1,\ldots,m. \tag{3.3}$$

Our problem revolves now about the stationary character of the quantity

$$S'=-\left[\lambda_0+\sum_{j=1}^{k}\lambda_jP_j\right]+\sum_{i=1}^{m}\beta_iO_i. \tag{3.4}$$

Taking as variational parameters the quantities P_j, we attain, by means of (2.7a),

$$0=\frac{\partial S'}{\partial P_j}=-\lambda_j+\sum_{i=1}^{m}\beta_i\frac{\partial O_i}{\partial P_j}. \tag{3.5}$$

Therefore,

$$\lambda_j=\sum_{i=1}^{m}\beta_i\frac{\partial O_i}{\partial P_j}, \tag{3.6}$$

and

$$\hat{\rho}_{\text{app}}=\exp\left[\lambda_0+\sum_{i=1}^{m}\beta_i\hat{o}_i\right], \tag{3.7}$$

where we have defined the "effective" operators

$$\hat{o}_i=\sum_{j=1}^{k}\frac{\partial O_i}{\partial P_j}\hat{P}_j, \tag{3.8}$$

which are linear combinations of operators of the chosen set, but with coefficients which depend upon the mean values P_j. $\hat{o}_i$ can be interpreted as the projection[12,13] of $\hat{O}_i$ onto the subspace spanned by the P_j's (see also Refs. 6 and 7).

By means of the property[14] [λ_o is considered a function of the remaining λ's through (2.5)]

$$\frac{\partial\hat{\rho}_{\text{app}}}{\partial\lambda_j}=\hat{\rho}_{\text{app}}\hat{P}_j^*, \tag{3.9}$$

with

$$\hat{P}_j^*=\int_0^1(\hat{\rho}_{\text{app}})^{-u}\hat{P}_j(\hat{\rho}_{\text{app}})^u du-\text{Tr}(\hat{\rho}_{\text{app}}\hat{P}_j), \tag{3.10}$$

the coefficients in (3.8) can be explicitly written as

$$\frac{\partial O_i}{\partial P_j}=\sum_l F_{il}G_{lj}^{-1}, \tag{3.11}$$

where

$$F_{il}=\frac{\partial O_i}{\partial\lambda_l}=\langle\hat{P}_l^*\hat{O}_i\rangle=\langle\hat{O}_i^*\hat{P}_l\rangle, \tag{3.12}$$

$$G_{jl}=\frac{\partial P_j}{\partial\lambda_l}=\langle\hat{P}_l^*\hat{P}_j\rangle=\langle\hat{P}_j^*\hat{P}_l\rangle. \tag{3.13}$$

The expression (3.7) is a formal solution for $\hat{\rho}_{\text{app}}$. We are thus led to a nonlinear system, since $\hat{\rho}_{\text{app}}$ depends on the mean values P_j that it determines (self-consistency), i.e.,

$$\text{Tr}(\hat{\rho}_{\text{app}}\hat{P}_j)=P_j,\quad j=1,\ldots,k. \tag{3.14}$$

The exception occurs if all operators $\hat{O}_i$ are linearly related to the $\hat{P}_j$'s in which case (3.8) implies

$$\sum_j\lambda_j\hat{P}_j=\sum_i\beta_i\hat{O}_i, \tag{3.15}$$

and the approximation becomes exact, so that we regain the familiar (information-theoretical) ground.

Since system (3.14) is of a nonlinear character, more than one solution may exist for fixed parameters β_i's, and not all of them will correspond to maxima of S'. Certainly, minima and saddle points will occur, as opposed to what happens in the case of the exact solution.

On the other hand, for fixed mean values O_i, the β_i's must be determined from (3.3), and will not, in general, coincide with the exact parameters λ_i's entering (2.4). In this case, the β_i's should be interpreted as effective Lagrange multipliers, i.e., the parameters for which the self-consistent solution yields the same predictions for the O_i's as the exact density operator. A general solution will not always exist in this case, since the range of mean values O_i spanned by (3.1) may be smaller than the exact one. At the same time, the nonlinearity may give rise to various simultaneous solutions for the β_i's, the best of which is in principle that which yields the highest entropy (see Sec. V).

The standard way to solve system (3.14), other than a direct maximization of S or S', is the iterative procedure

$$P_j^{i+1}=\mathrm{Tr}(\hat{\rho}^i_{\mathrm{app}}\hat{P}_j),\quad j=1,\ldots,k\ , \tag{3.16}$$

starting with an initial set of mean values P_j^0, with which $\hat{\rho}^0_{\mathrm{app}}$ is constructed via (3.8). The iteration is continued until self-consistency is reached, i.e., convergence in the mean values P_j. The procedure obviously converges if the self-consistent solution is a stable attractor, and if the initial chosen values lie in its basin of attraction.

It is worthwhile to notice that the important relationships (27a) and (27b) still hold within this approximation, i.e.,

$$\frac{\partial S}{\partial O_i}=-\beta_i\ , \tag{3.17a}$$

$$\frac{\partial S'}{\partial \beta_i}=O_i\ , \tag{3.17b}$$

due to the stationary condition (3.5), although λ_0 ceases to be, in general, identical with $-S'$,

$$S'=-\lambda_0-\sum_{i=1}^{m}\beta_i\langle\hat{o}_i-\hat{O}_i\rangle\ . \tag{3.18}$$

Moreover, the quantity $\partial S/\partial\beta_i$ is not identical with the sum of fluctuations $-\sum_j\beta_j(\langle\hat{O}_j\hat{O}_i\rangle-O_jO_i)$, contrary to what happens in the exact picture.

