Variational description of the nuclear free energy

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By means of a variational calculation, we place an upper bound on the finite-temperature free energy for nuclear systems which can be described by pseudospin Hamiltonians. The trial states are irreducible permutation invariant Gibbs states. The best trial state is the one which minimizes the free energy operator. We compare the upper bound with the numerically computed free energy for the Meshkov-Glick-Lipkin Hamiltonian for various values of nucleon number N and nuclear interaction strength V. For large N and/or $\beta(=1/kT)$ the best trial Gibbs state becomes a good approximation to the actual density operator. Somewhat surprisingly, the variational approach reveals the presence of a second order thermodynamic phase transition much more clearly than the numerical computation does, even though the former is only an approximation to the latter.

[NUCLEAR STRUCTURE Finite-temperature free energy, pseudospin Hamiltonian, variational description and phase transitions, atomic coherent states.]

I. INTRODUCTION

The study of finite-temperature nuclear physics has recently generated a great deal of interest.[1] The appearance of heavy-ion collision data[2] has been a major factor encouraging such investigations. In this work, we study primarily the behavior of nuclear matter at finite temperatures by studying the behavior of the associated nuclear free energy. The nuclear free energy can be estimated accurately for a large class of nuclear systems describable by pseudospin Hamiltonians.[3-5]

This class of Hamiltonians consists of all symmetrized Hermitian polynomials in the pseudospin operators. A general Hamiltonian $\hat{\mathcal{H}}$ in the class studied has the form[5]

$$\hat{h}_Q = \hat{\mathcal{H}}/N = \sum_{L=1}^{\text{finite}} \sum_{M=-L}^{L} A_M^L \mathcal{Y}_M^L(\vec{J}/N) . \tag{1.1}$$

Here N is the number of nucleons present, the nuclear interaction parameters A_M^L have order of magnitude unity and are independent of N, the $\mathcal{Y}_M^L$ are irreducible spherical tensor operators, and the homogeneous form of $\hat{\mathcal{H}}/N$ is required by thermodynamic considerations, in particular, by the requirement that a thermodynamic limit exists.[6,7] The study of the general pseudospin Hamiltonian (1.1) is facilitated by introducing the atomic coherent state representation.[8,9]

Upper and lower bounds on the ground state energy E_g were constructed[4] for the general Hamiltonian (1.1) using the atomic coherent state Q and P representations. These bounds differ by a number of order $\ln N$. Bounds on the finite-temperature free energy $F(\beta)$ ($\beta = 1/k_B T$) were also constructed[5]; these bounds also differ by a number of order $\ln N$. As a result, in the nuclear matter limit ($N \to \infty$), these bounds (divided by N) converge to exact expressions for the ground state energy per nucleon and the free energy per nucleon.

In the case of finite N the upper and lower bounds on the ground state energy were compared[4] with the exact ground state energy eigenvalue for the pseudospin Hamiltonian (1.1) with $A_0^1 = \epsilon$, $A_2^2 = A_{-2}^2 = V/2$, $A_M^L = 0$ otherwise, studied originally by Meshkov, Glick, and Lipkin (MGL).[3] It was found that the upper limit, provided by the minimum of the Q representation of the MGL Hamiltonian, was a good approximation to the ground state energy eigenvalue. This, in turn, suggested that the atomic coherent states $|J,\Omega\rangle$, with $J = N/2$, provided a useful set of trial wave functions for a variational treatment of this problem. This allows for a particularly vivid representation of both the ground state and the ground state energy phase transition, since the atomic coherent states for fixed J exist in one to one correspondence with the points on the surface of the (Bloch) sphere.

In the absence of interactions ($A_2^2 = A_{-2}^2 = 0$ in the MGL Hamiltonian) the variational ground state "points to" the South Pole. When the interaction parameters are sufficiently large, the variational ground state ceases to point toward the South Pole. A second order ground state energy (nuclear shape) phase transition occurs as the ratio $|V|/\epsilon$ increases through 1.[4] This is evident already both from the exact ground state

energies[3] and the estimated ground state energies[4] but it becomes especially clear in the nuclear matter limit.[5]

Although we now have a very vivid picture of the ground state energy phase transition in terms of variational states, we have no corresponding picture for the accompanying thermodynamic phase transition. It is the purpose of the present work to provide such a picture.

In order to make the present work as self-contained as possible, we collect in Sec. II the properties of SU(2) coherent states which are required. In Sec. III we review the variational calculation of the upper bound for the ground state free energy. This calculation is used as a model for the computation of the upper bound on the nuclear free energy, which is carried out in Sec. IV. The upper bound is compared with the exact free energy, computed for the Meshkov-Glick-Lipkin Hamiltonian in Sec. V. The thermodynamic second order phase transition is discussed in Sec. VI. We relegate to Appendix A a derivation of the most general form for an N-particle permutation-invariant operator, and the description of such irreducible operators in the atomic coherent state representation. In Appendix B we describe how the piecewise linear upper bound on the nuclear free energy is constructed.

