Lower Bounds to the Many-Body Problem Using Density Matrices*

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Variation principles for obtaining lower bounds by means of density matrices are applied to a number of many-body problems. This is done by means of restrictions derived from the study of exacly solvable models. Two classes of problems are considered: (a) obtaining a lower bound to the ground-state energy of a system of particles, and (b) obtaining a lower bound to the Helmholtz free energy. For the first case an exact lower bound is obtained for the ground-state energy of the particle-conserving Bogoliubov Hamiltonian. Of particular significance in the nonzero temperature case is a rigorous lower bound to the free energy of the Ising model with small external field at low temperatures.

I. INTRODUCTION

ALTHOUGH variation principles have been used for some time in obtaining energy levels for the quantum mechanical many-body problem, the systematic application of variational principles involving density matrices (to be defined) has only developed very recently. To illustrate the basic idea involved, we recall that in obtaining a lowest-energy eigenvalue E_0 for some Hamiltonian H, one tries to minimize $\int\psi^*(1,2,\cdots,N)H\psi(1,2,\cdots,N)d1, d2, \cdots, dN$ by varying this expression over all normalized symmetrized functions $\psi(1,2,\cdots,N)$. For two-body interactions, this is equivalent to minimizing $\mathrm{tr}H^{(2)}\Gamma^{(2)}$, where

$$H^{(2)}=\tfrac{1}{2}N[T(1)+T(2)]+\tfrac{1}{2}N(N-1)v(12),$$

provided $\Gamma^{(2)}(1',2'|1,2)$ is an N-representable normalized density matrix, i.e., it comes from integrating some function of the form $\sum_i\lambda_i\psi_i^*(1',2',3,\cdots,N)\times\psi_i(1,2,3,\cdots,N)(\lambda_i\geq 0, \sum_i\lambda_i=1)$ over the coordinates 3 to N.[1] If the latter restriction is disregarded, then minimizing $\mathrm{tr}H^{(2)}f^{(2)}$ over all functions $f^{(2)}(1',2'|1,2)$ of four arguments satisfying $\mathrm{tr}f^{(2)}=1$ (which is a larger set of functions than the set of N-representable density matrices $\Gamma^{(2)}$ and includes $\Gamma^{(2)}$ as a subset) results in obtaining either E_0 exactly or a value less than E_0.[2] Usually one will not be so fortunate as to obtain precisely E_0 except for the most trivial cases.

If all the conditions needed to guarantee that a function $f^{(2)}(1',2'|1,2)$ of four arguments is an N-representable density matrix were known, then we could simply minimize subject to $f^{(2)}$ satisfying these restrictions and obtain E_0 exactly. However, a usable set of restrictions has yet to be found. Minimizing subject to no restrictions on $f^{(2)}$ will give a poor lower bound in many problems of interest.

In Sec. II of this paper, density-matrix methods are used on some models to see just how well these methods work. Section II A starts with an explanation of some of the properties of density matrices and includes a variational principle which involves minimizing subject to an inequality constraint. Section II B reviews the method of minimizing subject to inequality constraints and in Sec. II C this is actually carried out for the Ising model. A less accurate but much simpler variational principle is then derived in Sec. II D and is applied to the Ising model for comparison with the results of Sec. II C. Section II E describes how these principles can be applied to the infinite-boson problem.

Section III has to do with statistical mechanics at finite temperatures. The quantum variation principle mentioned above is actually the zero-temperature limit of a more general one in statistical mechanics. Section III A contains the derivation of a variation principle for obtaining a lower bound to the free energy. This principle is then applied in Sec. III B to the Ising model with a small external magnetic field.

II. DENSITY MATRIX METHODS

A. Properties of Density Matrices

It will be convenient to distinguish between density matrices and N-representable density matrices. Two-particle density matrices $f^{(2)}(1',2'|1,2)$ are functions of four arguments which satisfy the following conditions:

Non-negativity of $f^{(2)}$ as an operator;

$$(g,f^{(2)}g)\geq 0 \text{ for } any\ g(1,2). \tag{1}$$

Hermiticity;

$$f^{(2)}(1',2'|1,2)=(f^{(2)}(1,2|1',2'))^*. \tag{2}$$

Symmetry;

$$\begin{aligned}f^{(2)}(1,2|1',2')&=\pm f^{(2)}(2,1|1',2')\\&=\pm f^{(2)}(1,2|2',1').\end{aligned} \tag{3}$$

(This is for quantum systems, the plus sign for bosons and the minus sign for fermions.)

Normalization;

$$\mathrm{tr}f^{(2)}=1. \tag{4}$$

The normalized N-representable two-particle density matrix $\Gamma^{(2)}(1',2'|1,2)$ is a function which comes from integrating some function of the form

$$\sum_i\lambda_i\psi_i^*(1',2',3,\cdots,N)\psi_i(1,\cdots,N)$$

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[1] A. J. Coleman, Rev. Mod. Phys. 35, 668 (1963).

[2] C. Garrod and J. K. Percus, J. Math. Phys. 5, 1756 (1964).

over the coordinates 3 to N, where the functions ψ_i are symmetric or antisymmetric under interchange of a pair of particles for bosons or fermions. Not all of the density matrices $f^{(2)}$ will come from integrating over such functions, so that $f^{(2)}$ is a larger set than $\Gamma^{(2)}$, and includes the latter as a subset.

