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Finite temperature projected calculations in the static path approximation

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Particle number projected calculations are examined within the context of the static path approximation. A different evaluation of the thermal average energy is also employed, which is seen to provide the correct behaviour at low temperature and is more appropriate for projected calculations. The evaluation of the energy level density is also discussed. Application to a pairing hamiltonian is made.

There have recently been various attempts to derive microscopic approaches which can go beyond the conventional finite temperature mean field approximations in finite systems, in particular projected (before variation) mean field methods [1], the static path approximation (SPA) [2–5] and the inclusion of correlations [6,7]. The SPA is a successful method for calculating nuclear level densities and thermal averages based on the Hubbard–Stratonovich transformation [8] and the ensuing path integral representation of the partition function. It was shown that integrating just over the static paths, an accurate description of the thermal average energy could be obtained for systems described by attractive interactions expressed as sums of squares of one-body operators. The method yields the smooth thermal behaviour characteristic of finite systems and is exact at high temperatures.

The approach exhibits however in its standard form some shortcomings at low temperatures, such as omission of Fock terms and the possibility of a negative slope in the average energy as $T\to 0$. In this work we examine particle number projected calculations [1,7] within the framework of the SPA. We show at the same time a straightforward means to improve the low temperature behaviour, by recourse to a different evaluation of the average energy, which also allows to effectively recover the Fock terms.

We consider a hamiltonian which can be written as $\hat{H}=\hat{H}_0-\frac{1}{2}\sum_i\lambda_i\hat{O}_i^2$, with $\lambda_i>0$ and $\hat{O}_i$ and $\hat{H}_0$ hermitic one-body operators. The SPA leads to the following approximate expression for the partition function [2],

$$Z=\left[\prod_i\left(\frac{\lambda_i\beta}{2\pi}\right)^{1/2}\right]\times\int_{-\infty}^{\infty}\exp\left(-\tfrac{1}{2}\beta\sum_i\lambda_i x_i^2\right)\mathrm{Tr}\exp[-\beta\hat{h}(x)]\,\mathrm{d}x\,, \tag{1}$$

where $\beta=T^{-1}$, $x=\{x_i\}$ denotes the set of averages of the fields associated with each operator $\hat{O}_i$ (which become integration variables in the SPA), $\mathrm{d}x\equiv\prod_i\mathrm{d}x_i$, and

$$\hat{h}(x)=\hat{H}_0-\mu\hat{N}-\sum_i\lambda_i x_i\hat{O}_i\,. \tag{2}$$

Eq. (1) is exact if the operators $\hat{O}_i$ commute among themselves and with $\hat{H}_0$, and is thus exact in the limit $T\to\infty$ [2]. The energy was evaluated in the original approach as

$$E=-\partial\ln Z/\partial\beta+\mu N\,, \tag{3}$$

which allows for an expedient calculation of the level density [3,4], but exhibits some shortcomings at low temperatures, such as the possibility of a negative

specific heat due to an improper cancellation of the temperature dependent prefactor as $T\to 0$ [3]. Moreover, only the Hartree energy is obtained in the present case from (3) as $T\to 0$, without the contribution of the Fock terms.

In the present work we shall employ a different evaluation based on the SPA statistical operator $\hat{D} \propto \int_{-\infty}^{\infty} \exp\{-\beta[\frac{1}{2}\sum_i \lambda_i x_i^2 + \hat{h}(x)]\}\mathrm{d}x$. We define the mean energy as

$$E \equiv \mathrm{Tr}\,\hat{D}\hat{H} = \frac{1}{Z'}\int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\beta \sum_i \lambda_i x_i^2\right) z(\beta, x) H(\beta, x)\mathrm{d}x\,, \tag{4}$$

where $z(\beta, x) = \mathrm{Tr}\exp[-\beta\hat{h}(x)]$,

$$H(\beta, x) = \frac{1}{z(\beta, x)}\mathrm{Tr}\exp[-\beta\hat{h}(x)]\hat{H} \equiv \langle \hat{H}\rangle_x, \tag{5}$$

and $Z' = \int_{-\infty}^{\infty}\exp(-\frac{1}{2}\beta\sum_i\lambda_i x_i^2) z(\beta, x)\mathrm{d}x$. If traces are taken in a grand canonical (GC) ensemble, (5) is the usual finite temperature Wick's theorem average