II. ATOMIC COHERENT STATES

The atomic coherent state $|J,\Omega\rangle$ is obtained by applying the SU(2) rotation Ω to the spin state $|J,J\rangle$ (Ref. 9):

$$|J\Omega\rangle = U(\Omega)|J,J\rangle\,, \qquad U(\Omega) = \exp\frac{\theta}{2}(e^{i\phi}J_- - e^{-i\phi}J_+)\,. \tag{2.1}$$

The coherent states $|J,\Omega\rangle$ exists in one to one correspondence with points (θ,ϕ) on the surface of the Bloch sphere. These states are nonorthogonal and overcomplete. They have a host of interesting properties which have been extensively summarized elsewhere.[10] For the purpose of the present work only the following three properties are required. They are as follows:

(1) Every operator $\hat{G}$ which maps a J-invariant subspace into itself has both a P representative $P_J(\hat{G};\Omega)$ and a Q representative $Q_J(\hat{G};\Omega)$ which are defined as follows[9]:

$$\hat{G} = \frac{2J+1}{4\pi}\int \left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle P_J(\hat{G};\Omega)\left\langle\begin{matrix}J\\ \Omega\end{matrix}\right| d\Omega\,,$$
$$Q_J(\hat{G};\Omega) = \left\langle\begin{matrix}J\\ \Omega\end{matrix}\right|\hat{G}\left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle \tag{2.2}$$

where $d\Omega = \sin\theta d\theta\, d\phi$.

The P and Q representatives of $\hat{G}$ are functions defined over the surface of the Bloch sphere.

(2) The P and Q representatives of the irreducible spherical tensor operators $\mathcal{Y}^L_M(\vec{J})$ are proportional to the corresponding spherical harmonic functions[11]

$$P_J(\mathcal{Y}^L_M(\vec{J});\Omega) = \frac{(2J+1+L)!}{(2J+1)!\,2^L}\,Y^L_M(\Omega)\,,$$
$$Q_J(\mathcal{Y}^L_M(\vec{J});\Omega) = \frac{(2J)!}{(2J-L)!\,2^L}\,Y^L_M(\Omega)\,. \tag{2.3}$$

(3) The P and Q representatives of $\hat{G}$ can be used to put bounds on the trace of Hermitian operators $\exp\hat{G}$ in the space of dimension $2J+1$ as follows:

$$\frac{2J+1}{4\pi}\int e^{Q_J(\hat{G};\Omega)}d\Omega \le \mathrm{Tr}_J e^{\hat{G}} \le \frac{2J+1}{4\pi}\int e^{P_J(\hat{G};\Omega)}d\Omega\,. \tag{2.4}$$

The lower bound is due to Bogoliubov, the upper bound is due to Lieb.[12]

The P and Q representatives of the general pseudospin Hamiltonian are easily constructed using (2.3) and the homogeneity relation $\mathcal{Y}^L_M(\vec{J}/N) = N^{-L}\mathcal{Y}^L_M(\vec{J})$.

III. TRIAL STATES FOR A VARIATIONAL CALCULATION: $T=0$

Since the atomic coherent states $|J,\Omega\rangle$ are overcomplete, any state $|\psi\rangle$ in the $(2J+1)$ dimensional subspace has an integral representation of the form

$$|\psi\rangle = \int \left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle f(\Omega)d\Omega\,. \tag{3.1}$$

For the MGL Hamiltonian, it is known that the ground state lies in the SU(2)-invariant subspace with maximum allowed $J=N/2$. This is true for all psuedospin Hamiltonians (1.1).[5] In particular, the ground state eigenfunction can always be represented in the form (3.1) with $J=N/2$.

If we choose a class of trial states of the form

$$|\psi_{\mathrm{tr}}\rangle = \left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle,\quad J=N/2 \tag{3.2}$$

for a variational calculation, then we find

$$E_g \le \min_\Omega \left\langle\begin{matrix}J\\ \Omega\end{matrix}\right|\hat{\mathcal{H}}\left|\begin{matrix}J\\ \Omega\end{matrix}\right\rangle, \le \min_\Omega Q_J(\hat{\mathcal{H}};\Omega)\,,\quad J=N/2\,. \tag{3.3}$$

Thus, the existence of the Q representative of

$\hat{\mathcal{H}}$ as the upper bound on the ground state energy is tantamount to choosing the coherent states (3.2) as trial state for a variational calculation. Furthermore, the near equality[4] between E_g and $Q_{N/2}(\hat{\mathcal{H}};\Omega_0)$, where Ω_0 minimizes $Q_{N/2}(\hat{\mathcal{H}};\Omega)$, suggests that $|J=N/2,\Omega_0\rangle$ is a good approximation to the exact ground state eigenfunction (3.1) for the MGL Hamiltonian. This in turn suggests that the function $f(\Omega)$ is sharply peaked around Ω_0.