The present general self-consistent approach yields a lower bound to S and S' for fixed values of the O_i's and β_i's, respectively, if traces are taken over the same space used in the exact description, since we are restricting the maximization procedure to a particular set of density operators. It provides us with an instantaneous approximate description of the system in terms of the operators $\hat{P}_j$.

IV. GENERALIZED STATISTICAL MEAN-FIELD APPROACH

We shall examine in this section the important situation in which the chosen set of Eq. (3.1) consists of single-particle (s.p.) fermion operators, in order to reobtain some well-known results that arise as a special case of our more general treatment. The approximation becomes thus equivalent to a mean-field approach, embedded within a completely general statistical context. The most general density operator constructed with s.p. operators will be of the form (see also Refs. 7 and 11)

$$\hat{\rho}=\exp\left\{\lambda_0+\sum_{i,j}[\lambda_{ij}c_i^\dagger c_j+\tfrac{1}{2}(\gamma_{ij}c_ic_j+\gamma_{ij}^*c_j^\dagger c_i^\dagger)]\right\}\ , \tag{4.1}$$

where $c_i^\dagger$ (c_i) creates (annihilates) a fermion in the state labeled by the quantum number i. The Hermiticity of $\hat{\rho}$ implies $\lambda_{ij}=\lambda_{ji}^*$ and we can set $\gamma_{ij}=-\gamma_{ji}$. Defining an Hermitic matrix M of multipliers

$$M=\begin{bmatrix}\Lambda & -\Gamma^*\\ \Gamma & -\Lambda^*\end{bmatrix}\ , \tag{4.2}$$

such that $\Lambda_{ij}=\lambda_{ij}$, $\Gamma_{ij}=\gamma_{ij}$, the operator (4.1) can be rewritten as

$$\hat{\rho}=\exp[\lambda_0'+\tfrac{1}{2}(Z^\dagger MZ)]\ , \tag{4.3}$$

where

$$\lambda_0'=\lambda_0+\tfrac{1}{2}\mathrm{tr}(\Lambda)\ ,$$

and

$$Z^+=(c_i^\dagger,\ldots,c_L^\dagger,c_1,\ldots,c_L)\ ,$$

Z being its adjoint. L denotes the total number of accessible s.p. states. The fermion anticommuting relationships may be condensed in the tensorial product $ZZ^\dagger+[(Z^\dagger)^{\mathrm{tr}}Z^{\mathrm{tr}}]^{\mathrm{tr}}=I$, where I is the identity of $2L\times 2L$. The full s.p. density matrix can be defined as[15]

$$D=\begin{bmatrix}A & B\\ -B^* & I-A^*\end{bmatrix}=I-\langle ZZ^\dagger\rangle\ , \tag{4.4}$$

where $A_{ij}=\langle c_j^\dagger c_i\rangle$ is the s.p. density matrix, while $B_{ij}=\langle c_jc_i\rangle$ is usually referred to as the s.p. pairing tensor.

$\hat{\rho}$ can be written in diagonal form by means of a Bogoliubov transformation[15] $Z'=WZ$, such that the matrix $M'=WMW^\dagger$ is diagonal, in which case,

$$\hat{\rho}=\exp\left[\lambda_0''+\sum_i\lambda_ic_i'^\dagger c_i'\right]\ , \tag{4.5}$$

where $\lambda_0''=\lambda_0+\frac{1}{2}\mathrm{tr}(\Lambda-\Lambda')$. Hence,

$$\langle c_i'c_j'\rangle=0,\quad \langle c_i'^\dagger c_j'\rangle=f_i\delta_{ij}\ ,$$

and $(c_i'^\dagger c_i')^*=c_i'^\dagger c_i'-f_i$ [cf. (3.10)]. The matrices F and G [(3.12) and (3.13)] can thus be interpreted as correlations. In particular, in a grand canonical (GC) ensemble, G becomes diagonal in the primed basis, and we obtain for f_i the well-known expression $f_i=[1+\exp(-\lambda_i)]^{-1}$. Therefore, in a general basis,

$$D=[I+\exp(-M)]^{-1}\ . \tag{4.6}$$

The mean value of any one-body observable $\hat{O}=\frac{1}{2}Z^+QZ$ can be cast as

$$\langle\hat{O}\rangle=\tfrac{1}{2}\mathrm{tr}(QD)\ , \tag{4.7}$$

where tr denotes the trace in the extended $2L$ dimensional s.p. space. In particular, we attain the following expression for the entropy:

$$S=-\lambda_0-\tfrac{1}{2}\mathrm{tr}(MD)\ , \tag{4.8}$$

which in a grand canonical ensemble is identical with the well-known formula

$$S=-\sum_i[f_i\ln(f_i)+(1-f_i)\ln(1-f_i)]$$
$$=-\mathrm{tr}(D\ln D)\ . \tag{4.9}$$

We would like to remark here that in the case of incomplete s.p. information (i.e., a partially known density matrix D), (4.6) yields a system of equations, namely,

$$0=M_{ij}=-[\ln(D^{-1}-I)]_{ij} \; , \tag{4.10}$$

which determines the inferred values of the remaining unknown elements, via the maximum entropy principle.