In estimating the lowest energy eigenvalue for some Hamiltonian H, one obtains the correct E_0 if $\Gamma^{(2)}$ is varied so as to minimize the expression $\mathrm{tr}H^{(2)}\Gamma^{(2)}$. Thus, if $\mathrm{tr}H^{(2)}f^{(2)}$ is varied over $f^{(2)}$, $\min_{f^{(2)}} \mathrm{tr}H^{(2)}f^{(2)}$ will not be greater than E_0, i.e., $\min_{f^{(2)}} H^{(2)}f^{(2)}\leq E_0$, and one obtains a lower bound.

Restricting $f^{(2)}$ further by conditions satisfied by $\Gamma^{(2)}$ can improve the lower bound. Any N-representable two-particle density matrix $\Gamma^{(2)}$ will satisfy the condition $\mathrm{tr}H_{\mathrm{mod}}{}^{(2)}\Gamma^{(2)}\geq E_0{}^{\mathrm{mod}}$, where $E_0{}^{\mathrm{mod}}$ is the ground-state energy corresponding to the Hamiltonian H_{mod}. When this condition is combined with the others, the variational principle takes the form

$$\min_{f^{(2)}} \mathrm{tr}H^{(2)}f^{(2)}\leq E_0, \tag{5}$$

where

$$\mathrm{tr}H_{\mathrm{mod}}{}^{(2)}f^{(2)}\geq E_0{}^{\mathrm{mod}}, \tag{6}$$

and $f^{(2)}$ satisfies conditions (1) through (4).

We might well expect that if H_{mod} is a good approximation to H, then the lower bound will be very close to the exact ground-state energy. Model Hamiltonians exist in the theory of spin waves, the theory of the electron gas, and of superfluidity, which are supposed to approximate the exact Hamiltonians. The latter case will be discussed in Sec. II E; however, it is appropriate to choose a special test case (the Ising model) to see how the lower bound obtained by this method approaches E_0 as H_{mod} begins to look like H. It is of course clear that if $H_{\mathrm{mod}}{}^{(2)}=H^{(2)}$ and thereby $E_0{}^{\mathrm{mod}}=E_0$, then (5) and (6) yield correctly $\mathrm{tr}H^{(2)}f^{(2)}=E_0$, but this is a singular situation with a very high degeneracy in $f^{(2)}$.

B. Minimizing Subject to Inequalities

In general, suppose one wants to find the minimum of some function $F(x,y,\cdots)$ subject to the condition $g(x,y,\cdots)\geq 0$. Assuming that F and g are continuous, as are their first derivatives, we first find all relative minima of F subject to no condition; those relative minima which satisfy $g(x,y,\cdots)<0$ are discarded. Next, we find the relative minima of F which are on the boundary described by $g(x,y,\cdots)=0$ (e.g., by use of Lagrange multipliers). The smallest of the relative minima of the two procedures is then the solution to our problem.

In our case, the problem is intrinsically simpler, because $F=\mathrm{tr}H^{(2)}f^{(2)}$ is a linear function of $f^{(2)}$ satisfying linear equalities (normalization, symmetry, Hermitian condition). F can therefore only achieve its minimum on the boundary of the region it is restricted to by any inequalities which are imposed. Furthermore, when the region is convex (the average of two density matrices is a guaranteed density matrix), the minimum must occur at an isolated point (or line segment, etc., in case of degeneracy). There are no additional relative minima, and so the only question is whether the minimum of $\mathrm{tr}H^{(2)}f^{(2)}$ with nonnegative $f^{(2)}$ already satisfies $g\geq 0$ or whether it occurs on the boundary $g=0$. We shall adopt the terminology (i) the minimum of F satisfies $g\geq 0$; g is inactive; (ii) the minimum of F is at $g<0$: g is active, and we must then choose the minimum of F subject to the restriction $g=0$.

Thus, when we wish to minimize $\mathrm{tr}H^{(2)}f^{(2)}$ over all pair density matrices subject to $\mathrm{tr}H_{\mathrm{mod}}{}^{(2)}f^{(2)}\geq E_0{}^{\mathrm{mod}}$, (i) and (ii) become, respectively,

$$\begin{aligned} &\text{(i)}\quad \delta\,\mathrm{tr}(H^{(2)}-\lambda)f^{(2)}=0;\quad E_0\geq\lambda,\\ &\text{(ii)}\quad \delta\,\mathrm{tr}(H^{(2)}-\gamma H_{\mathrm{mod}}{}^{(2)}-\lambda)f^{(2)}=0, \end{aligned} \tag{7}$$

subject to

$$\mathrm{tr}H_{\mathrm{mod}}{}^{(2)}f^{(2)}=E_0{}^{\mathrm{mod}};\quad E_0\geq\lambda+\gamma E_0{}^{\mathrm{mod}}.$$

Here we consider all variations δ maintaining the characteristic properties of a density matrix except for normalization. It is to be noted that in general there will be just one N-representable density matrix $f_s{}^{(2)}$ which satisfies $\mathrm{tr}H_{\mathrm{mod}}{}^{(2)}f_s{}^{(2)}=E_0{}^{\mathrm{mod}}$ and many which are not N-representable. When (ii) is active, one of the latter will in fact be obtained (unless H_{mod} happens to coincide with H).