IV. TRIAL STATES FOR A VARIATIONAL CALCULATION: $T>0$

At finite temperatures a quantum mechanical system is not in a pure state, but rather a statistical superposition of states. The state of such a system must be represented by a density operator $\hat{\rho}$ (known as the "Gibbs state").[6]

We show in Appendix A that the most general permutation-invariant operator for a system of N identical particles can be represented in the form

$$\hat{\rho}=\sum_{J=0\text{or}1/2}^{N/2}\frac{2J+1}{4\pi}\int\sum_{\alpha=1}^{Y(N,J)}\left|\begin{matrix}J\\ \Omega,\alpha\end{matrix}\right\rangle P_J(\Omega)\left\langle\begin{matrix}J\\ \Omega,\alpha\end{matrix}\right|d\Omega \tag{4.1}$$

in the atomic coherent state representation. The outer sum is over all J values which can occur by combining N pseudospin $\frac{1}{2}$ nucleons;

$$Y(N,J)=(2J+1)N!\left[\left(\tfrac{1}{2}N+J+1\right)!\left(\tfrac{1}{2}N-J\right)!\right]^{-1} \tag{4.2}$$

is the number of times the angular momentum J occurs, and $\alpha=1,2,\ldots,Y(N,J)$ indexes the $Y(N,J)$ different SU(2)-invariant subspaces of dimension $2J+1$. Expression (4.1) is the finite-temperature analog of the zero-temperature statement (3.1). The analogs of the trial pure state (3.2) are the trial Gibbs states

$$\hat{\rho}_{\text{tr}}=d\sum_{\alpha=1}^{Y(N,J)}\left|\begin{matrix}J\\ \Omega\alpha\end{matrix}\right\rangle\left\langle\begin{matrix}J\\ \Omega\alpha\end{matrix}\right|, \tag{4.3}$$

where d is a constant to be computed.

The corresponding pictorial representation of these trial states is apparent: The states (4.3) exist in one to one correspondence with points on spherical shells of radii $r=J/N$. In the nuclear matter limit, the states (4.3) exist in one to one correspondence with points in the interior of, or on the boundary of, a sphere of radius $\frac{1}{2}$.

The appropriate trial Gibbs state is the state which minimizes the free energy operator

$$\hat{F}=\hat{H}-T\hat{S}. \tag{4.4}$$

Since

$$E=\langle\hat{H}\rangle=\text{Tr}\hat{\rho}\hat{H} \tag{4.5}$$

and

$$S=-k_B\text{Tr}\hat{\rho}\ln\hat{\rho}=\text{Tr}\hat{\rho}(-k_B\ln\hat{\rho}), \tag{4.6}$$

the entropy operator is $-k_B\ln\hat{\rho}$ and the free energy operator is

$$\hat{F}=\hat{H}-T(-k_B\ln\hat{\rho})=\hat{H}+\beta^{-1}\ln\hat{\rho}. \tag{4.7}$$

For a variational calculation, the trial states (4.3) provide an upper bound on the free energy

$$\begin{aligned}F=\langle\hat{F}\rangle&=\text{Tr}\hat{\rho}\hat{F}\\ &\leqslant\text{Tr}\hat{\rho}_{\text{tr}}\hat{H}+k_BT\,\text{Tr}\hat{\rho}_{\text{tr}}\ln\hat{\rho}\\ &\leqslant\text{Tr}\hat{\rho}_{\text{tr}}\hat{H}+k_BT\,\text{Tr}\hat{\rho}_{\text{tr}}\ln\hat{\rho}_{\text{tr}}.\end{aligned} \tag{4.8}$$

The second term on the right hand side of (4.8) can be computed as follows. We note that

$$\begin{aligned}&\hat{\rho}_{\text{tr}}=d\sum_{\alpha=1}^{Y(N,J)}|\psi_\alpha\rangle\langle\psi_\alpha|,\\ &\text{Tr}\hat{\rho}_{\text{tr}}=\text{Tr}d\sum_{\alpha=1}^{Y(N,J)}|\psi_\alpha\rangle\langle\psi_\alpha|\\ &\quad=d\sum_{\alpha=1}^{Y(N,J)}\langle\psi_\alpha|\psi_\alpha\rangle=dY=1,\\ &\text{Tr}\hat{\rho}_{\text{tr}}^{\,2}=\text{Tr}\left(d\sum_{\alpha=1}^{Y(N,J)}|\psi_\alpha\rangle\langle\psi_\alpha|\right)\left(d\sum_{\alpha'=1}^{Y(N,J)}|\psi_{\alpha'}\rangle\langle\psi_{\alpha'}|\right)\\ &\quad=d^2\sum_{\alpha=1}^{Y(N,J)}\sum_{\alpha'=1}^{Y(N,J)}\langle\psi_{\alpha'}|\psi_\alpha\rangle\langle\psi_\alpha|\psi_{\alpha'}\rangle=d^2Y=d\\ &\quad\cdots\\ &\text{Tr}\hat{\rho}_{\text{tr}}^{\,n+1}=d^n=[Y(N,J)]^{-n}.\end{aligned} \tag{4.9}$$

The second line of (4.9) comes from the normalization condition on density operators ($\text{Tr}\hat{\rho}=1$). If $\ln X=\sum c_jx^j$ is any convergent expansion for $\ln X$,

$$\begin{aligned}\text{Tr}\hat{\rho}_{\text{tr}}\ln\hat{\rho}_{\text{tr}}&=\text{Tr}\hat{\rho}_{\text{tr}}\sum_j c_j(\hat{\rho}_{\text{tr}})^j\\ &=\sum_j c_j[Y(N,J)]^{-j}\\ &=-\ln Y(N,J).\end{aligned} \tag{4.10}$$

