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Static Path Approximation for the Nuclear Partition Function

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We propose to approximate the many-body partition function for a system of interacting Fermions by summing static paths of the Hubbard–Stratonovich representation. We demonstrate with a simple two-level model that the approximation is superior to finite temperature Hartree theory. Corrections to the approximation to second order in the inverse temperature are readily evaluated.

1. INTRODUCTION

The behavior of nuclei at high excitation energy is an interesting topic of study with new experimental probes available. However, the theory needs to be much improved from the present state. Standard many-body theory yields the finite temperature Hartree approximation, which is applied with a Brueckner or phenomenological effective interaction. The main physical shortcoming of Hartree theory is that the single mean field does not allow enough fluctuations to describe any sort of fluctuation phenomena at high temperature. Fluctuating mean fields have been incorporated in an ad hoc manner by computing a free energy surface in the space of nuclear shape degrees of freedom [1]. We would like an approximation that contains the same physics, but can be derived from a systematic theoretical framework.

The Hubbard–Stratonovich repesentation [2], of the partition function seems to provide a suitable framework. The Hartree approximation is contained as a definite approximation to the path integral. Namely, one replaces the integral by the integrand for this path. In our approximation we also start with static paths, but integrate over all such paths rather than simply take the most important. Since each static path is identical to a mean field configuration, the approximation in some way sums over fluctuations in the mean field. It should therefore be superior to a single-field approximation.

Our interest in this method is due to our belief that the technique can be applied to semi-realistic nuclear Hamiltonians. The integration over paths would be done by a Monte Carlo sampling method. Essentially, the work involved corresponds to calculating a single Hartree–Fock iteration for each sampled path. This would require considerably more work than is done in present calculations, but it is not out of bounds of what can be contemplated with present-day computers. Before

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embarking on a lengthy project using this approximation, we need to have some idea of its utility. In the paper, we apply the method to a simple model Hamiltonian to see how well it works.

In Section 2, the static path approximation to the partition function is defined. It is applied to the model Hamiltonian in Section 3. Higher order corrections are discussed in Section 4, while comparison with Hartree calculations is discussed in Section 5. Section 6 contains some concluding remarks.

2. Partition Function in Hubbard–Stratonovich Representation

The starting point of our discussion is the functional representation of the partition function. For simplicity we will consider the grand canonical partition function

$$Z = \mathrm{tr}\{e^{-\beta(\hat{H}-\mu\hat{N})}\}, \tag{2.1}$$

where $\hat{N}$ is the particle number operator, $\hat{H}$ the Hamiltonian of the system, and β the inverse temperature. We will refer to β as the time variable, due to the similarity of the exponential in (2.1) with the evolution operator.

We now require that the Hamiltonian be the sum of a one-body operator, $\hat{K}$, and two-body interactions that can be written as a negative definite quadratic form in one-body operators $\hat{\rho}_\alpha$,

$$\hat{H} = \hat{K} - \sum_\alpha \lambda_\alpha \hat{\rho}_\alpha \hat{\rho}_\alpha, \qquad \lambda_\alpha > 0. \tag{2.2}$$

The exponential in Eq. (2.1) is replaced by the Trotter product of L time slices, and the exponential on each slice is expressed as an integral over one-body Hamiltonians using the Hubbard–Stratonovich transformation. The partition function then has the appearance

$$\begin{aligned} Z = \lim_{L\to\infty} \prod_\alpha \left(\frac{\beta\lambda_\alpha}{\pi L}\right)^{L/2} \int \prod_{l\alpha} d\sigma_\alpha(t_l) \exp\left(-\frac{\beta}{L}\sum_{\alpha l} \lambda_\alpha \sigma_\alpha(t_l)^2\right) \\ \times \mathrm{Tr}\left\{\prod_l \exp\left(-\frac{\beta}{L}(\hat{h}[\sigma(t_l)] - \mu\hat{N})\right)\right\}, \end{aligned} \tag{2.3}$$

where l labels the time slices. The one-body Hamiltonian $\hat{h}$ is given by

$$\hat{h}[\sigma(t)] = \hat{K} - \sum_\alpha 2\lambda_\alpha \sigma_\alpha(t)\, \hat{\rho}_\alpha. \tag{2.4}$$