$$\langle \hat{H}\rangle_x = \langle \hat{H}_0\rangle_x - \tfrac{1}{2}\sum_i \lambda_i(\langle \hat{O}_i\rangle_x^2 + \gamma_i)$$

with γ_i the Fock or exchange terms (i.e., if $\hat{O}_i = \sum_{jk} A_{jk} c_j^\dagger c_k$, $\langle \hat{O}_i\rangle_x = \sum_{jk} A_{jk}\rho_{kj}$, $\gamma_i = \sum_{jklm} A_{jk}A_{lm} \times [\rho_{mj}(\delta_{kl} - \rho_{kl}) - t'_{jl}t_{km}]$, with $\rho_{kj} = \langle c_j^\dagger c_k\rangle_x$, $t_{jk} = \langle c_j c_k\rangle_x$, $t'_{jk} = \langle c_j^\dagger c_k^\dagger\rangle_x$).

It is apparent that (3) and (4) do not coincide (except when (1) is exact). The definition (4) is still exact at high temperatures (since $\hat{D}$ coincides with the exact density operator up to order $1/T$) but avoids the shortcomings at low temperatures since the temperature dependent prefactors are canceled out. Moreover, the Fock terms are in this way recovered in the average energy, leading (4) as $T\to 0$ to the full mean field energy evaluated in the state which minimizes the Hartree energy. Nevertheless, differences between (3) and (4) will be significant only at relatively small temperatures.

We note that $\exp(-\frac{1}{2}\beta\sum_i\lambda_i x_i^2) z(\beta, x) = \exp[-\beta \times f(\beta, x)]$, where $f(\beta, x) = \langle \hat{h}(x)\rangle_x - \frac{1}{2}\sum_i\lambda_i x_i^2 - Ts(\beta, x)$ can be interpreted as the Hartree-like thermodynamic potential in terms of the variables x_i [3] ($s(\beta, x)$ is the single particle entropy). Expression (4) looks thus similar (but is not equal) to the usual macroscopic "thermodynamic" average [9–11]. The present approach is however fully microscopic and leads to exact averages in the high temperature limit in the corresponding ensemble.

Let us consider now projected calculations in the context of the SPA. We note first that although for fixed x_i, $\hat{h}(x)$ may break relevant symmetries associated with the hamiltonian, they may be formally conserved in $\hat{D}$ after integration, in which case symmetries are still violated if traces are taken in an unrestricted GC ensemble.

For particle number projection, the canonical ensemble for a fixed particle number N_0 should be employed in the previous traces. For $[\hat{h}(x), \hat{N}] = 0$, this projection removes the statistical fluctuations in the particle number arising at finite temperature from the use of the GC ensemble (significant only for very small systems [7]), but is more relevant when $[\hat{h}(x), \hat{N}] \neq 0$ as in pairing hamiltonians, where it restores the broken symmetry [1] and suppresses thus the quantum fluctuations (existing in this case also at $T=0$). The canonical trace Tr_c can be obtained from the GC trace Tr_{GC} as

$$\begin{aligned}\mathrm{Tr}_c \exp[-\beta\hat{h}(x)]\begin{Bmatrix}1\\ \hat{H}\end{Bmatrix} &= \frac{1}{2\pi}\int_0^{2\pi}\mathrm{Tr}_{GC}\exp[\mathrm{i}\alpha(\hat{N}-N_0)] \\ &\times \exp[-\beta\hat{h}(x)]\begin{Bmatrix}1\\ \hat{H}\end{Bmatrix}\mathrm{d}\alpha \\ &= \frac{1}{2\pi}\int_0^{2\pi} z(\beta, x, \alpha)\begin{Bmatrix}1\\ H(\beta, x, \alpha)\end{Bmatrix}\mathrm{d}\alpha\,.\end{aligned} \tag{6}$$

We shall employ here a general and compact method for the evaluation of these type of traces. They pose no formal problem even if $[\hat{N}, \hat{h}(x)] \neq 0$, since $\hat{h}(x)$ is a one-body operator and the product of exponents of one-body operators is the exponent of a one-body operator [12]. Hence, $H(\beta, x, \alpha)$ is *again* given by the usual Wick's theorem expression. The exact projection entails thus an additional integral and in principle an additional one-body diagonalization if $[\hat{N}, \hat{h}(x)] \neq 0$. Similar considerations hold for other symmetries in which the projection operator can be expressed as the integral of exponents of one-body operators, as in angular momentum projection [13].