The first term on the right hand side of (4.8) is

$$\begin{aligned}\text{Tr}\hat{\rho}_{\text{tr}}\hat{H}&=\text{Tr}\left(d\sum_{\alpha=1}^{Y(N,J)}\left|\begin{matrix}J\\ \Omega,\alpha\end{matrix}\right\rangle\left\langle\begin{matrix}J\\ \Omega,\alpha\end{matrix}\right|\right)\hat{H}\\ &=d\sum_{\alpha=1}^{Y(N,J)}\left\langle\begin{matrix}J\\ \Omega\alpha\end{matrix}\right|\hat{H}\left|\begin{matrix}J\\ \Omega\alpha\end{matrix}\right\rangle.\end{aligned} \tag{4.11}$$

The expectation values are independent of the index α, so the summation in (4.11) is just the

Q representative of $\hat{H}$. Therefore the inequality on the free energy in (4.8) becomes

$$F \leq Q_J(\hat{H};\Omega) - T(k_B \ln Y(N,J)) . \tag{4.12}$$

This estimate must hold for all trial Gibbs states (4.3), so that

$$F \leq \underset{J,\Omega}{\text{Min}}\, Q_J(\hat{H};\Omega) - k_B T \ln Y(N,J) . \tag{4.13}$$

This is the upper bound on the free energy derived previously[5] in the nuclear matter limit, where $k_B \ln Y(N,J)$ has been interpreted as the nuclear entropy. As in Sec. III, the existence of the Q representative of $\hat{F}$ as the upper bound on the free energy is tantamount to using the Gibbs states (4.3) as trial states for a variational calculation. Further, if the free energy estimate from the variational calculation agrees closely with the exact free energy computed by diagonalizing the Hamiltonian, then for the J_0, Ω_0 which minimizes (4.4), $\hat{\rho}_{tr}$ is a good approximation to the nuclear Gibbs state and the weighting function $P_J(\Omega)$ is sharply peaked around J_0, Ω_0.

V. COMPARISON WITH EXACT FREE ENERGY

In order to estimate how good an approximation the best trial Gibbs state (4.3) is to the exact Gibbs state $\exp\beta(F-\hat{\mathcal{H}})$ we have chosen once again to work with the MGL Hamiltonian

$$\hat{\mathcal{H}} = \epsilon J_3 + \frac{V}{2N}(J_+^2 + J_-^2), \quad \epsilon = 1 . \tag{5.1}$$

The free energy $F(\beta)$ was computed numerically according to

$$e^{-\beta F} = \sum_{J=0\text{or}1/2}^{N/2} Y(N,J) \sum_{M=-J}^{+J} e^{-\beta E(J,M;V)} \tag{5.2}$$

for $N = 14$, 30, 50, and 70, and $V = 0.25$, 0.5, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.5, and 5.0. In each of these cases we have compared the free energy computed according to (5.2) with the upper bounds computed according to (4.13). The actual method for constructing the piecewise linear upper bound is described in Appendix B. The free energy and its upper bound are compared in the worst case ($V = 0.5$) in Fig. 1 for $N = 30$, 50, 70. It is clear from these figures that the difference between the upper bound and $F(\beta)$ is of the order of $\ln N$, so that

$$\underset{J,\Omega}{\text{Min}}\{Q_J(\hat{\mathcal{H}};\Omega) - \beta^{-1}\ln Y(N,J)\}/N$$

becomes a better approximation to $F(\beta)/N$ as N increases. In the thermodynamic limit their difference vanishes.[5]

The Q and P representatives of $\hat{\mathcal{H}}$ provide

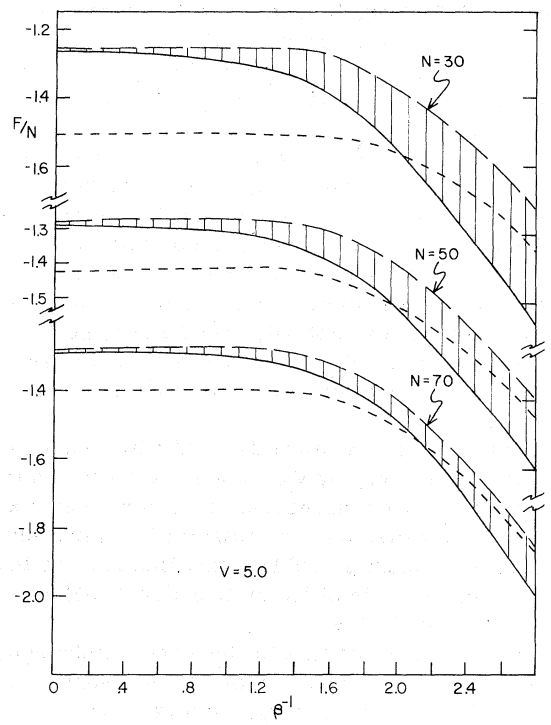

FIG. 1. The free energy per nucleon $F(\beta)/N$ (solid curve) is compared with the upper bound provided by the variational estimate (4.13) (long dashed curve). The function obtained by the substitution $Q_J(\hat{\mathcal{H}};\Omega) \to P_J(\hat{\mathcal{H}};\Omega)$ does not provide a rigorous lower bound on the free energy (short dashed curve). As N increases the variational estimate for $F(\beta)/N$ becomes an increasingly good approximation to the exact value of $F(\beta)/N$. These calculations were done for the MGL Hamiltonian with $V = 5.0$ and $N = 30$, 50, 70.