Let us assume now that the available information deals with the mean values $\{O_i, i=1,\ldots,m\}$, of general n-body fermion operators $\hat{O}_i$. The corresponding exact statistical operator becomes very difficult to deal with, so that it makes sense to work with s.p. statistical operators as a zeroth-order approximate description. In this case, statistical inference of mean values of operators $\hat{O}_i$ are easily computed, within the grand canonical ensemble, by recourse to the statistical version of Wick's theorem.[7]

The approximate density operator (3.7) reads

$$\hat{\rho}_{\text{app}}=\exp[\lambda_0+\tfrac{1}{2}Z^\dagger M(D)Z] \; , \tag{4.11}$$

where

$$M(D)=\sum_i \beta_i \begin{bmatrix} R^i-\Delta^{i*} \\ \Delta^i-R^{i*} \end{bmatrix} \equiv \sum_i \beta_i Q_i \; , \tag{4.12}$$

with

$$R^i_{lj}=\frac{\partial O_i}{\partial\langle c_l^\dagger c_j\rangle} \; , \tag{4.13a}$$

$$\Delta^i_{lj}=\frac{\partial O_i}{\partial\langle c_l c_j\rangle} \; . \tag{4.13b}$$

The expectation value of an n-body operator with respect to (5.1) becomes a polynomial of degree n in the elements of D. The operators $\hat{o}_i$ (3.8) are s.p. effective mean-field operators

$$\hat{o}_i=\tfrac{1}{2}Z^\dagger Q_i Z \; . \tag{4.14}$$

By means of Wick's theorem, it can be easily shown that $\langle\hat{o}_i\rangle=n\langle\hat{O}_i\rangle$, if $\hat{O}_i$ is an n-body operator.

The statistical operator (4.12) poses, for fixed parameters β_i, the nonlinear (matrix) equation [cf. (4.6)]

$$D=\{I+\exp[-M(D)]\}^{-1} \; , \tag{4.15}$$

which represents the generalized statistical Hartree-Fock-Bogoliubov (SHFB) equations in the grand canonical ensemble. The iterative procedure leads to $D^i=\{1+\exp[-M(D^{i-1})]\}^{-1}$. The iteration must be continued until convergence is reached in all the elements of D. Of course, many solutions may be encountered, starting with different initial density matrices D^0, and not in every situation is convergence guaranteed. A direct maximization of S or S' may provide one with a more convenient route in some cases (see Sec. V).

The usual static statistical HFB equations[2,3] are recovered when all observables $\hat{O}_i$ commute among themselves and with the Hamiltonian $\hat{H}$ of the system. In particular, the finite temperature HFB approach[2,3] is obtained when the operators $\hat{O}_i$ are restricted to the Hamiltonian and the number of particles, $\hat{N}$.

However, the present context is completely general, operators $\hat{O}_i$ being completely arbitrary. The generalized statistical mean-field approach provides an instantaneous approximate description of an arbitrary quantum system, based on s.p. observables. Besides, restricted mean-field approaches can be obtained by reducing the number of s.p. observables to be included in the exponent of $\hat{\rho}$. For instance, if the mean values $\langle c_i c_j\rangle$ are not relevant in the evaluation of the O_i's, they can be discarded, thus reducing the equations to half their size (SHF).

V. APPLICATION

A. The model

Let us illustrate our ideas with references to a nontrivial SU(2)×S(U2) model,[16–18] consisting of s.p. states $|p,\nu\rangle$, $p=1,\ldots,2\Omega$, $\nu=\pm1$. We define the following collective operators:

$$\hat{J}_+=\sum_p c^\dagger_{p+}c_{p-}=\hat{J}^\dagger_- , \quad \hat{J}_z=\tfrac{1}{2}\sum_{p,\nu}\nu c_{p\nu}c^\dagger_{p\nu} \; , \tag{5.1}$$

$$\begin{aligned} &\hat{Q}_+=\sum_p c^\dagger_{p+}c^\dagger_{p-}=\hat{Q}^\dagger_- \; , \\ &\hat{Q}_z=\tfrac{1}{2}\sum_{p,\nu}c^\dagger_{p\nu}c_{p\nu}-\Omega=\tfrac{1}{2}\hat{N}-\Omega \; , \end{aligned} \tag{5.2}$$

which satisfy an SU(2)×SU(2) algebra. We shall assume that the available information deals with expectation values of functions of the operators (5.1) and (5.2). The corresponding statistical operator in the mean-field approximation will thus be

$$\hat{\rho}=\exp(\lambda_0+\lambda\hat{J}_z+\tau\hat{J}_++\tau^*\hat{J}_-+\mu\hat{Q}_z+\eta\hat{Q}_++\eta^*\hat{Q}_-) \; . \tag{5.3}$$

The operator (5.3) can be written in diagonal form by means of rotations in the respective SU(2) spaces, equivalent to a Bogoliubov transformation of the fermion operators $c^\dagger_{p\nu}$, $c_{p\nu}$, i.e.,

$$\hat{\rho}=\exp(\lambda_0+\lambda'\hat{J}'_z+\mu'\hat{Q}'_z) \; , \tag{5.4}$$

where $\lambda'^2=\lambda^2+4|\tau|^2$, $\mu'^2=\mu^2+4|\eta|^2$, and

$$\begin{aligned} &\hat{J}'_z=\hat{J}_z\cos(\theta)-\tfrac{1}{2}[\hat{J}_+\sin(\theta)e^{(-i\phi)}+\hat{J}_-\sin(\theta)e^{(+i\phi)}] \\ &\hat{J}'_\nu=\hat{J}_\nu\cos^2(\theta/2)+\hat{J}_z\sin(\theta)e^{(i\nu\phi)} \\ &\qquad -\hat{J}_{-\nu}\sin^2(\theta/2)e^{(i2\nu\phi)} \; , \end{aligned} \tag{5.5}$$

with the Bloch angles determined by

$$\lambda=\lambda'\cos(\theta), \quad \tau=-\tfrac{1}{2}\lambda'\sin(\theta)e^{-i\phi} \; .$$