C. Lower Bound for the Ising Model using Density Matrices

We shall go through the details for obtaining a lower bound for the N-particle Ising model ground-state energy in a nonaxial magnetic field $\mathbf{B}$. The Hamiltonian is

$$H=-\epsilon\sum_{k=1}^{N}\sigma_k{}^z\sigma_{k+1}{}^z-B_z\sum_{k=1}^{N}\sigma_k{}^z-B_x\sum_{k=1}^{N}\sigma_k{}^x, \tag{8}$$

where σ^x and σ^z are the Pauli spin matrices. Here, we can restrict our attention to the nearest-neighbor density matrix $f^{(2)}$, which may be expanded in a complete set of two-particle wave functions

$$f^{(2)}(12|1'2')=\sum_{i,j,l=1}^{4} b_{ij}b_{lj}{}^*|\psi_i(12)\rangle\langle\psi_l(1'2')|. \tag{9}$$

The coefficients have been written so as to ensure nonnegativity of $f^{(2)}$ as an operator. For the complete set we can use the following: $|\psi_1\rangle=\uparrow\uparrow$, $|\psi_2\rangle=\frac{1}{2}\sqrt{2}(\uparrow\downarrow+\downarrow\uparrow)$, $|\psi_3\rangle=\downarrow\downarrow$, and $|\psi_4\rangle=\frac{1}{2}\sqrt{2}(\uparrow\downarrow-\downarrow\uparrow)$. The expression

$$\begin{aligned}\mathrm{tr}H^{(2)}f^{(2)}=N[&-\epsilon\,\mathrm{tr}\sigma_1{}^z\sigma_2{}^zf^{(2)}(1,2|1',2')\\ &-B_z\,\mathrm{tr}\sigma_1{}^zf^{(2)}(12|1'2')-B_x\,\mathrm{tr}\sigma_1{}^xf^{(2)}(12|1'2')]\end{aligned} \tag{10}$$

may now be evaluated in terms of the coefficients b_{ij}.

(We have intentionally handicapped ourselves by working with a non-symmetric Hamiltonian. If the symmetric form of the two-particle Hamiltonian is used instead of (10), $f^{(2)}$ can be taken as symmetric and an improved bound is obtained.) The normalization for $f^{(2)}(1,2|1'2')$ gives

$$\sum_{i,j=1}^{4}|b_{ij}|^2=1.$$

Minimization is performed by Lagrange's method of multipliers by forming $F=\mathrm{tr}H^{(2)}f^{(2)}-\lambda_1 N\sum|b_{ij}|^2$ and minimizing this over the coefficients b_{ij}. Solving the resulting 4×4 determinant for λ_1 gives

$$\lambda_1=\pm((\epsilon\pm B_z)^2+B_x^2)^{1/2}.$$

Now $\min_{f^{(2)}}\mathrm{tr}H^{(2)}f^{(2)}=\min N\lambda_1$ is a lower bound to the exact ground-state energy E_0 of H, so we obtain (for ϵ and B_z positive)

$$E_0\geq -N((\epsilon+B_z)^2+B_x^2)^{1/2}.$$

The resulting density matrix $f^{(2)}$ has the form

$$f^{(2)}(1,2|1',2')=|\Psi(1,2)\rangle\langle\Psi(1',2')|, \qquad (11)$$

where

$$|\Psi(1,2)\rangle=(B_x^2+(\lambda+\epsilon+B_z)^2)^{-1/2}\times[B_x|\uparrow\uparrow\rangle-(\lambda+\epsilon+B_z)|\downarrow\uparrow\rangle]$$
$$\lambda=-(B_x^2+(\epsilon+B_z)^2)^{1/2},$$

and $f^{(2)}$ is not in general an N-representable density matrix, if only by virtue of not satisfying in general the relation

$$\mathrm{tr}_1 f^{(2)}(1,2|1',2')=\mathrm{tr}_3 f^{(2)}(2,3|2',3').$$

We next consider applying the equality-inequality restriction on the density matrix with a model Hamiltonian for which the lower bound to the N-particle system of Eq. (8) approaches E_0 as $H_{\mathrm{mod}}\to H$. For the model Hamiltonian we choose

$$H_{\mathrm{mod}}=-\epsilon'\sum_{k=1}^{N}\sigma_k^z\sigma_{k+1}^z-B_z'\sum_{k=1}^{N}\sigma_k^z-B_x'\sum_{k=1}^{N}\sigma_k^x=\sum_{k=1}^{N}(H_{\mathrm{mod}}^{(2)})_k.$$

Since we have already obtained the minimum for procedure (i) [Sec. II B], we now evaluate

$$\min_{f^{(2)}} N\,\mathrm{tr}\{[H_1^{(2)}-\gamma(H_{\mathrm{mod}}^{(2)})_1-\lambda_1]f^{(2)}(1,2|1',2')\}$$

to obtain

$$\min\{-N[[(\epsilon-\gamma\epsilon')\pm(B_z-\gamma B_z')]^2+(B_x-\gamma B_x')^2]^{1/2}\}\equiv\mu N.$$

The parameter γ may be found by solving

$$\mathrm{tr}H_{\mathrm{mod}}^{(2)}f^{(2)}=E_0^{\mathrm{mod}}$$

using the results of (11) together with the appropriate substitutions $\epsilon\to\epsilon-\gamma\epsilon'$, $B_x\to B_x-\gamma B_x'$, $B_z\to B_z-\gamma B_z'$, and $\lambda\to\mu$. The roots of this equation are found to be

$$\gamma=-\{K^2(xx'+zz')-(Kz'-x')(Kz-x)\}/\{(Kz'-x')^2-K^2(x'^2+z'^2)\}\pm\{[K^2(xx'+zz')-(Kz'-x')(Kz-x)]^2-[(Kz'-x')^2-K^2(x'^2+z'^2)]\times[(Kz-x)^2-K^2(x^2+z^2)]\}^{1/2}/\{(Kz'-x')^2-K^2(x'^2+z'^2)\}, \qquad (12)$$

