# Thermal response of states of approximate angular momentum in the finite temperature restricted Hartree-Fock approximation

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(Received 2 December 1985)

The thermal response of states of approximate angular momentum in $^{24}$Mg with $J^{\pi}=8^{+}$ has been calculated in the finite temperature restricted Hartree-Fock approximation. Full angular momentum projection has been circumvented by the use of constraints on the total angular momentum $\hat{J}^2$ and the $z$ component $\hat{J}_z$. States with an abnormal occupation of the single particle orbitals at $T=0$ exhibit a discontinuity in the thermal response of their variational energy.

Most finite temperature Hartree-Fock (FTHF) calculations[1-3] are performed for the low-lying Hartree-Fock (HF) solutions, which, in general, are not eigenstates of the angular momentum operator. Since the exact Hamiltonian preserves rotational symmetry, it is of interest to study the thermal excitation of states of good angular momentum. At zero temperature an approximation method has been devised to calculate the excitation spectrum of states of a particular angular momentum.[4,5] The full angular momentum projection has been circumvented by the use of the constrained Hartree-Fock (CHF) method with constraints on the expectation values of the total angular momentum $\hat{J}^2$ (Refs. 6 and 7) and the $z$ component $\hat{J}_z$. If one only considers those states that are strongly localized about the desired angular momentum, that is, those for which $\Delta J^2=\langle[\hat{J}^2-J(J+1)]^2\rangle$ is small, it has been demonstrated that, in $^{24}$Mg, it is possible to obtain a good approximation to the excitation spectrum of states of a particular angular momentum.[4] Furthermore, this method may easily be extended to the finite temperature regime.

It has recently been demonstrated that quantum systems with few degrees of freedom display quantum statistical behavior,[8] even when the dimension of the Hilbert space is only $2^7$. In these numerical studies of the dynamics of finite quantum spin chains the system is well described by the canonical ensemble in spite of the fact that the density of states of the system was too irregular to be described by a Boltzmann factor. In the present calculations the number of $J=8$ many particle states at zero temperature in the model space considered is 329. In view of the aforementioned work we feel justified in applying quantum statistical mechanics to the $J=8$ states in $^{24}$Mg.

Finite temperature restricted Hartree-Fock calculations for the thermal excitation of the ground state have also been performed in other light nuclei.[3] In these calculations, as well as the calculations in heavier systems,[1,2] the level spacing of the lowest-lying Hartree-Fock states at zero temperature is expected to be of roughly the same magnitude as that for the constrained $J=8$ states in $^{24}$Mg. In all of these calculations one uses the grand canonical ensemble with the Fermi distribution for the thermal occupation probability of the single particle states.

For the states in the yrast band, finite temperature Hartree-Fock-Bogoliubov cranking equations have also been evaluated numerically by a number of groups.[9-12] In these calculations the full angular momentum projection has been circumvented by means of a constraint on the expectation value of the one-body operator $\hat{J}_x$, but no attempt has been made to ascertain how strongly localized the solutions are about the desired angular momentum. Furthermore, no anomalous behavior in the thermal response of the states in the yrast band has been observed at very low temperatures. This is probably due to the fact that the equation of constraint involves a one-body operator, and that only the lowest-lying solution of the cranking equations is considered. At higher temperatures a critical temperature exists above which backbending disappears.

The use of the two-body $\hat{J}^2$ constraint in zero temperature CHF calculations, which has previously been successfully implemented,[4-7] leads to an anomalous occupation of the single particle orbitals, in which the lowest lying orbitals are not all occupied. The thermal excitation of such solutions in the grand canonical ensemble will inevitably lead to discontinuities between the zero and finite temperature results. The present calculation is the first to demonstrate this behavior.