The field variables $\sigma_\alpha(t)$ thus appear as single-particle potentials, and the

integration of (2.3) is taken over all values of the fields. The limit of Eq. (2.3) as the width of the time slices β/L goes to zero is written formally as a path integral,

$$Z = \int D[\sigma]\, e^{S_{\text{eff}}[\sigma]} \tag{2.5a}$$

in terms of the effective action

$$S_{\text{eff}}[\sigma] = -\int_0^\beta dt \sum_\alpha \lambda_\alpha \sigma_\alpha(t)^2 + \ln \operatorname{tr}\left\{ T \exp\left(-\int_0^\beta dt (\hat{h}[\sigma(t)] - \mu\hat{N}) \right) \right\}. \tag{2.5b}$$

Here T denotes the time-ordering operator. Equation (2.5) will be referred to as the continuous time limit. The trace is taken over the many-body states of the system. In the grand canonical ensemble, the trace reduces to the determinant [3]

$$\operatorname{tr}\left\{ T \exp\left(-\int_0^\beta dt\, (\hat{h}[\sigma(t)] - \mu\hat{N}) \right) \right\} = \det(1 + U_\sigma), \tag{2.6}$$

where U_σ is a matrix representation of the single-particle evolution operator,

$$U_\sigma = T \exp\left(-\int_0^\beta dt\, (h[\sigma(t)] - \mu) \right) = \lim_{L\to\infty} \prod_l \exp\left(-\frac{\beta}{L} (h[\sigma(t_l)] - \mu) \right). \tag{2.7}$$

In general, the evolution operator is untractable and an approximation scheme is required to evaluate the effective action (2.5). One approximation would be to expand the functional $h[\sigma]$ as a Taylor series around the static field, σ^0, which yields the maximum of the effective action. However, only the zeroth order term is easily evaluated. Namely, the determinant becomes trivial in the basis of eigenstates of the single-particle matrix $h[\sigma^0]$,

$$\det(1 + U_\sigma) = \prod_k (1 + \exp(-\beta(\varepsilon_k - \mu))), \tag{2.8}$$

where ε_k are the eigenvalues of $h[\sigma^0]$. This would give the Hartree solution for the partition function, while the second order terms give the RPA corrections [4].

However, the approximation may be largely improved, by noting that the relation (2.8) applies to all time-independent paths σ. We therefore expand the effective action (2.5) as a power series around the static path

$$\bar{\sigma}_\alpha = \frac{1}{\beta}\int_0^\beta dt\, \sigma_\alpha(t) = \lim_{L\to\infty} \frac{1}{L} \sum_l \sigma_\alpha(t_l) \tag{2.9}$$

which is defined for each path $\sigma_\alpha(t)$. Here $\bar{\sigma}_\alpha$ is the average of $\sigma_\alpha(t)$ over the interval β. The expansion is formally similar to the well-known expansion about the mean field, but is carried out here for all constant values of the field. The static path approximation is obtained by considering only the static paths in the evolution

operator. Corrections to the static path approximation are taken into account by considering fluctuations of the Hubbard–Stratonovich field around the static paths $\bar{\sigma}_\alpha$.

In the static path approximation, the integration is performed over the variables $\bar{\sigma}_\alpha$. We therefore need a transformation to a new set of variables that contains $\bar{\sigma}_\alpha$. This may be done conveniently by Fourier-expanding the fields $\sigma_\alpha(t_l)$. For L finite and odd, we may write

$$\sigma_\alpha(t_l) = \sum_{n=-(L-1)/2}^{n=(L-1)/2} c_{\alpha,n} \exp\left(i\frac{2\pi n}{L} l\right), \qquad c_{\alpha,-n} = c_{\alpha,n}^* \tag{2.10}$$

noting that $\sigma_\alpha(t)$ is real. The integration is performed over the fields $c_{\alpha,0}$, $\mathrm{Re}(c_{\alpha,n})$, $\mathrm{Im}(c_{\alpha,n})$, $n = 1, \ldots, (L-1)/2$, where the field $c_{\alpha,0}$ is equal to $\bar{\sigma}_\alpha$. For small fluctuations the single-particle Hamiltonian $h[\sigma]$ is split into two parts,