where $z\equiv\epsilon\pm B_z$, $z'\equiv\epsilon'\pm B_z'$, $x\equiv B_x$, $x'\equiv B_x'$, and

$$K=\frac{-B_x'\pm[B_x'^2+[E_0^{\mathrm{mod}}/N+\epsilon'+B_z'][\epsilon'+B_z'-E_0^{\mathrm{mod}}/N]]^{1/2}}{[-E_0^{\mathrm{mod}}/N-\epsilon'-B_z']}; \qquad (13)$$

with the signs being chosen so that γ satisfies

$$\mathrm{tr}H_{\mathrm{mod}}^{(2)}f^{(2)}=E_0^{\mathrm{mod}}$$

and minimizes μ. Knowing ϵ, B_x, B_x', B_z, B_z', and E_0^{mod}, one may obtain γ from (12) and (13). Denoting the solution to procedure (ii) by E_{ii}, then

$$E_{ii}=\gamma E_0^{\mathrm{mod}}-N[(\epsilon-\gamma\epsilon'\pm B_z\mp\gamma B_z')^2+(B_x-\gamma B_x')^2]^{1/2}. \qquad (14)$$

If one lets $\epsilon'\to\epsilon$, $B_x'\to B_x$, and $B_z'\to B_z$, then γ reduces to 1, and since $E_0^{\mathrm{mod}}\to E_0$, $E_{ii}\to E_0$.

Numerical results have been obtained for the case $N=3$. Of course $E_0^{\mathrm{mod}}(\epsilon',B_x',B_z')$ must be known to be able to use the variational principle. The solution to E_0^{mod} for $N=3$ has been found in the appendix by the use of exact wave functions. For $\epsilon'=\epsilon$ and $B_z'=B_z$,

$$\mu=-N[(\epsilon+B_z)^2(1-\gamma)^2+(B_x-\gamma B_x')^2]^{1/2}.$$

Putting in the values $\epsilon'/B_z=\epsilon/B_z=2$, $B_z'/B_z=1$, and $B_x/B_z=3.5$ and evaluating E_{ii} from (14), one finds that for B_x'/B_z close to 3.5, E_{ii} is the lower bound E_{LB}, and a graph of the lower bound for this problem is shown in Fig. 1. The lower bound approaches E_0 $(=-12.784B_z)$ linearly from both sides of $B_x'/B_z=3.5$. Fig. 2 shows the exact levels of H.

D. A Second Variational Principle for Obtaining a Lower Bound to the Ground-State Energy

In this section we derive a variational principle which turns out to be the limit as the temperature goes to zero of another variational principle developed later for the free energy. We present it in this section in order to make a comparison with the previous variational principle (5) and (6).

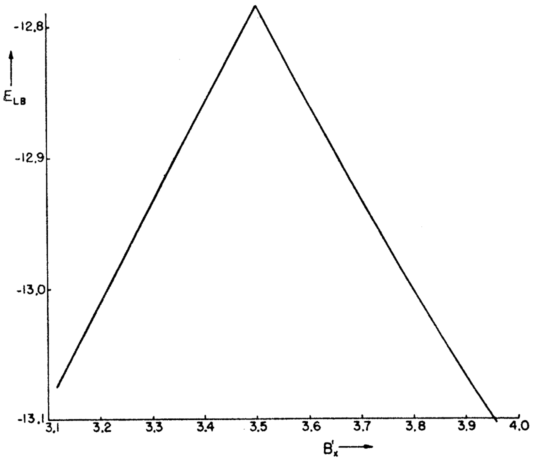

FIG. 1. Lower bound to the ground-state energy of the Hamiltonian H in units of B_z [$=\frac{1}{2}gm_B\times$ (z component of magnetic field), where m_B is the Bohr magneton] versus B_x' [$=\frac{1}{2}gm_B\times$ (x component of the external magnetic field for the model Hamiltonian H_{mod})] in units of B_z for $N=3$.

To start, let $\Gamma^{(2)}$ be an N-representable 2-particle density matrix which comes from the ground-state wave function of H. Then

$$E_0=\text{tr}H^{(2)}\Gamma^{(2)}\geq\text{tr}(H^{(2)}-H_{\text{mod}}{}^{(2)})\Gamma^{(2)}+E_0{}^{\text{mod}}$$
$$\geq\min_{f^{(2)}}(H^{(2)}-H_{\text{mod}}{}^{(2)})f^{(2)}+E_0{}^{\text{mod}},$$

so that our variational principle becomes

$$E_0\geq\min_{f^{(2)}}\text{tr}(H^{(2)}-H_{\text{mod}}{}^{(2)})f^{(2)}+E_0{}^{\text{mod}}. \tag{15}$$

Applying this to the example of the previous section, we obtain $\min_{f^{(2)}}\text{tr}(H^{(2)}-H_{\text{mod}}{}^{(2)})f^{(2)}=-N|B_x-B_x'|$ (for $\epsilon=\epsilon'=2$, $B_z=B_z'=1$), so

$$E_{\text{LB}}=-N|B_x-B_x'|+E_0{}^{\text{mod}}.$$

A graph of this result is represented by the solid line in Fig. 3. For comparison, the result of the previous section is shown dotted. For this example, the first variational principle gives a better bound than does the second one, but the latter is definitely simpler to apply. It can be shown that a suitable application of the weaker principle for the full class of models $\{\lambda H_{\text{mod}}\}$ is equivalent to the strong principle for the single model H_{mod}.