In the present work we formulate and solve the constrained finite temperature restricted Hartree-Fock (CFTHF) equations with constraints on the expectation values of the total angular momentum $\hat{J}^2$ and its $z$ component $\hat{J}_z$. As in FTHF, one minimizes the thermodynamic potential $\Omega=\langle\hat{H}\rangle_T-TS-\mu N$ with respect to the HF orbitals $\psi_v(r)$ and the single particle thermal occupation probabilities $f_v$, given the constraint

$$\sum f_v=N\ . \tag{1}$$

Now, however, the additional constraints

$$\langle\hat{J}^2\rangle_T=J(J+1)\ , \tag{2}$$

$$\langle\hat{J}_z\rangle_T=K\ , \tag{3}$$

 

are imposed. Here $\langle\ \rangle_T$ designates the ensemble average at temperature $T$, where $T$ denotes the absolute temperature. The chemical potential is denoted by $\mu$, the number of particles by $N$, and the entropy by $S$, where

$$S=-\sum_\nu f_\nu \ln f_\nu+(1-f_\nu)\ln(1-f_\nu)\ . \tag{4}$$

Starting from a many-body Hamiltonian

$$\hat{H}=\hat{T}+\hat{U}+\hat{V}^{(2)}\ , \tag{5}$$

where $\hat{U}$ is a single particle potential and $\hat{V}^{(2)}$ is a two-body nuclear interaction, one obtains the following set of coupled CFTHF equations:

$$\hat{H}_{\rm cr}(\rho)\psi_\nu=\epsilon_\nu\psi_\nu \tag{6}$$

$$\mathrm{Tr}\rho=\sum_\nu f_\nu=\sum_\nu\{1+\exp[\beta(\epsilon_\nu-\mu)]\}^{-1}=N\ , \tag{7}$$

$$\langle\hat{J}^2\rangle_T=\sum_\nu f_\nu J_\nu^{2(1)}+\sum_{\mu\nu} f_\mu f_\nu J^{2(2)}_{\mu\nu\bar{\mu}\bar{\nu}}=J(J+1)\ , \tag{8}$$

$$\langle\hat{J}_z\rangle_T=\sum_\nu f_\nu J_{z\nu}=K\ , \tag{9}$$

where $\beta=1/kT$,

$$\hat{H}_{\rm cr}=\hat{H}(\rho)-\lambda\hat{J}^2(\rho)-\alpha\hat{J}_z\ , \tag{10}$$

and $\hat{H}(\rho)$ and $\hat{J}^2(\rho)$ are given by their matrix elements

$$\langle\mu\,|\,\hat{H}\,|\,\nu\rangle_T=\langle\mu\,|\,\hat{T}+\hat{U}\,|\,\nu\rangle+\sum_\tau\langle\mu\tau\,|\,\hat{V}^{(2)}\,|\,\tilde{\nu}\tau\rangle f_\tau\ , \tag{11}$$

$$\langle\mu\,|\,\hat{J}^2\,|\,\nu\rangle_T=\langle\mu\,|\,\hat{J}^{2(1)}\,|\,\nu\rangle+\sum_\tau\langle\mu\tau\,|\,\hat{J}^{2(2)}\,|\,\tilde{\nu}\tau\rangle f_\tau\ . \tag{12}$$

Note that $\hat{J}^2$ has been written as the sum of one- and two-body operators in the form

$$\hat{J}^2=\sum_{\mu\nu}\langle\mu\,|\,\hat{j}\cdot\hat{j}\,|\,\nu\rangle c_\mu^\dagger c_\nu+\sum_{\mu\nu\sigma\tau}\langle\mu\nu\,|\,\hat{j}\cdot\hat{j}\,|\,\sigma\tau\rangle c_\mu^\dagger c_\nu^\dagger c_\tau c_\sigma\ , \tag{13}$$

where the operators $c_\mu^\dagger$ refer to the Hartree-Fock orbitals $\psi_\mu$.