An analogous formula obviously holds for Q operators, with Bloch angles say, γ, ψ. The connection (4.6) between the relevant one-body expectation values and the corresponding Lagrange multipliers can be explicitly found in this case:

$$\langle\hat{J}_z\rangle=2\Omega j\lambda/\lambda', \quad \langle\hat{J}_+\rangle=4\Omega j\tau^*/\lambda' \; , \tag{5.6}$$

$$\langle\hat{Q}_z\rangle=2\Omega q\mu/\mu', \quad \langle\hat{Q}_+\rangle=4\Omega q\eta^*/\mu' \; , \tag{5.7}$$

where

$$j=\langle \hat{J}_z' \rangle /2\Omega=(f_+ - f_-)/2 \ , \quad (5.8)$$

$$q=\langle \hat{Q}_z' \rangle /2\Omega=(f_+ + f_- - 1)/2 \ , \quad (5.9)$$

with f_ν the mean quasiparticle occupation number. Without loss of generality, we can assume $j>0$, $q>0$, and $0\le\theta\le\pi$, $0\le\phi<2\pi$ (the same for γ,ψ).

Obviously, for $\eta\neq 0$, (5.3) should be dealt with in a GC ensemble. However, if $\eta=0$, other ensembles (i.e., canonical ones[19]) become feasible. In a GC ensemble, $f_\nu=\{1+\exp[-\frac{1}{2}(\mu'+\nu\lambda')]\}^{-1}$ and the entropy (4.9) can be written as

$$S=-2\Omega\sum_{\nu,\nu'}(\tfrac{1}{2}+\nu j+\nu' q)\ln(\tfrac{1}{2}+\nu j+\nu' q) \ . \quad (5.10)$$

S increases for decreasing values of j and q. The inverse relations

$$j=[\langle \hat{J}_z \rangle^2+\langle \hat{J}_+ \rangle\langle \hat{J}_- \rangle]^{1/2}/2\Omega \ ,$$

$$q=[\langle \hat{Q}_z \rangle^2+\langle \hat{Q}_+ \rangle\langle \hat{Q}_- \rangle]^{1/2}/2\Omega \ ,$$

together with (5.6)–(5.9), enable one to construct $\hat{\rho}$ from the knowledge of all the collective one-body mean values. Statistical inference becomes trivial in this case. A given expectation value will vanish if the corresponding multiplier vanishes [cf. (5.6)–(5.7)].

B. Self-consistent approach and effective multipliers

Let us first suppose that the available information consists of the set $\{\langle \hat{J}_z \rangle, \langle \hat{Q}_z \rangle, \langle \hat{Q}_+\hat{Q}_- \rangle\}$. The approximate description, based on (5.3), will now be constructed. By applying Wick's theorem, we find

$$p\equiv\langle \hat{Q}_+\hat{Q}_- \rangle/(2\Omega)^2=[\langle \hat{Q}_+ \rangle\langle \hat{Q}_- \rangle+(\langle \hat{N}^2 \rangle/4-\langle \hat{J}_z^2 \rangle-\langle \hat{J}_+ \rangle\langle \hat{J}_- \rangle)/2\Omega]/(2\Omega)^2$$
$$=q^2\sin^2(\gamma)+[n^2/4-j^2]/2\Omega \ , \quad (5.11)$$

where $n=\langle \hat{N} \rangle/2\Omega=2q\cos(\gamma)+1$. In what follows we shall concern ourselves with the case $N=2\Omega$ ($\langle \hat{Q}_z \rangle=0$), so that $\gamma=\pi/2$ ($\mu=0$) if $q\neq 0$. Hence,

$$q=[p-(\tfrac{1}{4}-j^2)/2\Omega]^{1/2} \ . \quad (5.12)$$

Maximum entropy implies $|\cos(\theta|=1(\tau=0)$, so that $j=|j_z|$, where $j_z=\langle \hat{J}_z \rangle/2\Omega$. On the other hand, ψ (phase of $\langle \hat{Q}_+ \rangle$) remains completely arbitrary, corresponding to the violation of particle number conservation [by (5.3)].

The corresponding effective multipliers (3.17a) are

$$\beta_1\equiv-\frac{\partial S}{\partial\langle \hat{J}_z \rangle}=[\lambda'+\mu' j/(2\Omega q)]j_z/j \ , \quad (5.13)$$

$$\beta_2\equiv-\frac{\partial S}{\partial\langle \hat{Q}_+\hat{Q}_- \rangle}=\mu'/(4\Omega q) \ , \quad (5.14)$$

$$\beta_3\equiv-\frac{\partial S}{\partial\langle \hat{Q}_z \rangle}=-\mu' n/(4\Omega q) \ , \quad (5.15)$$

where [cf. (5.4)]

$$\lambda'=-\frac{\partial S/N}{\partial j}=\ln\{[(\tfrac{1}{2}+j)^2-q^2]/[(\tfrac{1}{2}-j)^2-q^2]\} \ , \quad (5.16)$$

$$\mu'=-\frac{\partial SN}{\partial q}=\ln\{[(\tfrac{1}{2}+q)^2-j^2]/[(\tfrac{1}{2}-q)^2-j^2]\} \ . \quad (5.17)$$

Notice that both β_2 and β_3 vanish in the thermodynamic limit $2\Omega\to\infty$.