E. Lower Bound for the Particle-Conserving Bogoliubov Hamiltonian

By dropping certain terms in the exact Hamiltonian of a many-boson system in second-quantized form,

$$H=\frac{\hbar^2}{2m}\sum_{\mathbf{k}}k^2a_{\mathbf{k}}{}^\dagger a_{\mathbf{k}}+\frac{1}{2V}\sum_{\mathbf{kk}'}\sum_{\mathbf{q}\neq0}\tilde{v}(\mathbf{q})a_{\mathbf{k}}{}^\dagger a_{\mathbf{k}'}{}^\dagger a_{\mathbf{k}+\mathbf{q}}a_{\mathbf{k}'-\mathbf{q}}+\frac{1}{2}\frac{N(N-1)}{V}\tilde{v}(0), \tag{16}$$

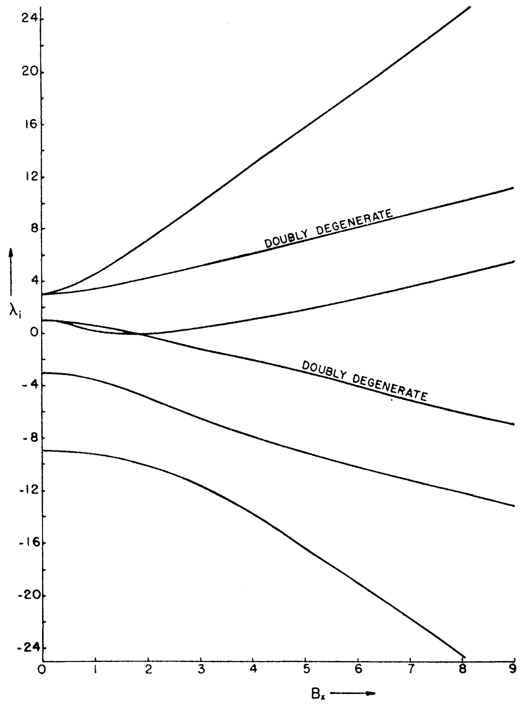

FIG. 2. Energy eigenvalues (in units of B_z) for the Hamiltonian H versus B_x (in units of B_z) for $N=3$.

where $\tilde{v}(\mathbf{q})\equiv\int e^{-i\mathbf{q}\cdot\mathbf{r}}v(\mathbf{r})d^3r$, one obtains the following reduced Hamiltonian:

$$H_{\text{mod}}=\frac{1}{2}\frac{N(N-1)}{V}\tilde{v}(0)+\frac{1}{2V}\sum_{\mathbf{k}\neq0}\tilde{v}(\mathbf{k})\{a_{\mathbf{k}}{}^\dagger a_{-\mathbf{k}}{}^\dagger a_0a_0+a_0{}^\dagger a_0{}^\dagger a_{\mathbf{k}}a_{-\mathbf{k}}\}+\sum_{\mathbf{k}\neq0}\left\{\frac{\hbar^2k^2}{2m}+\frac{\hat{N}_0}{V}\tilde{v}(\mathbf{k})\right\}a_{\mathbf{k}}{}^\dagger a_{\mathbf{k}}, \tag{17}$$

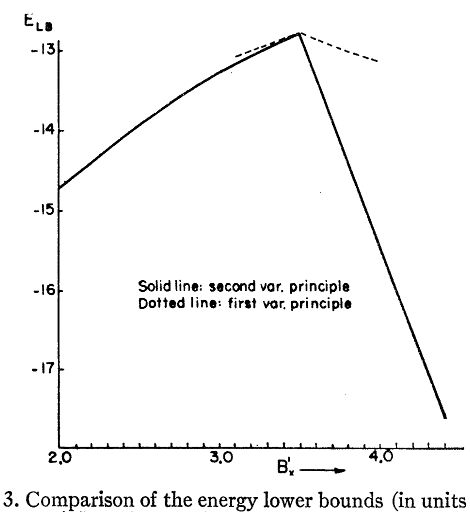

FIG. 3. Comparison of the energy lower bounds (in units of B_z) versus B_x' (in units of B_z) for the two variation principles.

where $\hat{N}_0 = a_0^\dagger a_0$. We call this the particle-conserving Bogoliubov Hamiltonian. The terms which have been deleted in going from Eqs. (16)–(17) are those with no zero momentum annihilation or creation operators, and those which contain only one $a_0^\dagger$ or one a_0.

Suppose we minimize the expectation of (17) using only the condition of (normalization and) positive definiteness of $\Gamma^{(2)}$. Since

$$\Gamma^{(2)}(mn|kl) = \langle a_k^\dagger a_l^\dagger a_m a_n \rangle , \tag{18}$$

this is clearly equivalent to the simple model condition

$$\langle \sum f_{kl} a_k^\dagger a_l^\dagger \sum \bar{f}_{nm} a_m a_n \rangle \geq 0 , \tag{19}$$