The above projection can be done both in the original expression (1) and in the corrected evaluation (4). However, as we shall see in a simple example, the new evaluation may be *essential* for proper projected energy evaluation.

The definition (4) poses on the other hand the problem of how to evaluate the corresponding energy level density. This quantity can in principle be exactly obtained as the inverse Laplace transform of the partition function. We can define in the present situation an *effective* partition function such that (we consider first a canonical ensemble) $E=-\partial \ln Z_{\rm eff}/\partial\beta$, with $Z_{\rm eff}=\int \rho_{\rm eff}(E)\exp(-\beta E)\,{\rm d}E$. Then we can proceed as usual and employ the saddle point approximation in the inverse transform [14], which leads to $\rho_{\rm eff}(E)=Z_{\rm eff}\exp(\beta E)/(-2\pi\,\partial E/\partial\beta)^{1/2}$. In *canonical* calculations, $Z_{\rm eff}$ can be obtained as

$$\ln Z_{\rm eff}(\beta)=-\int_{\beta_0}^{\beta} E(\beta)\,{\rm d}\beta+\ln Z_{\rm eff}(\beta_0)\,, \qquad (7)$$

with $E(\beta)$ determined according to (4). For β_0 it is convenient to choose a small value (T_0 high), where we can use the (projected) expression (1) for the canonical partition function at β_0, since at high T differences between both definitions are small. In finite shell model calculations, it is also possible to employ $\beta_0=0$, with $Z_{\rm eff}(0)$ the total number of accessible states for the given number of particles.

In the GC ensemble, we can proceed in the same way by defining the effective partition function along the path with constant N, which is just (7) plus the term $N[\alpha(\beta)-\alpha(\beta_0)]$, with $\alpha=\beta\mu$, and employing then the GC expression [14] $\rho_{\rm eff}(E,N)=Z_{\rm eff}\times\exp(\beta E-\alpha N)/(2\pi\sqrt{|J|})$ (J is the jacobian $\partial(E,N)/\partial(\beta,\alpha)$). Nevertheless, with the definition (4) the cross derivatives may not be equal, and $Z_{\rm eff}$ should be considered in this case just an approximation for the density evaluation.

As an application, we shall consider the case of a general n-level pairing hamiltonian,

$$\hat H=\sum_i \epsilon_i\hat N_i-G\hat P^\dagger\hat P\,, \qquad (8)$$

where $\hat N_i=\sum_p(c^\dagger_{pi}c_{pi}+c^\dagger_{\bar p i}c_{\bar p i})$ and $\hat P=\sum_{i,p}c_{\bar p i}c_{pi}$, with $p=1,\ldots,\Omega_i$ and $2\Omega_i$ the degeneracy of the level i. We note that $\hat P^\dagger\hat P=[\frac12(\hat P^\dagger+\hat P)]^2+[(\hat P^\dagger-\hat P)/2i]^2+\frac12(\hat N-\Omega)$ (with $\Omega=\sum_i\Omega_i$). In this case [3], the SPA statistical operator can be written as

$$\hat D\propto\int_0^\infty\int_0^{2\pi}\exp\{-\beta[\Delta^2/G+\hat h(\Delta,\phi)]\}\Delta\,{\rm d}\phi\,{\rm d}\Delta\,, \qquad (9)$$

where $\hat h(\Delta,\phi)=\sum_i\epsilon'_i\hat N_i-\Delta[\exp(i\phi)\hat P^\dagger+\exp(-i\phi)\times\hat P]+\frac12 G\Omega$, with $\epsilon'_i=\epsilon_i-\mu-\frac12 G$. The energy (4) becomes (the integrand will not depend on ϕ)

$$E=\frac{\int_0^\infty\exp(-\beta\Delta^2/G)z(\beta,\Delta)H(\beta,\Delta)\Delta\,{\rm d}\Delta}{\int_0^\infty\exp(-\beta\Delta^2/G)z(\beta,\Delta)\,\Delta\,{\rm d}\Delta}\,. \qquad (10)$$

There is a measure Δ arising from the two-dimensional character of the pairing field.