Let us consider now a less detailed description, based on the sole knowledge of $\langle \hat{Q}_z \rangle$ and $E=\langle \hat{H} \rangle$, with $\hat{H}=\hat{J}_z+G\hat{Q}_+\hat{Q}_-$. $\hat{H}$ can be interpreted as a Hamiltonian, with G the quasispin pairing[16] coupling constant. In the mean-field picture,

$$E/2\Omega=j_z+gp \ , \quad (5.18)$$

where $g=2\Omega G$. The particular values of $j=|j_z|$ and q are determined by maximizing (5.10) with the constraint (5.18). We are thus led to the "gap"-like equation

$$2q\lambda'+\mu'[-j_z/(jg)+j/\Omega]=0 \ , \quad (5.19)$$

which determines the optimized j, q. The sign of j_z is equal to that of E. For sufficiently large G, there will be a critical value of E, determined by the equation

$$-2\ln[(\tfrac{1}{2}+j)/(\tfrac{1}{2}-j)]=(\tfrac{1}{4}-j^2)^{-1}[-j_z/(jg)+j/\Omega] \ , \quad (5.20)$$

beyond which a solution with $q\neq 0$ will exist (see also Ref. 17). At the same time, a solution of (5.19) with $q=0$ is always feasible, with a vanishing value of the gap. However, the superconducting solution (that with $q\neq 0$) yields a higher entropy than the normal solution ($q=0$) when it exists. Thus, at the critical point given by (5.20), a phase transition (which can be proved to be of second order for sufficiently large G) arises in the self-consistent approach, as a result of the incomplete description. The corresponding effective multiplier is

$$\beta\equiv-\frac{\partial S}{\partial E}=\mu'/(2gq) \quad (5.21a)$$
$$=\lambda'/(j_z/j-gj/\Omega) \ , \quad (5.21b)$$

and $T=-1/\beta$ can be interpreted as the mean-field effective temperature.

In the normal solution, j can be directly determined from (5.18). We obtain in this case the same expression (5.21b) for β. Due to the smoothness of the transition, the two different β's coincide at the critical point.

Numerical results for S, β_1, β_2 and β are depicted in Figs. 1 and 2. The exact results have been computed in the full canonical ensemble[17] [dimension $\binom{4\Omega}{N}$], for $N=30$, using as "exact" multipliers $\beta_1^{\rm ex}=-\epsilon/T$, $\beta_2^{\rm ex}=-G/T$, with $\epsilon=1$, $G=-2.5/N$. The situation is thus similar to a system described by a quasispin pairing

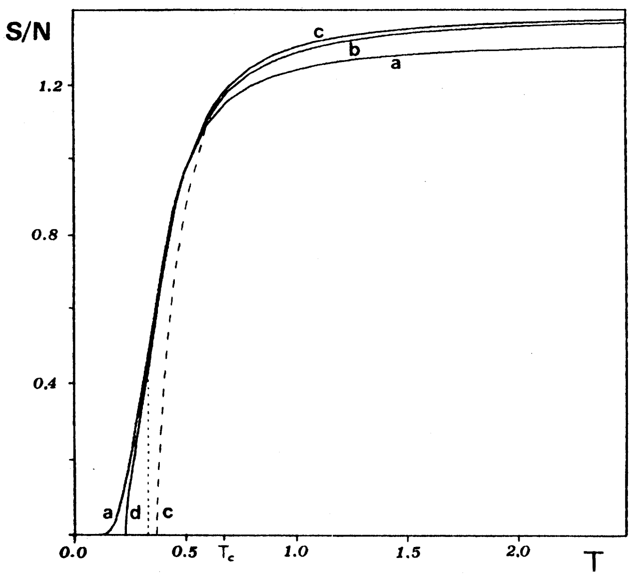

FIG. 1. Intensive entropies according to exact (*a*) and generalized mean-field (*b,c,d*) treatments, for the quasispin pairing system (Sec. V B), in terms of the exact temperature (in units of the energy difference ϵ between the unperturbed s.p. levels). (*b*) corresponds to the smooth, detailed description, (*c*) to the normal solution of (5.19) [unstable below T_c (dashed line)], and (*d*) to the superconducting solution ($T<T_c$). The dotted line indicates the beginning of the detailed description.

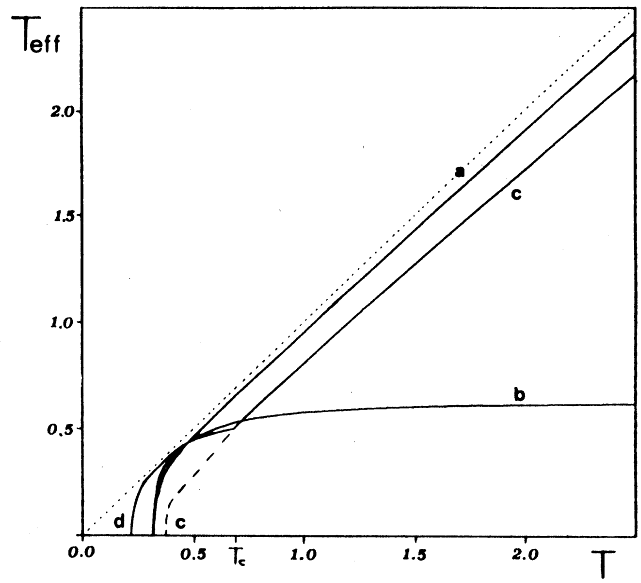

FIG. 2. Effective temperatures in the quasispin pairing system. (*a*) and (*b*) depict, respectively, $T_1=-\epsilon/\beta_1$ (5.13) and $T_2=-G/\beta_2$ (5.14) in the detailed description, whereas (*c*) and (*d*) depict $T=-1/\beta$ (5.21) according to the normal and superconducting solutions. The straight dotted line represents the exact temperature.