(owing to the fact that $A^\dagger A$ is a non-negative operator) a rudimentary form of the "Q-condition" of Garrod and Percus. As we have previously observed, the lower bound for E_0 is then precisely the ground-state energy of the effective 2-body Hamiltonian $H^{(2)}$. For (17), $H^{(2)}$ is given by

$$\begin{aligned} H_{\text{mod}}^{(2)} = \frac{1}{2}\frac{N(N-1)}{V}\bar{v}(0) &+ \frac{N}{2}\Big[\frac{p_1^2+p_2^2}{2m} + (N-1)\bar{v}(\mathbf{r}_1-\mathbf{r}_2)I(1)I(2) \\ &+ (N-1)I(1)I(2)\bar{v}(\mathbf{r}_1-\mathbf{r}_2) \\ &+ (N-1)(v^*(1)I(2)+I(1)v^*(2))\Big] , \end{aligned} \tag{20}$$

where

$$\bar{v}(\mathbf{r}) = v(\mathbf{r}) - \bar{v}(0)/N , \quad I(1)f(\mathbf{r}_1) = \frac{1}{V}\int f(\mathbf{r}_1')d\mathbf{r}_1' ,$$

$$v^*(1)f(\mathbf{r}_1) = \frac{1}{V}\int \bar{v}(\mathbf{r}_1-\mathbf{r}_1')f(\mathbf{r}_1')d\mathbf{r}_1' .$$

But Garrod[3] has proven that the lower bound ground-state variational problem for such a translation invariant system may rigorously be degraded to that of its relative coordinate, and so we may choose instead

$$H' = \frac{1}{2}\frac{N(N-1)}{V}\bar{v}(0) + \frac{N}{2}\Big[\frac{p^2}{m} + (N-1)(\bar{v}(r)I + I\bar{v}(r))\Big] . \tag{21}$$

H' of (21) is separable in k space, and we readily find the energy dispersion for $\bar{E} = E - \frac{1}{2}[N(N-1)/V]\bar{v}(0)$,

$$\frac{\bar{E}}{N} = \frac{1}{4}\left(\frac{N-1}{V}\right)^2 \sum_{k\neq 0} \frac{\bar{v}(\mathbf{k})^2}{\bar{E}/N - \hbar^2k^2/2m} . \tag{22}$$

It is clear that for this bound, $-E/N \propto N^{1/2}$ as $N \to \infty$ in the ground state, which therefore does not saturate—i.e., does not correspond to an extensive system.

[3] C. Garrod, Phys. Fluids **9**, 1764 (1966).

Blatant failure of the minimal criterion $E/N \to$ constant as $N \to \infty$ in the ground state is typical when the model used accomplishes only the requirement of positive definiteness. There is, however, another simple basically kinematical condition. Classically, it is the stability condition $g_k \geq -1/n$ which prevents unphysical density fluctuations. Here it exploits the simple model relation

$$\langle \sum f_{kl} a_k^\dagger a_l \sum \bar{f}_{nm} a_m^\dagger a_n \rangle \geq 0 , \tag{23}$$

and hence the positive definiteness of the matrix $\langle a_k^\dagger a_l a_m^\dagger a_n \rangle$. This is the "$G$-condition":

$$G(kl;nm) \equiv \langle a_k^\dagger a_m^\dagger a_l a_n \rangle + \delta_{lm}\langle a_k^\dagger a_n \rangle \tag{24}$$

is positive definite. In particular, consider only the 2×2 submatrix or Schwarz inequality condition

$$\begin{aligned} |\langle a_0^\dagger a_0^\dagger a_{\mathbf{k}} a_{-\mathbf{k}} \rangle| &= |\langle a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_0 a_0 \rangle| \leq (\langle \hat{N}_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle + \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle)^{1/2} \\ &\quad \times (\langle \hat{N}_0 a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} \rangle + \langle \hat{N}_0 \rangle)^{1/2} . \end{aligned} \tag{25}$$

Minimizing $\langle H_{\text{mod}} \rangle$ of (17) by using only (25), indeed weakened by replacing $\langle \hat{N}_0 \rangle$ by N, we find (assume $\bar{v}(\mathbf{k}) \geq 0$)

$$\begin{aligned} E = \sum \{ [\alpha(\mathbf{k})T_{\mathbf{k}} + \rho\bar{v}(\mathbf{k})]\rho(\mathbf{k}) - \rho\bar{v}(\mathbf{k})[1+\alpha(\mathbf{k})/N]^{1/2} \\ \times [\rho(\mathbf{k})(1+\rho(-\mathbf{k}))]^{1/2} \} + \tfrac{1}{2}(N^2/V)\bar{v}(0) , \end{aligned} \tag{26}$$

where

$$T_{\mathbf{k}} = \hbar^2k^2/2m , \quad \rho = N/V , \quad \rho(\mathbf{k})N = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \hat{N}_0 \rangle ,$$
$$\alpha(\mathbf{k})\rho(\mathbf{k}) \equiv \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle .$$

This still must be varied over the independent quantities $\rho(\mathbf{k})$ and $\alpha(\mathbf{k})$. Varying over $\rho(\mathbf{k})$ by setting $\partial E/\partial\rho(\mathbf{k}) = 0$ [and noting that $\rho(\mathbf{k}) = \rho(-\mathbf{k})$ in the ground state],

$$\begin{aligned} E(\alpha) = -\tfrac{1}{2}\sum_{\mathbf{k}\neq 0} \{ T_{\mathbf{k}}\alpha(\mathbf{k}) + \rho\bar{v}(\mathbf{k}) - [(T_{\mathbf{k}}\alpha(\mathbf{k}) + \rho\bar{v}(\mathbf{k}))^2 \\ - \rho^2\bar{v}(\mathbf{k})^2(1+\alpha(\mathbf{k})/N)]^{1/2} \} + \tfrac{1}{2}(N^2/V)\bar{v}(0) . \end{aligned} \tag{27}$$