$$\begin{aligned} h[\sigma(t_l)] &= h_{\bar{\sigma}} + h_c(t_l) \\ h_{\bar{\sigma}} &= \hat{K} - \sum_\alpha 2\lambda_\alpha \hat{\rho}_\alpha \bar{\sigma}_\alpha - \mu \\ h_c(t_l) &= -\sum_{n>0} \sum_\alpha 2\lambda_\alpha \hat{\rho}_\alpha \, 2\,\mathrm{Re}\left[c_{\alpha,n} \exp\left(i\frac{2\pi n}{L} l\right)\right], \end{aligned} \tag{2.11}$$

and h_c is treated as a perturbation. The exponential of h_c is expanded in powers of $c_{\alpha,n}$ including up to quadratic terms

$$\begin{aligned} &\lim_{L\to\infty} \prod_l \exp\left(-\frac{\beta}{L} h[\sigma(t_l)]\right) \\ &\quad \approx \exp(-\beta h_{\bar{\sigma}}) - \int_0^\beta dt \exp(-t h_{\bar{\sigma}})\, h_c(t) \exp(-(\beta - t)\, h_{\bar{\sigma}}) \\ &\quad + \int_0^\beta dt \int_t^\beta dt' \exp(-t h_{\bar{\sigma}})\, h_c(t) \exp(-(t'-t)\, h_{\bar{\sigma}})\, h_c(t') \exp(-(\beta - t')\, h_{\bar{\sigma}}). \end{aligned} \tag{2.12a}$$

Here $h_c(t)$ is the continuum limit of (2.11)

$$h_c(t) = -\sum_{n>0} \sum_\alpha 2\lambda_\alpha \hat{\rho}_\alpha \, 2\,\mathrm{Re}[c_{\alpha,n} \exp(i\omega_n t)], \qquad \omega_n = \frac{2\pi n}{\beta}. \tag{2.12b}$$

Taking the trace of (2.12) causes the second term on the right hand side to vanish. Thus corrections to the static path approximation are of quadratic or higher order terms in the fluctuating fields. However, when evaluating the trace as a determinant, cf. Eq. (2.6), the term in Eq. (2.12) that is linear in h_c must be included in

the determinant for the relation (2.6) to be valid to second order in h_c. The integrals (2.12) are evaluated by working in a basis that diagonalizes the matrix representation of $h_{\bar{\sigma}}$. This is carried out in a model calculation in Section 4.

Keeping only the first term of the expansion (2.12) yields the static path approximation to the partition function

$$Z = \prod_{\alpha} \left(\frac{\beta \lambda_\alpha}{\pi} \right)^{1/2} \int \prod_{\alpha} d\bar{\sigma}_\alpha \exp\left(-\beta \sum_{\alpha} \lambda_\alpha \bar{\sigma}_\alpha^2 \right) \mathrm{Tr}\{\exp(-\beta(\hat{h}_{\bar{\sigma}}))\}. \tag{2.13}$$

Expectation values treated in this approximation are amenable to Monte Carlo sampling. Note that static solutions of the mean field are included in the integration domain of (2.13). Thus (2.13) has the potential to be a better approximation to Z than the usual mean-field theory, especially if contributions from several mean field solutions are important.

The static path approximation is exact when the kinetic and the potential energy operators in (2.2) commute. In the limit of high temperature, i.e., for $\beta \to 0$, one can neglect the noncommutativity between these operators, the error in the partition function being of the order β^3. Therefore the proposed approximation gives the correct high temperature limit.

3. Application to a Model Hamiltonian

The technique of the Hubbard–Stratonovich transformation and the approximation of the partition function introduced in the previous section can be elucidated in a simple two-level model. The Hamiltonian is taken to be

$$\begin{aligned} \hat{H} &= \hat{K} - \lambda \hat{\rho}^2, \qquad \lambda > 0 \\ \hat{K} &= d(\hat{N}_2 - \hat{N}_1) \\ \hat{\rho} &= \hat{A}^\dagger + \hat{A}, \end{aligned} \tag{3.1a}$$

where

$$\begin{aligned} \hat{N}_1 &= \sum_{\nu=1}^{N} c_{1\nu}^\dagger c_{1\nu}, \qquad \hat{N}_2 = \sum_{\nu=1}^{N} c_{2\nu}^\dagger c_{2\nu}, \\ \hat{A}^\dagger &= \sum_{\nu=1}^{N} c_{1\nu}^\dagger c_{2\nu}, \qquad \hat{A} = \sum_{\nu=1}^{N} c_{2\nu}^\dagger c_{1\nu}. \end{aligned} \tag{3.1b}$$

The number of particles is given by N, as for half-filled shell. In the grand canonical ensemble, Eq. (2.1), this corresponds to having a chemical potential $\mu = 0$, independent of temperature.