Hamiltonian at a temperature T, with ϵ the energy difference between unperturbed s.p. levels. In what follows, all temperatures and coupling constants will thus be given in units of ϵ. Mean-field results have been obtained utilizing exact averages (instead of exact multipliers). This allows us to examine the approach from a viewpoint different from the conventional one.[17]

In the more detailed description, the mean-field solution exists only for $T>T_{c1}\sim 0.34$, starting with a nonvanishing value of the entropy (see Fig. 1). For $T<T_{c1}$, $j+q>0.5$ [see (5.8) and (5.9)], so that the exact averages cannot be reproduced by recourse to an operator of the form (5.3). The slope of S at the threshold temperature is infinite, since λ' and μ' diverge as $\ln(T-T_{c1})$ [see (5.16) and (5.17)]. For the same reason, the effective temperatures $T_1=-\epsilon/\beta_1$, $T_2=-G/\beta_2$ (see Fig. 2), which coincide with T in the exact treatment, vanish as $1/\ln(T-T_{c1})$. Notice however that for $T>T_{c1}$, the mean-field description is smooth in this case, with no phase transitions.

On the other hand, in the less detailed description, the superconducting self-consistent solution exists for $T>T_{c2}\sim 0.22$, starting with a vanishing value of S (since $j=0$, initially). The normal solution becomes feasible for $T>T_{c3}\sim 0.37$, and remains the only solution for $T>T_c\sim 0.68$ (critical temperature). Only when the information is restricted to $\langle\hat{H}\rangle$ (and $\langle\hat{Q}_z\rangle$) is a phase transition encountered. The entropy is obviously higher in this case, due to the smaller amount of informational input. The initial slopes of the entropies and the initial values of the effective temperatures behave as in the previous situation.

The behavior of the effective multipliers depend strongly on the nature of the corresponding observable. In general, we can see that mean-field descriptions are "cooler" than exact pictures, although crossing points may in principle occur. In the detailed description, as $T\to\infty$, both j and q vanish, so that $\lambda'\sim 8j$, $\mu'\sim 8q$. Therefore, β_1 vanishes, whereas $\beta_2\to 2/\Omega$. This explains the behavior (at high temperatures) of the multiplier associated with the two-body observable (see Fig. 2). The effective coupling constant β_2/β_1 (equal to G in the exact picture) diverges in the detailed mean-field description as $T\to\infty$. This fact actually predicts the phase transition occurring in the less detailed description, where β_2/β_1 is constrained to a constant value. In this case, the effective multiplier behaves similar to β_2 for $T<T_c$, and to β_1 for $T>T_c$, indicating the strongest contribution to $\langle\hat{H}\rangle$.

C. Lower bound for the entropy

The standard mean-field treatment does not provide one with a lower bound to the exact canonical entropy, since it works in the GC ensemble. Although it is (in principle) possible to consider (5.3) in a canonical ensemble, just by replacing the expression for f_ν with an appropriate numerical value, the approach would be constrained in this case to that situation for which $\eta=0$. Hence, it would be unable to cope with information about $\hat{Q}_+\hat{Q}_-$. We shall examine, within the context of the generalized self-consistent treatment of Sec. III, the possibility of enlarging the set of relevant observables to be included in the exponent of $\hat{\rho}$, by adding particular two-body observables, while preserving, at the same time, its "tractability." Thus, we propose the new trial density operator

$$\hat{\rho}=\exp(\lambda_0+\lambda\hat{J}'_z+\sigma\hat{J}'^2_z+\zeta\hat{J}^2+\kappa\hat{Q}^2) , \quad (5.22)$$

where we have omitted terms depending on $\hat{Q}_z$ since we shall work in a canonical ensemble. Operator (5.22) conserves the number of particles, and besides, is diagonal in a standard $SU(2)\times SU(2)$ basis.[17]

When the generalized self-consistent approach, based on (5.22), is applied to the situations described in the previous subsection, it yields *exact* results, since $\hat{Q}_+\hat{Q}_-=\hat{Q}^2-\hat{Q}_z^2+\hat{Q}_z$, and therefore, observables about which information is available, are spanned by the chosen operators [see (3.15)]. In this situation, $\sigma=\zeta=0$, while λ and κ coincide with exact multipliers β_1^{ex} and β_2^{ex}, respectively.

As a more challenging example, we shall examine the case where information is also given about $\hat{O}=\frac{1}{2}(\hat{J}_+^2+\hat{J}_-^2)$, in addition to $\langle\hat{J}_z\rangle$, $\langle\hat{Q}_+\hat{Q}_-\rangle$, and $\langle\hat{Q}_z\rangle$. The exact treatment requires, in this case, a diagonalization of $\ln(\hat{\rho})$. The standard mean-field treatment yields in this context,

$$\langle\hat{O}\rangle=(2\Omega-1)/4\Omega(\langle\hat{J}_+\rangle^2+\langle\hat{J}_-\rangle^2)$$
$$=2\Omega(2\Omega-1)j^2\sin^2(\theta)\cos(2\phi) , \quad (5.23)$$