In the GC ensemble, $z(\beta,\Delta)=\prod_i\{2\exp[-\beta(\epsilon_i-\mu)][1+\cosh(\beta\lambda_i)]\}^{\Omega_i}$, with $\lambda_i=\sqrt{\epsilon_i'^2+\Delta^2}$ the quasiparticle energy, and

$$H(\beta,\Delta)=\sum_i\epsilon_i\langle\hat N_i\rangle$$

$$-G\left(\langle\hat P^\dagger\rangle\langle\hat P\rangle+\tfrac14\sum_i\langle\hat N_i\rangle^2/\Omega_i\right), \qquad (11)$$

where

$$\langle\hat N_i\rangle=\Omega_i[1-(1-2f_i)\epsilon'_i/\lambda_i]\,,$$

$$\langle\hat P\rangle=\tfrac12\Delta\exp(i\phi)\sum_i\Omega_i(1-2f_i)/\lambda_i\,, \qquad (12)$$

with $f_i=[1+\exp(\beta\lambda_i)]^{-1}$. The Fock term (equal in this case to $-G\sum_{pi}\langle c^\dagger_{pi}c_{pi}\rangle\langle c^\dagger_{\bar p i}c_{\bar p i}\rangle$) is represented by the last term in the bracket of (11) and is obviously of order $1/\Omega$ in comparison with the direct term.

We consider now the particle number projected calculation. We note first that (9) strictly *conserves* the particle number symmetry, $[\hat D,\hat N]=0$ (the integration over ϕ cancels terms with unequal powers of $\hat P$ and $\hat P^\dagger$). Nevertheless, this symmetry is broken in the GC traces. The projected traces can in this case be straightforwardly calculated using (6) and SU(2) disentangling relationships (see for instance ref. [15]), as $c^\dagger_{pi}c^\dagger_{\bar p i}$, $c_{\bar p i}c_{pi}$, and $\frac12(c^\dagger_{pi}c_{pi}+c^\dagger_{\bar p i}c_{\bar p i}-1)$ satisfy an SU(2) algebra. We obtain (we set now $\mu=0$)

$$z(\beta,\Delta,\alpha)$$

$$=\exp[i\alpha(\Omega-N_0)]\prod_i[2\exp(-\beta\epsilon_i)\,z_i]^{\Omega_i}, \qquad (13)$$

$$z_i = 1 + \cosh(\beta\lambda_i)\cos\alpha - \mathrm{i}\frac{\epsilon'_i}{\lambda_i}\sinh(\beta\lambda_i)\sin\alpha\,. \qquad (13\ \text{cont'd})$$

The function $H(\beta, \Delta, \alpha)$ has obviously the same form as (11), but with the new elements

$$\langle \hat{N}_i \rangle = \Omega_i \left[1 + \left(\mathrm{i}\cosh(\beta\lambda_i)\sin\alpha - \frac{\epsilon'_i}{\lambda_i}\sinh(\beta\lambda_i)\cos\alpha \right) \Big/ z_i \right], \qquad (14)$$

$$\langle \hat{P} \rangle = \tfrac{1}{2}\Delta \exp[\mathrm{i}(\phi+\alpha)] \sum_i \Omega_i \sinh(\beta\lambda_i)/\lambda_i z_i, \qquad (15)$$

and $\langle \hat{P}^\dagger \rangle = \langle \hat{P} \rangle^* (z_i^*/z_i)$. The ensuing integrals (6) can be done analytically (the integrands are polynomials in $\cos\alpha$, $\sin\alpha$).

Results for a half filled two level pairing model ($\Omega_1 = \Omega_2 = \frac{1}{2}N$, $\epsilon_2 = -\epsilon_1 = \epsilon$) are shown in figs. 1 and 2 and compared with the exact canonical results [6]. We also show full finite temperature BCS results (Fock terms included [6]) for a proper comparison with mean field approximations and the energy obtained from the classical "thermodynamic" average, following the prescription of ref. [10], which involves the same amount of work as (10). In GC calculations, $\mu = -\frac{1}{2}G$.

We note first that the energy obtained from (4) (cf. 10) exhibits the correct low temperature behaviour, both in GC and projected calculations, with no negative slopes. The Fock terms are recovered and are responsible in the GC calculation for the difference with the energy obtained from (3) as $T \to 0$. It is seen that the projection practically covers the remaining difference with the exact energy as $T \to 0$. Moreover, the most important corrections arising in the projected calculation are contained in the projected evaluation of the Fock term, which entails that almost no improvement for the energy is obtained from the original definition in a projected calculation. In fact, this projected energy (not shown) differs only slightly from the unprojected one at all temperatures and also exhibits the incorrect behaviour at low T.