The choice of the Hamiltonian is motivated by the similarity of a Nilsson Hamiltonian plus a quadrupole–quadrupole interaction [5] and allows comparison

with an exact solution. As in the Lipkin–Meshov–Glick model [6], the solutions to the Hamiltonian (3.1) can be characterized by quasi-spin quantum numbers. The operators $\hat{A}^\dagger$, $\hat{A}$, and $\frac{1}{2}(\hat{N}_1 - \hat{N}_2)$ obey the angular momentum commutation relations of J_+, J_-, and J_z, respectively. With the use of these quasi-spin operators the Hamiltonian (3.1) may be written

$$H = -4\lambda(J_x)^2 - 2dJ_z. \tag{3.2}$$

The total angular momentum J is a constant of motion. For the lowest energy eigenstate it is given by the maximum value of the z-component, $J = J_{z,\max} = N/2$.

In the form (3.2), the Hamiltonian can be given a nice geometrical interpretation of a single particle of angular momentum J in a quadrupole, oblate deformed nucleus with symmetry axis x, and cranked with the frequency $2d$ around the z-axis [7]. In the large N limit, the solution of the Hamiltonian may be obtained by a semiclassical approximation. Namely, the trajectory of the motion of the angular momentum vector is given by the intersection of the parabolic cylinder (3.2) and the sphere,

$$J^2 = J_x^2 + J_y^2 + J_z^2. \tag{3.3}$$

The minimum energy solution is given in Table I. Note that for frequencies $2d < 8\lambda J$, the Hamiltonian possess two degenerate minima of opposite signs of J_x, while at frequencies $2d > 8\lambda J$, only one minimum appears, at $J_x = 0$. Thus a phase transition occurs with the order parameter $\langle J_x \rangle$ when the frequency $2d$ is increased beyond $8\lambda J$. In the following, it is shown that this phase transition also occurs when the temperature is increased to $T = 2\lambda J$. This is similar to the BCS theory for pairing phase transitions.

The partition function in the Hubbard–Stratonovich transformation (2.3) is

$$Z = \lim_{L\to\infty} \left(\frac{2\beta\lambda}{\pi}\right)^{L/2} 2^{-1/2} \int dc_0 \prod_{n>0} d\,\mathrm{Re}(c_n)\, d\,\mathrm{Im}(c_n)$$
$$\times \exp\left(-\beta\lambda c_0^2 - 2\beta \sum_{n>0} |c_n|^2\right) \mathrm{Tr}\left\{T \exp\left(-\int_0^\beta dt\, (h_{\bar{\sigma}} + h_c)\right)\right\}, \tag{3.4a}$$

TABLE I

Minimum Energy Solutions of the Hamiltonian (3.2) in the Semiclassical Approximation.

	J_x	J_z	E
$2d < 8\lambda J$	$\pm(J^2 - d^2/16\lambda^2)^{1/2}$	$d/4\lambda$	$-4\lambda J^2 - d^2/4\lambda$
$2d > 8\lambda J$	0	J	$-2dJ$

where

$$h_{\bar{\sigma}} = \hat{K} - 2\lambda\hat{\rho}c_0, \qquad h_c = -2\lambda\hat{\rho}\sum_{n>0} 2\,\mathrm{Re}[c_n \exp(i\omega_n t)]. \tag{3.4b}$$