and $\langle\hat{J}_z\rangle=2\Omega j\cos(\theta)$. Maximum entropy implies $|\cos(2\phi)|=1$ (in order to obtain a minimum value of j), and therefore, $j=(j_z^2+|o|)^{1/2}$, $tg^2(\theta)=j_z^2/|o|$, where $o=\langle\hat{O}\rangle/[2\Omega(2\Omega-1)]$. The s.p. self-consistent operator (5.3) can thus be found, except for the sign of τ (i.e., the sign of $\langle\hat{J}_y\rangle$), which remains undetermined (degenerate solution). This fact corresponds to the violation of the parity $\hat{P}=\exp(i\pi\hat{J}_z)$ ($[\hat{P},\hat{O}]=0$) by the operator (5.3). The expression for the new effective multiplier is

$$\beta_4\equiv-\frac{\partial S}{\partial\langle\hat{O}\rangle}=[\lambda'+\mu'j/(2\Omega q)]sg(o)/[2j(2\Omega-1)] , \quad (5.24)$$

whereas β_1, β_2, and β_3 remain as given by (5.13)–(5.15).

On the other hand, within the new self-consistent approach based on (5.22), one obtains, using (5.5),

$$\langle\hat{O}\rangle=\tfrac{1}{2}\sin^2(\theta)\cos(2\phi)(3\langle\hat{J}'^2_z\rangle-\langle\hat{J}^2\rangle) , \quad (5.25)$$

and obviously $\langle\hat{J}_z\rangle=\langle\hat{J}'_z\rangle\cos(\theta)$. Therefore, according to (3.6), $\sigma=-3\zeta$. For fixed θ,ϕ, the parameters λ, ζ, and κ must be determined numerically. In addition, the Bloch angles can be chosen so as to maximize the entropy. Again, $|\cos(2\phi)|=1$ (the degeneracy in the sign of $\langle\hat{J}_y\rangle$ still remains), while θ must be determined from

$$\frac{\partial S}{\partial\theta}\propto\lambda\langle\hat{J}_z\rangle\sin^4(\theta)+4\zeta\langle\hat{O}\rangle\cos^3(\theta)=0 . \quad (5.26)$$

The effective multipliers are, using (3.17) and (5.26),

$$\beta_1=\lambda/\cos(\theta) , \quad (5.27)$$

$$\beta_4=-2\zeta/\sin^2(\theta) , \quad (5.28)$$

while $\beta_2=\kappa$.

Numerical results are shown in Figs. 3 and 4. The approximate treatments have been obtained again utilizing "exact" averages. We have used as exact multipliers $\beta_1^{ex}=-\epsilon/T$, $\beta_2^{ex}=-G/T$, $\beta_4^{ex}=-V/T$, with $\epsilon=1$, $G=-2.5/N$, $V=-2.5/(N-1)$, and again, $N=30$. The situation is now similar to a system described by a quasispin pairing plus monopole Hamiltonian,[16,17] at a temperature T. For these values of the coupling constants, we attain a deformed ground state.

The mean-field behavior is the same as in the previous situation. In both cases, the s.p. entropy lies above the exact entropy for high enough T, and moreover, the difference increases with T. On the other hand, the lower bound given by (5.22) is extremely accurate (except, perhaps, in the transition zone) and the difference with the exact values decreases as T increases. Besides, the new approximate solution exists for a larger range of T values. The nonvanishing value of the exact entropy at very low temperatures is due to the quasidegeneracy of the "deformed" ground state.

The predictions for the effective temperatures T_2 and $T_4=-V/\beta_4$ are very similar in the s.p. description, and differ from the fairly accurate values obtained for T_1. On the other hand, the new approach provides a quite accurate prediction of T_2, a small improvement in T_4 (which now increases as $T\to\infty$) and a small loss of accuracy in T_1, which is now "mixed" with T_4 through (5.26).

Finally, we would like to remark that predictions of the intensive entropy S/N made by both the s.p. mean-field approach and the new self-consistent approach based on (5.22) improve as N increases, becoming exact in the thermodynamic limit $N\to\infty$ (see, for instance, Ref. 17).

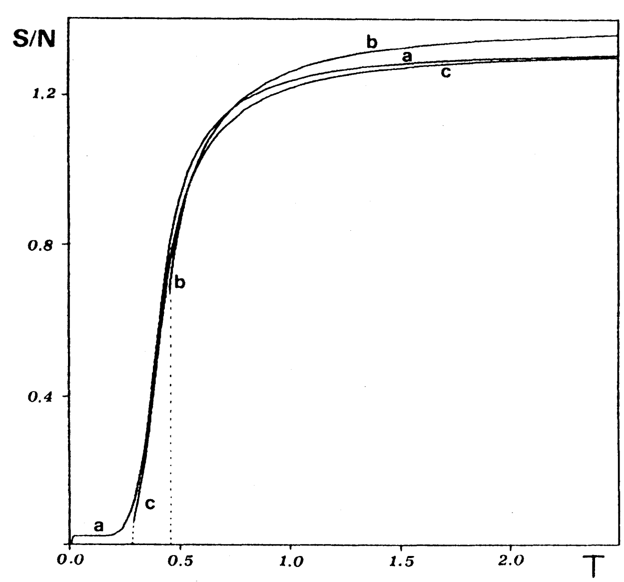

FIG. 3. Intensive entropies in the quasispin pairing plus monopole system (Sec. V C). (*a*) corresponds to exact results, (*b*) to the detailed mean-field description, and (*c*) to the higher-order self-consistent description (5.22). Dotted lines indicate threshold points.