rigorous upper and lower bounds on the nuclear ground state energy, by the Bogoliubov and Lieb inequalities (2.4) for $J = N/2$, $\hat{G} = -\beta\hat{\mathcal{H}}$, in the $T \to 0$ limit. The Q representative of $\hat{F}$ provides a rigorous upper bound on the free energy by the variational computation (4.13). However, there is no argument that can be used to show that the P representative of $\hat{F}$ is a rigorous lower bound on $F(\beta)$. [Such an argument could be made only if there were a factor such as β or N in the exponent in (2.4) which became very large. This is why the P representative is a rigorous lower bound only for the ground state ($\beta \to \infty$) and in the thermodynamic limit ($N \to \infty$).] The short dashed lines in Fig. 1 are the curves

$$\underset{J,\Omega}{\text{Min}}\, P_J(\hat{\mathcal{H}};\Omega) - \beta^{-1}\ln Y(N,J) . \tag{5.3}$$

It is certainly clear that (5.3) does not provide a lower bound for $F(\beta)$. However, in the $T \to 0$

limit, (5.3) does, in fact, provide a rigorous lower bound on the ground state energy. It is clear that the upper bound [(4.13) with $T \to 0$] is a much better approximation to the ground state energy.

From Fig. 1 we see that for fixed N, the best trial Gibbs state becomes an increasingly poor approximation to the correct density operator as the temperature increases. This is because the trial Gibbs state involves only a single value of J at any temperature T whereas the exact density operator includes not only that J value, but others as well. Moreover, the other J values occur with increasing probability as the temperature increases.

For fixed temperature the trial Gibbs state becomes an increasingly good approximation as the particle number increases. This is because the width of the distribution $P_J(\Omega)$ [in (4.1)] increases around the most probable J only like $\ln N$, so that the relative width of the distribution $P_J(\Omega)$ decreases like $\ln N/N$.

Figure 1 reveals that the best trial Gibbs state is a reasonable approximation to the density operator when either β is large or N is large.

VI. PHASE TRANSITION TEMPERATURE

In the nuclear matter limit ($N \to \infty$), the thermodynamic phase transition has a very graphic representation. In the case of finite N, the free energy $F(\beta)$ (5.2) is a smooth function of β. It is as difficult to make statements about thermodynamic phase transitions in this numerical calculation case as it was to make statements about ground state energy phase transitions from the numerical ground state energy calculations carried out initially by Meshkov, Glick, and Lipkin.

As in the ground state case, so also in the thermodynamic case, the variational calculation very clearly exhibits the phase transition when it occurs. In the ground state case, the second order ground state energy phase transition occurs as a function of increasing nuclear interaction parameter V when the minimum of

$$\mathrm{Min}_{\Omega} Q_J(\hat{\mathcal{H}}_{\mathrm{MGL}};\Omega) = \mathrm{Min}_{J=N/2} \left[J\cos\theta + \frac{V}{2N} J(J-\tfrac{1}{2}) \times \sin^2\theta (e^{2i\phi} + e^{-2i\phi}) \right] \tag{6.1}$$

moves from $\theta = \pi$ to $\theta \neq \pi$. This occurs for $|V| = (1 - N^{-1})^{-1}$. In the thermodynamic case, the most likely value of J decreases from $J \simeq \sqrt{N}/2$ at very high temperatures, to $J = N/2$ at $T = 0$. If $\mathrm{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega)$ occurs at $\theta = \pi$ for high temperatures when $J \simeq \sqrt{N}/2$, but at $\theta \neq \pi$ at $T = 0$ when $J = N/2$, then at some intermediate temperature the minimum will move from $\theta = \pi$ (spherical) to $\theta \neq \pi$ (deformed). For the MGL Hamiltonian this transition occurs for $2J - 1 \simeq N/|V|$. The temperature at which this second order thermodynamic phase transition occurs is given approximately by

$$\beta_c = \ln[Y(N,J)/Y(N,J+1)]\,|_{J \simeq N/2|V|+1/2}\,. \tag{6.2}$$

We show in Fig. 2 the upper bound on $F(\beta)/N$ for $V = 0.25$, 0.5, 5.0, and $N = 70$. The point of departure of the upper bound from the zero interaction bound ($V = 0$) indicates the rough location of the phase transition. These estimates for the location of the second order thermodynamic phase transition are close to the thermodynamic phase transition temperatures which can be determined exactly in the thermodynamic limit from the analytic expression[5]

$$|V| \tanh \tfrac{1}{2}\beta_c = 1\,. \tag{6.3}$$

The phase transition temperatures for $N = 70$ and $V = 2.5$, 3.5, 5.0 are compared with the phase