The projected calculation, using (4), yields thus the correct high *and* low T limits, whereas at intermediate temperatures the discrepancy with the exact results, although reduced, remains. Higher order terms in the expansion of the path integral (see for instance refs. [2,5]) would still be required, although they are not easy to evaluate in a general situation. Results arising from the thermodynamic average, although smooth, are not exact at high temperature (they lie below the exact average) and only give a qualitative agreement. The level density obtained in the present approach, using the effective partition function, is in all cases of the same quality as that obtained from (1), except that the lower limit of the energy domain is extended. In fact, where the saddle point approximation is reliable, a projected calculation is in principle not necessary.

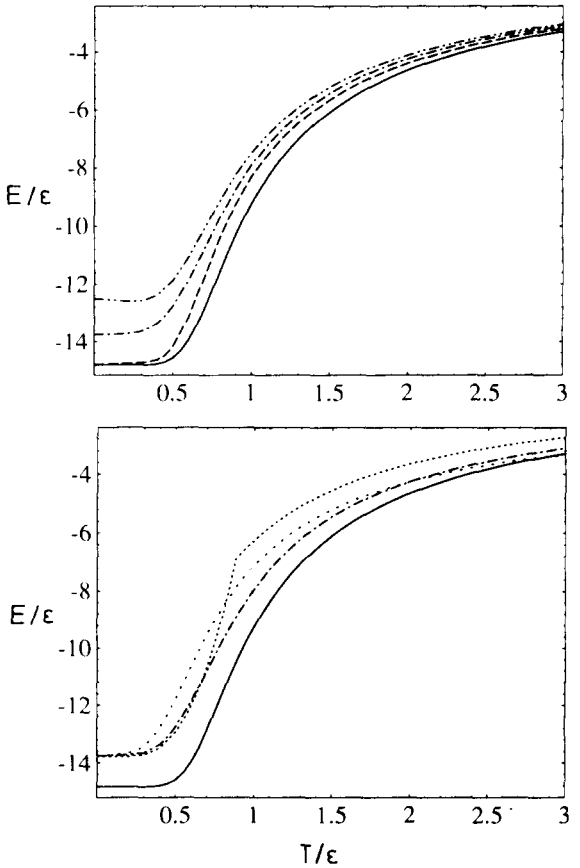

Fig. 1. Mean energy as a function of temperature in the two level pairing model for $GN/2\epsilon = 2$, and $N = 10$. In the upper figure, – corresponds to the exact canonical average, –···– to the unprojected SPA using the conventional definition (3), –·– to the definition (4), also unprojected, and —— to the projected calculation using (4). In the bottom figure, ... depicts full BCS results and · · · the thermodynamical average. Remaining details as in the upper figure.

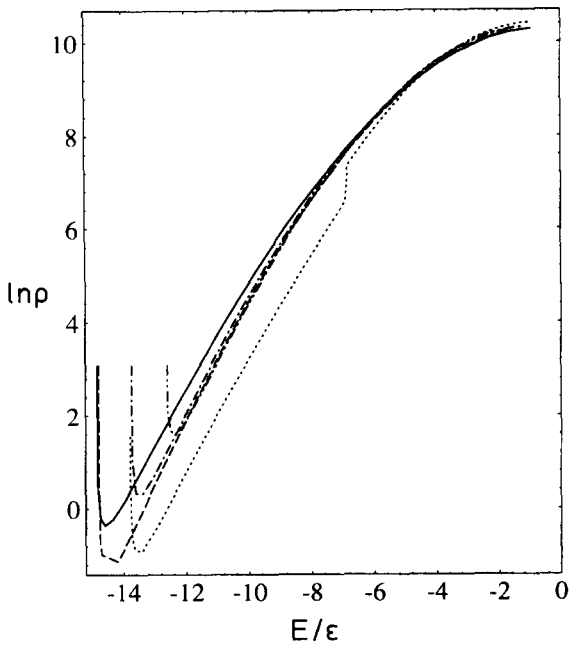

Fig. 2. Energy level density in the saddle point approximation. Same details as fig. 1.

In conclusion, we have shown that by recourse to a straightforward redefinition of the energy ensemble average, it is possible to improve the low temperature prediction of thermodynamic quantities in the context of the SPA. Moreover, the new definition is more adequate for finite temperature projected calculations, which were shown to be feasible within the context of the SPA and which improve further the low temperature limit. We note finally that rigorous projection before variation methods within the finite temperature mean field approximations are faced with the problem of the evaluation of the (projected) entropy [1], so that the SPA provides a suitable alternative framework for the implementation of projection methods at finite temperature.

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