The single-particle Hamiltonian $h[\sigma]$ is diagonal in the indices v, Eq. (3.1), and the $2N \times 2N$ matrix representation of $h[\sigma]$ is split into N identical 2×2 submatrices. The static path approximation to the partition function is obtained by neglecting h_c in Eq. (3.4) and applying the relations (2.6), (2.8). The integral over c_n, $n \neq 0$, is trivial, yielding

$$\begin{aligned} Z_{\bar{\sigma}} &= 2^N \left(\frac{\beta\lambda}{\pi}\right)^{1/2} \int d\bar{\sigma} \exp(-\beta\lambda(\bar{\sigma})^2)(1+\cosh(\beta\bar{s}))^N \\ \bar{s} &= (d^2 + (2\lambda\bar{\sigma})^2)^{1/2}. \end{aligned} \tag{3.5}$$

We evaluate the remaining integral in the stationary phase approximation. For small values of β, $N\lambda\beta < 1$, the integrand in (3.5) has a maximum at $\bar{\sigma} = 0$, and the partition function becomes

$$Z_{\bar{\sigma}} \approx 2^N (1+\cosh(\beta d))^N \left(1 - \frac{2N\lambda}{d}\tanh\left(\frac{\beta d}{2}\right)\right)^{-1/2}. \tag{3.6}$$

From the partition function, we can obtain the total energy. At high temperature, $T > N\lambda$, the energy can be expanded in powers of β,

$$E_{\bar{\sigma}} = -\frac{\partial}{\partial\beta}(\ln Z_{\bar{\sigma}}) = -\frac{1}{2}N\lambda - \frac{1}{2}Nd^2\beta - \frac{1}{2}(N\lambda)^2\beta - \frac{1}{2}(N\lambda)^3\beta^2 + \frac{1}{8}N\lambda d^2\beta^2 + o(\beta^3). \tag{3.7}$$

When the temperature is decreased, the stationary point $\bar{\sigma} = 0$ becomes a local minimum of the action. In the limit $\beta \to \infty$ and for $d < 2N\lambda$, the integrand has two symmetric maxima at $\bar{\sigma} = \pm\sqrt{(2\lambda N)^2 - d^2}$. Again, the stationary phase approximation may be applied to give

$$Z_{\bar{\sigma}} \approx \exp\left(\beta N^2\lambda + \beta\frac{d^2}{4\lambda}\right)\left(1 - \left(\frac{d}{2\lambda N}\right)^2\right)^{-1/2} \tag{3.8}$$

and the ground state energy is obtained,

$$E_0 = -N^2\lambda - \frac{d^2}{4\lambda}, \qquad d < 2N\lambda. \tag{3.9}$$

This is equivalent to the semiclassical result obtained above, cf. Table I. Note that the ground state energy is given by the mean field only. That is, the quadratic correction given by the last term in (3.8) does not contribute to the energy.

4. Higher Order Corrections

The second order corrections to the partition function are readily obtained from Eq. (2.12). The operator h_c is expressed in the basis that diagonalizes $h_{\bar{\sigma}}$ and the integrations are now straightforward but tedious. The resulting expression is inserted in the effective action (2.5b), which is expanded to second order in the fields c_n, $n>0$. The Gaussian integral over these fields is performed, leading to the partition function

$$Z_{\bar{\sigma}} = 2^N \left(\frac{\beta\lambda}{\pi}\right)^{1/2} \int d\bar{\sigma} \exp(-\beta\lambda(\bar{\sigma})^2)(1+\cosh(\beta\bar{s}))^N$$
$$\times \prod_{n>0} \left(1 - 2N\lambda(d/\bar{s})^2 \frac{\bar{s}}{(\bar{s})^2 + (\omega_n/2)^2} \tanh(\beta\bar{s}/2)\right)^{-1}. \tag{4.1}$$

It is instructive to obtain this result, making use of a technique discussed in Ref. [8] where it is applied to real time evolution operators. We are looking for the eigenvalues of the evolution operator

$$T\exp\left(-\int_0^\beta dt(h_{\bar{\sigma}} + h_c)\right)\phi_k = e^{-\beta\varepsilon_k}\phi_k. \tag{4.2}$$

Instead of solving (4.2) directly, we note that the states

$$\psi_k(t) = e^{t\varepsilon_k} T\exp\left(-\int_0^t dt'(h_{\bar{\sigma}} + h_c)\right)\phi_k \tag{4.3}$$

are solutions to the equivalent boundary value problem

$$\left(\frac{\partial}{\partial t} + h_{\bar{\sigma}} + h_c\right)\psi_k(t) = \varepsilon_k\psi_k$$
$$\psi_k(0) = \psi_k(\beta). \tag{4.4}$$