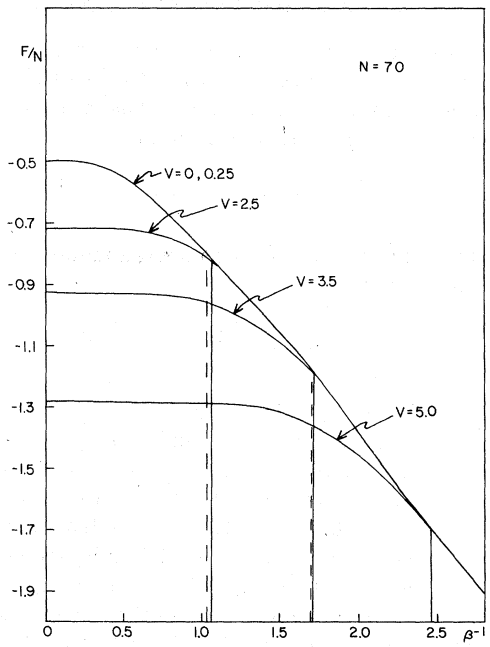

FIG. 2. The upper bound on $F(\beta)/N$ is plotted for the MGL Hamiltonian with $N = 70$ and $V = 0$, 2.5, 3.5, 5.0. For $0 < V < 1.0$, the upper bound is that given for $V = 0$. For $V > (1 - \frac{1}{70})^{-1}$, the temperature at which the upper bound departs from the $V = 0$ upper bound indicates the approximate temperature at which the thermodynamic phase transition takes place (solid lines). The thermodynamic phase transition temperature in the nuclear matter limit is shown by a dashed curve, which is not resolved for $V = 5.0$.

transition temperatures for $N \to \infty$ in Fig. 2.

We would like to point out that the phase transition problem has also been studied by Holzwarth.[13]

VII. SUMMARY AND CONCLUSIONS

For pseudospin Hamiltonians the nuclear ground state can be represented exactly by a superposition (3.1) of atomic coherent states drawn from the subspace with $J=N/2$. The atomic coherent states themselves can be used as trial states for a variational estimate of the nuclear ground state energy (3.2). The estimate is a good approximation to the exact ground state energy, suggesting that the corresponding atomic coherent state is a good approximation to the exact ground state wave function, or alternatively, that the weighting function $f(\Omega)$ appearing in (3.1) is sharply peaked about the value Ω_0 which minimizes $Q_J(\hat{\mathcal{H}};\Omega)$.

The nuclear density operator $\hat{\rho}=\exp\beta(F-\hat{\mathcal{H}})$ can be represented exactly by a superposition (4.1) of irreducible Gibbs states. These Gibbs states themselves can be used as trial states for a variational estimate of the nuclear free energy. This estimate is a reasonable approximation to the exactly computed free energy. The approximation becomes better as $T \to 0$ or as $N \to \infty$. This suggests that the corresponding Gibbs state is a good approximation to the exact density operator, or alternatively, that the weighting function $P_J(\Omega)$ appearing in (4.1) is sharply peaked about the values J_0, Ω_0 which minimize (4.13).

The free energy upper bound is a piecewise linear function which is easily constructed. The temperature at which the second order thermodynamic phase transition occurs may be determined more easily from the upper bound than from the exactly computed free energy. For large N the phase transition temperature is given to good approximation by (6.3), which determines the critical temperature $T_c=1/k\beta_c$ for $|V|>1$ in the thermodynamic limit.

Both for finite N and in the thermodynamic limit, the atomic coherent state representation provides a very graphic description of both the nuclear ground state and the nuclear Gibbs state. The point (a) on the Bloch sphere surface which minimizes the Hamiltonian corresponds to the best trial ground state, and the point (b) in the Bloch sphere which minimizes the free energy operator corresponds to the best trial Gibbs state. These points move as (a) the nuclear interaction parameters change and as (b) the temperature changes. The departure of the point from the south polar axis $\theta=\pi$ indicates (a) a second order ground state energy phase transition and (b) a second order thermodynamic phase transition.

APPENDIX A

In this appendix, we derive the expression for the density operator ("Gibbs" state) expanded in the ACGT[9] representation.

The most general operator on the N-particle pseudospinor Hilbert space $\mathcal{H}$ of the Hamiltonian can be written as

$$\theta_p=\sum_{JJ'}\sum_{\substack{MM'\\ \alpha\alpha'}}\left|\begin{matrix}J\lambda\\ M\alpha\end{matrix}\right\rangle A^{JJ'}_{M\alpha,M'\alpha'}\left\langle\begin{matrix}J'\lambda'\\ M'\alpha'\end{matrix}\right| . \tag{A1}$$

In the above expression, J indexes an SU(2) irreducible representation of dimension $2J+1$ and M indexes the orthornormal basis vectors for the representation. The pseudospinor space is invariant under the permutation group P_N which permutes the labels of the N-fold degenerate states in the upper and lower levels. The label $\tilde{\lambda}=(\lambda_1,\lambda_2)$ indexes a P_N irreducible representation of dimension

$$\dim(\tilde{\lambda})=\frac{N!\,(2J+1)}{(\frac{1}{2}N+J+1)!\,(\frac{1}{2}N-J)!}=Y(N,J) . \tag{A2}$$