But $\langle a_{\mathbf{k}}^\dagger \hat{N}_0 a_{\mathbf{k}} \rangle / \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \leq N-1$, so that $\alpha(\mathbf{k}) \geq 1$, and since $\partial E(\alpha)/\partial\alpha(\mathbf{k}) \geq 0$, the minimum occurs at $\alpha(\mathbf{k}) = 1$. A lower bound to the ground-state energy of H_{mod} is then given by the Bogoliubov energy

$$\begin{aligned} E_B = -\tfrac{1}{2}\sum_{\mathbf{k}\neq 0} \{ T_{\mathbf{k}} + \rho\bar{v}(\mathbf{k}) - [(T_{\mathbf{k}} + \rho\bar{v}(\mathbf{k}))^2 - \rho^2\bar{v}(\mathbf{k})^2]^{1/2} \} \\ + \tfrac{1}{2}(N^2/V)\bar{v}(0) , \end{aligned} \tag{28}$$

which now satisfies $E/N \to$ const as $N \to \infty$ at fixed ρ.

Even Eq. (28) is not the best bound available from the present elementary viewpoint, for the obvious condition $\sum_{k\neq 0} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \leq N$ may fail to be satisfied (granted, the Bogoliubov model is not very suitable under this circumstance). Of course, one may expect to do much better if the full G-condition is utilized.

III. LOWER BOUNDS TO THE FREE ENERGY USING DENSITY MATRICES

A. Variation Principles for the Free Energy

There exist a number of variation principles giving an upper bound to the free energy. Peierls's variational principle bounds the partition-function Q by the following inequality

$$Q \geq \sum_n e^{-\beta(\Phi_n, H\Phi_n)},$$

where $[\Phi_n]$ is an arbitrary orthonormal set of wave functions. This in turn puts an upper limit on the free energy.

A variational principle due to Gibbs is the following:

$$F \leq \mathrm{tr}\{\rho(H+kT\ln\rho)\},$$

where ρ is an arbitrary normalized density, and $F = -kT\ln\mathrm{tr}[\exp(-\beta H)]$. This principle reduces in the limit of $T=0$ to the standard quantum-mechanical variational principle

$$E_0 \leq \mathrm{tr}\rho H.$$

It is quite easy to show that Gibbs's variational principle is equivalent to what is known as Bogoliubov's variation principle, which is

$$F \leq F_{\mathrm{mod}} + \mathrm{tr}\{(H-H_{\mathrm{mod}})\Gamma_{\mathrm{mod}}{}^N\}, \tag{29}$$

where $\Gamma_{\mathrm{mod}}{}^N$ and F_{mod} are the statistical density matrix and free energy corresponding to some Hamiltonian H_{mod}.

If the two systems are interchanged in (29), then there results after rearranging the inequality

$$F \geq \mathrm{tr}\{(H-H_{\mathrm{mod}})\Gamma^N\} + F_{\mathrm{mod}}$$
$$\geq \min_{f^N}\{(H-H_{\mathrm{mod}})f^N\} + F_{\mathrm{mod}},$$

so that a lower bound to the free energy is given by

$$F \geq \min_{f^N}\mathrm{tr}\{(H-H_{\mathrm{mod}})f^N\} + F_{\mathrm{mod}}, \text{ where } \mathrm{tr}f^N = 1, \tag{30}$$

or by

$$F \geq \min_{f^{(2)}}\mathrm{tr}\{(H^{(2)}-H_{\mathrm{mod}}{}^{(2)})f^{(2)}\} + F_{\mathrm{mod}}, \tag{31}$$

where $\mathrm{tr}f^{(2)}=1$.

Note that in the limit that $T=0$, (31) reduces to (15).

B. Lower Bound to the Free Energy of the Two-Dimensional Ising Model

The Ising model in a magnetic field in two dimensions has the following Hamiltonian:

$$H = -\epsilon \sum_{m,n=1}^{\surd N} \sigma_{m,n}{}^z \sigma_{m,n+1}{}^z - \epsilon \sum_{m,n=1}^{\surd N} \sigma_{m,n}{}^z \sigma_{m+1,n}{}^z - B \sum_{m,n=1}^{\surd N} \sigma_{m,n}{}^z,$$

where m and n refer to the row and column of a lattice site. For a model system we choose the field-free case

$$H_{\mathrm{mod}} = -\epsilon' \sum_{m,n=1}^{\surd N} \sigma_{m,n}{}^z \sigma_{m,n+1}{}^z - \epsilon' \sum_{m,n=1}^{\surd N} \sigma_{m,n}{}^z \sigma_{m+1,n}{}^z.$$

This system has for its free energy

$$F_{\mathrm{mod}}(\epsilon')/N = f_{\mathrm{mod}}(\epsilon') = -kT\ln(2\cosh 2\beta\epsilon') - \frac{kT}{2\pi}\int_0^\pi d\phi \ln\tfrac{1}{2}[1+(1-\kappa^2\sin^2\phi)^{1/2}],$$

where

$$\kappa(\epsilon') = 2\tanh 2\beta\epsilon'/\cosh 2\beta\epsilon'.$$

It can be shown that

$$\min_{f^N}\mathrm{tr}[(H-H_{\mathrm{mod}})f^N]/N = -2\Delta - B, \quad \Delta \geq -B/4$$
$$= 2\Delta, \quad \Delta \leq -B/4,$$

where $\Delta = \epsilon - \epsilon'$ and we consider only positive B. A lower bound to the Helmholtz free energy is given according to (30) by