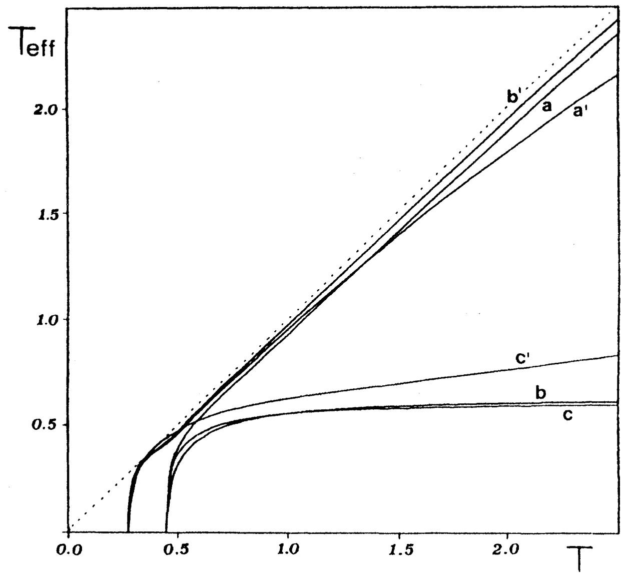

FIG. 4. Effective temperatures for the system of Fig. 3. (*a*), (*b*), and (*c*) correspond to $T_1 = -\epsilon/\beta_1$, $T_2 = -G/\beta_2$, and $T_4 = -V/\beta_4$ (5.24) in the detailed mean-field description, whereas (*a'*), (*b'*), and (*c'*) depict the same quantities in the higher-order approach.

VI. CONCLUSIONS

We have presented a quite general self-consistent approximation for statistical operators. The basic idea is to replace the exponent of $\hat{\rho}$ [i.e., to approximate $\ln(\hat{\rho})$] by a linear combination of a "chosen" set of observables, in order to attain a tractable density operator.

In the particular case where this set consists of s.p. operators, the formalism here presented allows for a very general and simple derivation of the statistical Hartree-Fock-Bogoliubov approximation, which extends standard thermal mean-field treatments within a completely general statistical context.

However, it should be stressed that within the present context, it is possible to improve upon the generalized mean-field description, obtaining self-consistent approximations of a higher order. A straightforward yet tractable extension can be attained, for instance, by choosing a set of commuting operators, diagonal in an appropriate known basis, which includes two-body (or higher) observables in addition to s.p. ones. In this case, no diagonalization is required for computing traces, and the matrices F and G [(3.12) and (3.13)] can be easily evaluated as correlations.

The formalism has been illustrated in a solvable nuclear model, utilizing information about observables which mock up short- and long-range interactions.[17] Both mean-field and higher-order self-consistent treatments have been examined, and constructed directly from the knowledge of a given set of mean values.

The present work may perhaps enlarge the scope of the possible applications of mean-field theories and self-consistent treatments, and clarify some aspects of their interpretation. In particular, the richness of the nuclear many-body problem manifests itself in fashions that entail going beyond conventional mean-field theories.[20] It is to be hoped that the present effort may constitute a step in this direction.

R.R. acknowledges support by the Buenos Aires Province Research Comission, (CICPBA), and A.P. was supported as a member of the National Research Council (CONICET) of Argentina.

[1] D. J. Thouless, *The Quantum Mechanics of Many Body Systems* (Academic, New York, 1961).

[2] A. L. Goodman, Nucl. Phys. **A352**, 30 (1981); **A352**, 45 (1981).

[3] M. Brack and P. Quentin, Nucl. Phys. **A352**, 45 (1981).

[4] E. T. Jaynes, Phys. Rev. **106**, 620 (1957); **108**, 171 (1957).

[5] A. Katz, *Principles of Statistical Mechanics* (Freeman, San Francisco, 1967).

[6] R. Balian, Y. Alhassid, and H. Reinhardt, Phys. Rep. **131**, 1 (1986).

[7] H. Reinhardt, R. Balian, and Y. Alhassid, Nucl. Phys. **A413**, 475 (1984).

[8] R. Balian and M. Veneroni, Ann. Phys. (N.Y.) **164**, 334 (1985); **174**, 229 (1987); R. Balian and N. L. Balazs, *ibid.* **179**, 97 (1987).

[9] D. Otero, A. Plastino, A. Proto, and G. Zannoli, Phys. Rev. A **26**, 1209 (1982).

[10] J. Aliaga, M. Negri, D. Otero, A. Plastino, and A. Proto, Phys. Rev. A **35**, 2304 (1987); **36**, 3427 (1987); E. Duering, D. Otero, A. Plastino, and A. Proto, Phys. Rev. A **32**, 2455 (1985).

[11] R. Rossignoli and A. Plastino, Phys. Rev. C **36**, 1595 (1987).

[12] N. Tishby and R. Levine, Phys. Rev. A **30**, 1477 (1984); Y. Alhassid and R. Levine, Phys. Rev. C. **20**, 1775 (1979).

[13] B. Robertson, Phys. Rev. **144**, 151 (1966).

[14] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957); Rep. Prog. Phys. **29**, 255 (1966).

[15] P. Ring and P. Schuck, *The Nuclear Many Body Problem* (Springer-Verlag, New York, 1980).

[16] M. Cambiaggio and A. Plastino, Z. Phys. A **288**, 153 (1978).

[17] R. Rossignoli and A. Plastino, Phys. Rev. C **32**, 1040 (1985).

[18] R. Rossignoli, A. Plastino, and J. Vary, Phys. Rev. C **37**, 314 (1988).

[19] R. Rossignoli and A. Plastino, Phys. Rev. C **30**, 1360 (1984).

[20] C. N. Papanicolas and V. Pandharipande, Phys. Today **42**, S56 (1989).