The label α indexes the orthogonal basis vectors for the representations. It should be noted that the label $\tilde{\lambda}$ is, in fact, redundant, since[9]

$$\lambda_1+\lambda_2=N \quad \text{and} \quad \lambda_1-\lambda_2=2J . \tag{A3}$$

The pseudospin operators are invariant under the operations of the permutation group P_N. Therefore, the Hamiltonian and density operator must also be invariant under P_N. The subset of operators (A1) invariant under P_N obeys $p\,\theta_p p^{-1}=\theta_p$ or

$$p\,\theta_p=\theta_p p , \quad p\in P_N . \tag{A4}$$

The permutation group operation on the bra and ket vectors in (A1) is

$$\begin{aligned} p\left|\begin{matrix}J\lambda\\ M\alpha\end{matrix}\right\rangle &=\left|\begin{matrix}J\lambda\\ M\beta\end{matrix}\right\rangle \Gamma^{\lambda}_{\beta\alpha}(p) ,\\ \left\langle\begin{matrix}J'\lambda'\\ M'\alpha'\end{matrix}\right| p &=\Gamma^{\lambda'}_{\alpha'\beta'}(p)\left\langle\begin{matrix}J'\lambda'\\ M'\beta'\end{matrix}\right| . \end{aligned} \tag{A5}$$

Here the invariant condition of (A4) may now be written as

$$\left|\begin{matrix}J\lambda\\M\beta\end{matrix}\right\rangle \Gamma^{\lambda}_{\beta\alpha}(p) A^{JJ'}_{M\alpha M'\alpha'} \left\langle\begin{matrix}J'\lambda'\\M'\alpha'\end{matrix}\right| = \left|\begin{matrix}J\lambda\\M\alpha\end{matrix}\right\rangle A^{JJ'}_{M\alpha M'\alpha'} \Gamma^{\lambda'}_{\alpha'\beta'}(p) \left\langle\begin{matrix}J'\lambda'\\M'\beta'\end{matrix}\right| . \quad \text{(A6)}$$

The outer products $|\rangle\langle'|$ are linearly independent basis vectors which span the linear vector space of operators on the N-particle pseudospin space. By standard theorems of linear vector space theory, the coefficients of corresponding basis vectors can be equated:

$$\Gamma^{\lambda}_{\alpha\beta}(p) A^{JJ'}_{M\beta M'\alpha'} = A^{JJ'}_{M\alpha M'\beta'} \Gamma^{\lambda'}_{\beta'\alpha'}(p), \quad p \in P_N . \quad \text{(A7)}$$

It is useful to regard the coefficients A, for fixed J,M,J',M', as a matrix with β,α' (or α,β') as the row and column indices. Then (A7) is a matrix equation. Since Γ^{λ} and $\Gamma^{\lambda'}$ are irreducible, we can exploit Schur's lemmas:

1. $A=0$ when $\lambda\neq\lambda'$, or equivalently from (A3), $J\neq J'$.

2. If $\lambda=\lambda'$, $A^{JJ'}_{M\alpha M'\beta}$ is a multiple of a unit matrix.

Combining the results of these two lemmas, we find

$$A^{JJ'}_{M\alpha M'\alpha} = A^{J}_{MM'} \delta_{JJ'} \delta_{\alpha\alpha'} . \quad \text{(A8)}$$

Therefore, the most general permutation invariant operator is

$$\theta_p = \sum_{J,MM'} \sum_{\alpha} \left|\begin{matrix}J\\M\alpha\end{matrix}\right\rangle A^{J}_{MM'} \left\langle\begin{matrix}J\\M'\alpha\end{matrix}\right| . \quad \text{(A9)}$$

Since every projector of the form $|J,M\rangle\langle J,M'|$ can be written in diagonal form in the atomic coherent state representation,[9] we have the alternative representation to (A9)

$$\theta_P = \sum_J \frac{2J+1}{4\pi} \int \sum_{\alpha} \left|\begin{matrix}J\\\Omega\alpha\end{matrix}\right\rangle P_J(\Omega) \left\langle\begin{matrix}J\\\Omega\alpha\end{matrix}\right| d\Omega . \quad \text{(A10)}$$

In the nuclear matter limit, it is possible to convert the sum over J into an integral over $r=J/N$ to give the following expression for the permutation-invariant operator in the atomic coherent state representation

$$\theta_p = \frac{N^2}{4\pi} \int r\,dr\,d\Omega \sum_{\alpha} \left|\begin{matrix}J=rN\\\Omega\quad\alpha\end{matrix}\right\rangle P(r,\Omega) \left\langle\begin{matrix}J=rN\\\Omega\quad\alpha\end{matrix}\right| , \quad \text{(A11)}$$

where the integral extends throughout a sphere of radius $\frac{1}{2}$ with a slightly altered measure.