$$F_{\mathrm{low}} = F_{\mathrm{mod}}(\epsilon-\Delta) - 2\Delta - B, \quad \Delta \geq -B/4$$
$$F_{\mathrm{low}} = F_{\mathrm{mod}}(\epsilon-\Delta) + 2\Delta, \quad \Delta \leq -B/4$$

valid for all $\epsilon - \Delta \geq 0$. This expression may now be maximized over Δ. We consider only the case $B/\epsilon \ll 1$. $f_{\mathrm{mod}}(\epsilon-\Delta)$ can then be expanded to first order to obtain

$$f_{\mathrm{mod}}(\epsilon-\Delta) = f_{\mathrm{mod}}(\epsilon) + \Delta\coth 2\beta\epsilon[1+(2/\pi)\kappa' K_1(\kappa)], \tag{32}$$

where

$$\kappa' = 2\tanh^2 2\beta\epsilon - 1 \quad \text{and} \quad K_1(\kappa) = \int_0^{\pi/2}\frac{d\phi}{(1-\kappa^2\sin^2\phi)^{1/2}}.$$

If one further considers this expression for very low temperatures, i.e., $\beta\epsilon \gg 1$, then

$$f_{\mathrm{low}} = f_{\mathrm{mod}}(\epsilon) - B - 8\Delta e^{-8\beta\epsilon}, \quad \Delta \geq -B/4$$
$$f_{\mathrm{low}} = f_{\mathrm{mod}}(\epsilon) + 4\Delta - 8\Delta e^{-8\beta\epsilon}, \quad \Delta \leq -B/4$$

and the maximum occurs at $\Delta = -B/4$. Our result is

$$f_{\mathrm{low}} \cong f_{\mathrm{mod}}(\epsilon) - B(1-2e^{-8\beta\epsilon}), \quad B/\epsilon \ll 1, \ \beta\epsilon \gg 1,$$

to first order in B/ϵ, keeping only the leading terms in a low-temperature expansion. Setting $\Delta = -B/4$ and evaluating $-(\partial f_{\mathrm{low}}/\partial B)_{B=0}$ for expression (32) then gives an upper bound to the spontaneous magnetization, and for $\beta\epsilon \gg 1$, one obtains

$$-\left(\frac{\partial f_{\mathrm{low}}}{\partial B}\right)_{B=0} = 1 - 2e^{-8\beta\epsilon},$$

keeping only the two leading terms in the expansion. Yang[4] has calculated the magnetization (see the article

[4] C. N. Yang, Phys. Rev. 85, 809 (1952).

by Schultz, Mattis, and Lieb[5] for comments on this calculation) to be

$$m=\left[\frac{(1+x^2)(1-6x^2+x^4)^{1/2}}{(1-x^2)^2}\right]^{1/4},\quad T<T_c$$

where $x=e^{-2\beta\epsilon}$ and $\sinh 2\epsilon/kT_c=1$. The two leading terms (at small temperature) of this result are in agreement with our result. At higher temperatures, the difference between the two magnetizations is considerable. The variational principle (30) is more suited for lower temperatures in this case because it emphasizes the energetic contribution of the applied field, as opposed to its entropic contribution.

APPENDIX: ENERGY EIGENVALUES FOR $N=3$

For $N=3$, we may expand the eigenfunctions Ψ_E of H in a complete set of 3-particle wave functions

$$\Psi_E(1,2,3)=\sum_{i=1}^{8} C_i\psi_i(1,2,3),$$

where

$$\begin{aligned}\psi_1&=(+++), & \psi_5&=(--+),\\ \psi_2&=(++-), & \psi_6&=(-+-),\\ \psi_3&=(+-+), & \psi_7&=(+--),\\ \psi_4&=(-++), & \psi_8&=(---).\end{aligned}$$

Then minimizing is equivalent to solving

$$\frac{\partial}{\partial C_i}(\langle\Psi_E|H|\Psi_E\rangle-\lambda\langle\Psi_E|\Psi_E\rangle)=0,$$

which results in the determinantal equation

$$\begin{vmatrix}\lambda+3(J+B_x) & B_x & B_x & B_x & 0 & 0 & 0 & 0\\ B_x & (\lambda+B_z-J) & 0 & 0 & 0 & B_x & B_x & 0\\ B_x & 0 & (\lambda+B_z-J) & 0 & B_x & 0 & B_x & 0\\ B_x & 0 & 0 & (\lambda+B_z-J) & B_x & B_x & 0 & 0\\ 0 & 0 & B_x & B_x & (\lambda-B_z-J) & 0 & 0 & B_x\\ 0 & B_x & 0 & B_x & 0 & (\lambda-J-B_z) & 0 & B_x\\ 0 & B_x & B_x & 0 & 0 & 0 & (\lambda-J-B_z) & B_x\\ 0 & 0 & 0 & 0 & B_x & B_x & B_x & \lambda+3(J-B_z)\end{vmatrix}=0.$$

Four roots can be factored out of this equation, namely,

$$\lambda_1=\lambda_2=J+(B_x^2+B_z^2)^{1/2},$$

$$\lambda_3=\lambda_4=J-(B_x^2+B_z^2)^{1/2},$$

leaving the quartic

$$\begin{aligned}\lambda_i^4+4J\lambda_i^3-2[5(B_x^2+B_z^2)+J^2]\lambda_i^2\\ +12J(B_z^2-J^2-3B_x^2)\lambda_i\\ +9(J^2-B_z^2-B_x^2)^2=0,\quad i=5,6,7,8\end{aligned}$$

to determine the remaining roots. The ground-state energy E_0 corresponds to the smallest λ_i ($i=1$ to 8).

[5] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).