The complete set of solutions to (4.4) is given as

$$\psi_{k,n}(t) = \psi_k(t)\exp(i\omega_n t), \qquad \varepsilon_{k,n} = \varepsilon_k + i\omega_n. \tag{4.5}$$

From (4.4), (4.5), we can obtain the energies ε_k as a perturbation expansion in the interaction h_c. We write $\varepsilon_k = \varepsilon_k^{(0)} + \varepsilon_k^{(2)}$, where the unperturbed energies $\varepsilon_k^{(0)}$ are the eigenvalues of $h_{\bar{\sigma}}$, the corresponding eigenstates $\psi_k^{(0)}$ being time-independent, and $\varepsilon_k^{(2)}$ are the second order energy terms

$$\varepsilon_k^{(0)} = \pm\bar{s}$$
$$\varepsilon_k^{(2)} = \sum_{k',n} \frac{|(\psi_k^{(0)}|h_c|\psi_{k',n}^{(0)})|^2}{\varepsilon_k^{(0)} - \varepsilon_{k',n}^{(0)}}. \tag{4.6}$$

In (4.6), the matrix element of h_c involves integration over time. Inserting h_c from Eq. (3.4) the energies become

$$\varepsilon_k = \pm\left(\bar{s} + (4\lambda)^2 \frac{d^2}{\bar{s}} \sum_{n>0} \frac{|c_n|^2}{(2\bar{s})^2 + \omega_n^2}\right). \tag{4.7}$$

Making use of (2.8), we can now expand the effective action to second order in c_n. Again, performing the Gaussian integrals over c_n, $n>0$, leads to the result (4.1).

The last term in Eq. (4.1) stems from the second derivative of the action with respect to c_n, and the expression is valid only when the second derivative is negative definite. Thus the Gaussian integral diverges for a certain range of parameters, when the last term contains negative factors, implying that quartic or higher order corrections may be important for evaluation of the correction to the static path approximation. In this case, the static path approximation does not sample the optimal paths of the partition function.

At high temperatures however, $\beta N\lambda < 1$, the second order correction converges, which is also the case when evaluated at the stationary mean field solution for smaller temperatures. As in Eq. (3.7), the energy may be expanded in powers of β. This leads to a correction of the energy of second order in β

$$\begin{aligned} E_\sigma &= E_{\bar{\sigma}} + E_c \\ E_c &= -\tfrac{1}{2} N\lambda d^2 \beta^2 + o(\beta^3), \qquad \beta N\lambda < 1. \end{aligned} \tag{4.8}$$

The energies obtained with the use of the Hubbard–Stratonovich transformation may be compared to an exact calculation. This has been carried out in the canonical ensemble. Noting that all terms of the energy expansion in β (4.8) contain quadratic or lower orders in d, the exact energy has been calculated including second order terms in the kinetic energy $\hat{K}$. Doing so, agreement up to order $1/N$ with the results (3.6), (4.8) is obtained. This suggests that the approximations applied here contain all terms in the energy expansion up to second order in β.

It is noted from the energy expansion in β, that approximating the Hubbard–Stratonovich fields by time-independent fields becomes a good approximation in the large N limit. This is essentially in agreement with the success of mean-field theories in heavy well-deformed nuclei. At small values of N, however, and for not too high temperatures, the time fluctuations of the Hubbard–Stratonovich fields become important, as seen from the energy correction (4.8).

5. Comparison to Finite Temperature Hartree and Hartree–Fock Theory

Nuclear microscopic calculations at high excitation energy have traditionally been carried out with the finite temperature Hartree or Hartree–Fock approaches.

It is therefore instructive to compare these techniques with the Hubbard–Stratonovich transformation in the static path approximation, as applied to the present model.

The Hartreee and the Hartree–Fock single-particle Hamiltonians may both be obtained as mean-field solutions to the path integral [9]. This is accomplished by adding linear terms in the fields $\sigma_\alpha(t_l)$, in the Trotter expansion of the evolution operator. Although adding such linear terms does not change the path integral carried out in the full space of the auxiliary fields $\sigma_\alpha(t_l)$, it alters the constant path approximation to the integral. In the present formulation, the constant path approximation contains as stationary paths the Hartree mean-field solutions, while the connection to Hartree–Fock is unclear.