APPENDIX B

The upper bound on the finite-temperature free energy of the MGL Hamiltonian for an N-nucleon system is given by (4.13)

$$F(\beta) \leq \operatorname*{Min}_{J,M} J\cos\theta + VJ(J-\tfrac{1}{2})\sin^2\theta\left(\frac{e^{2i\phi}+e^{-2i\phi}}{2}\right) - k_B T \ln Y(N,J) . \quad \text{(B1)}$$

This bound is easily constructed for all temperatures as follows. First, we find the minimum value of $Q_J(\hat{\mathcal{H}};\Omega)$ for each value of J. For the MGL Hamiltonian

$$\operatorname*{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega) = -J, \quad 2|V|(J-\tfrac{1}{2}) < 1$$

$$\operatorname*{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega) = -\frac{J}{2}\left[2|V|(J-\tfrac{1}{2}) + \frac{1}{2|V|(J-\tfrac{1}{2})}\right], \quad 2|V|(J-\tfrac{1}{2}) > 1 . \quad \text{(B2)}$$

For fixed J, the upper bound $\operatorname{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega) - kT\ln Y(N,J)$ is simply a straight line for which the y intercept is $\operatorname{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega)$ and the slope is $-k_B \ln Y(N,J)$. As J decreases from its maximum value $N/2$, the y intercept increases (becomes less negative) while the slope becomes more negative.

The free energy is bounded above by the envelope of straight lines. This envelope is most easily computed by determining the intersection points of successive lines. The straight line associated with $J=N/2$ is horizontal because $\ln Y(N,N/2)=\ln 1=0$. The value of k_BT at which the horizontal line intersects the straight line associated with $J=N-1$ is easily computed from

$$\operatorname*{Min}_{\Omega} Q_{N/2}(\hat{\mathcal{H}};\Omega) = \operatorname*{Min}_{\Omega} Q_{N/2-1}(\hat{\mathcal{H}};\Omega) - k_B T \ln Y(N,N/2-1) . \quad \text{(B3)}$$

More generally, the temperature at which the successive straight lines associated with J and $J-1$ intersect is given by

$$\operatorname*{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega) - k_B T \ln Y(N,J) = \operatorname*{Min}_{\Omega} Q_{J-1}(\hat{\mathcal{H}};\Omega) - k_B T \ln Y(N,J-1) , \quad \text{(B4)}$$

$$k_B T = \frac{\operatorname{Min}_{\Omega} Q_{J-1}(\hat{\mathcal{H}};\Omega) - \operatorname{Min}_{\Omega} Q_J(\hat{\mathcal{H}};\Omega)}{\ln Y(N,J-1) - \ln Y(N,J)} .$$

This result can be simplified further by noting that the difference of the logarithmic multiplicity factors is simply the logarithm of a ratio:

$$\ln[Y(N,J-1)/Y(N,J)] = \ln \frac{2J-1}{2J+1} \frac{\frac{1}{2}N+J+1}{\frac{1}{2}N-J+1} .$$

This construction is illustrated in Fig. 3 for $N = 30$.

From this figure we can see that as the temperature increases the most probable value of J becomes smaller. This occurs physically because the system moves toward increasing entropy ($s = \ln Y(N,J)$) and $Y(N,J)$ increases as J decreases, up to a point. The value of J for which the entropy is maximum is given approximately by $J \simeq \sqrt{N}/2$. For smaller values of J, the multiplicity $Y(N,J)$ decreases. As a result, in the high temperature limit the best trial Gibbs state (4.2) has $J \simeq \sqrt{N}/2$.

This upper bound construction gives a better indication of the thermodynamic phase transition than does the numerical computation (5.2) of $F(\beta)$. The phase transition occurs when the minimum of $Q_J(\hat{\mathcal{H}};\Omega)$ moves off the south polar axis $\theta = \pi$[5] as a function of decreasing temperature. For the MGL Hamiltonian, this occurs for a J value determined from $2|V|(J-\frac{1}{2}) = 1$ (cf. B.2). Thus, this piecewise linear approximation to the upper board on $F(\beta)$ reveals clearly that a second order thermodynamic phase transition occurs at the temperature at which the two straight lines with $J = J_c = [1/2|V| + \frac{1}{2}]$ and $J = J_c + 1$ intersect ($[x]$ is the greater integer or half integer in x, depending on whether N is even or odd).

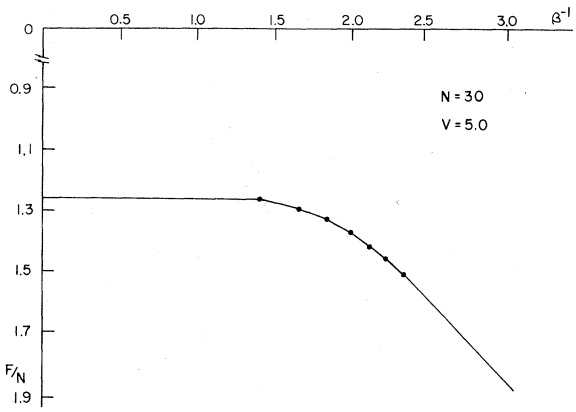

FIG. 3. The upper bound on $F(\beta)/N$ is computed here for the MGL Hamiltonian with $N = 30$ and $V = 5.0$. For fixed J, the upper bound (4.13) is a straight line with slope $-k_B \ln Y(N,J)$ and zero intercept $\mathrm{Min}_\Omega Q(\hat{\mathcal{H}};\Omega)$. The $(F/N, \beta^{-1})$ intersection points of all adjacent $(J, J+1)$ pairs of lines are computed, and the piecewise linear upper bound is drawn by "connecting the dots," as in a child's coloring book.

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