The Hartree solution to the partition function are obtained by replacing the integrand of Eq. (3.5) by its maximum value, that is, neglecting the correction factors in Eqs. (3.6), (3.8), stemming from the quadratic corrections. At temperatures above the phase transition, $T > N\lambda$, the Hartree mean field is given by $\bar{\sigma} = 0$, and from Eq. (3.6), the Hartree energy is readily obtained,

$$E_{\mathrm{H}} = -\frac{\partial}{\partial\beta}(\ln Z_{\bar{\sigma}}) \approx -\frac{1}{2} N d^2 \beta + o(\beta^3), \tag{5.1}$$

much different from the result (3.7). For $\beta \to \infty$ and $d < 2N\lambda$, the ground state energy (3.9) is obtained from the Hartree solution, as discussed below Eq. (3.9).

In the present model, the Hartree–Fock equations are easily solved. Noting that the Hamiltonian (3.1) is symmetric under any permutation of the indices v, the finite temperature Hartree–Fock Hamiltonian is given as

$$h_{\mathrm{HF}} = h_0 + \sum_{t=1}^{2N} f_t \sum_{jk} \{ |j\rangle\langle t|k\rangle\, V_{kj} \langle k|t\rangle\langle j| - |j\rangle\langle t|k\rangle\, V_{kj}\langle j|t\rangle\langle k| \}, \tag{5.2a}$$

where

$$\begin{aligned} &V_{+v,+v'} = V_{-v,-v'} = -2\lambda, && V_{+v,-v'} = V_{-v,+v'} = 2\lambda \\ &(h_0)_{+v,+v'} = (h_0)_{-v,-v'} = \lambda,\ \delta(v,v') && (h_0)_{+v,-v'} = (h_0)_{-v,+v'} = d,\ \delta(v,v') \end{aligned} \tag{5.2b}$$

and $|j\rangle$, $|k\rangle$ are the single-particle wavefunctions that diagonalize the interaction $\hat{\rho}$ (3.1),

$$|+v\rangle = \frac{1}{\sqrt{2}}(|1v\rangle + |2v\rangle), \qquad |-v\rangle = \frac{1}{\sqrt{2}}(|1v\rangle - |2v\rangle). \tag{5.3}$$

The Fermi occupation numbers, $f_t = (1 + \exp(\beta\varepsilon_t))^{-1}$, are given by the Hartree–Fock energies ε_t, and the states $|t\rangle$ denote the single-particle eigenstates to the Hartree–Fock Hamiltonian. For temperatures above the phase transition, $T > N\lambda$,

and for $d < \lambda N$, all Hartree–Fock energies become degenerate, $\varepsilon_i = 0$, and the total energy is given as

$$E_{HF} = -\frac{1}{2} N\lambda, \qquad \beta < \frac{1}{N\lambda}. \tag{5.4}$$

Thus, the Hartree–Fock approximation lacks a β-expansion of the energy and only the constant term in Eq. (3.7) is obtained in the high temperature limit.

6. Conclusions

We have shown that the static path approximation in the Hubbard–Stratonovich representation of the partition function is useful to treat a simple Hamiltonian similar to the Lipkin–Meshov–Glick model. At high temperature, the static path approximation is superior to the finite temperature Hartree approximation. Our static path treatment is also superior to Hartree–Fock, which in the present model is diseased and does not have a high energy expansion. We recently learned of a similar study of the Lipkin model by Alhassid and Zingman [10]. These authors consider only the Hamiltonian subspace of maximally symmetric configurations. Their conclusion which is similar to ours, is based on numerical comparison with their exact partition function.

We also examined second order corrections to the static paths. These corrections are well-behaved at high temperatures, but become uncontrollable at lower temperatures. Despite this, the static path approximation is rather accurate as the temperature goes to zero. In any case, one must be cautious in low temperature applications. We are encouraged by the overall utility of the approximation to apply it to a more realistic model. We are now considering models with a three dimensional spatial structure and separable interactions, that reduce to Nilsson Hamiltonians in the Hartree approximation.

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