For the HF equations at zero temperature the HF ground state is usually one in which the lowest $N$ single particle orbitals are occupied. As temperature increases, the occupation probabilities follow a Fermi distribution, where, again, the single particle states lowest in energy have the highest occupation probability. In the CFTHF method the occupation probabilities are also given by a Fermi distribution,

$$f_\nu=\{1+\exp[\beta(\epsilon_\nu-\mu)]\}^{-1}\ , \tag{14}$$

where the $\epsilon_\nu$ now denote the modified single particle energies of the constrained Hamiltonian, $\hat{H}_{\rm cr}$. Again, the single particle states with the lowest (modified) energy have the highest occupation probabilities.

At zero temperature, however, the solutions of the CHF equations are not necessarily ones in which the lowest single particle orbitals are occupied. In the calculations of Ref. 4 several low-lying solutions in fact have a particle-hole structure (see Figs. 2 and 3). This is probably due in part to the fact that one of the equations of constraint involves a two-body operator that, for certain solutions, enhances the importance of the two-body contribution to the variational energy. For such abnormal states a discontinuity between the zero and finite temperature solutions may occur.

In the present work we have performed a calculation of the thermal response of the $J^\pi=8^+$ and $K=-7$ states with total isospin $I=0$ in $^{24}$Mg. The $^{24}$Mg nucleus has been taken to consist of an inert $^{16}$O core plus eight active valence particles in the $2s$-$1d$ shell. The thermal response of the core was neglected in the present calculation because one expects, as in the case of the thermal response of the HF ground state, this contribution to be minimal for $T\lesssim 1$ MeV. In the $2s$-$1d$ shell we used an effective Hamiltonian with the Vary-Yang interaction,[13] including additional third order corrections to the $G$ matrix to provide a more complete accounting of the core polarization effects,[14] and the following single particle energies:

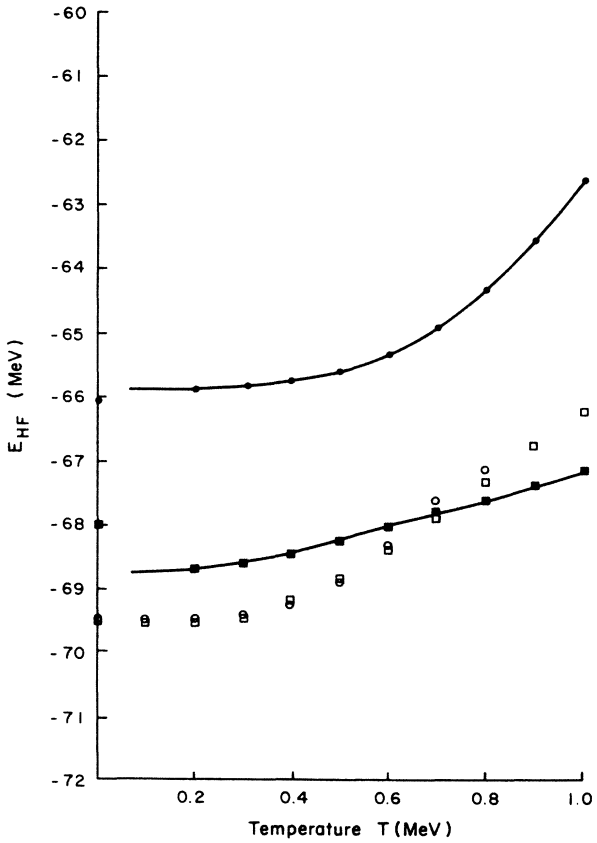


FIG. 1. The variational energies of some of the energetically lowest-lying solutions of the CFTHF equations of a function of temperature. The two delocalized solutions whose CHF variational energies are $-69.506$ MeV and $-69.476$ MeV are designated by open squares and circles, respectively. The localized solutions whose CHF variational energies are $-68.085$ MeV and $-66.069$ MeV are designated by solid squares and circles, respectively. Solid curves have been drawn through the CFTHF results which are localized in angular momentum.

TABLE I. The variance of the angular momentum distribution, $\Delta J^2=\langle[\hat{J}^2-J(J+1)]^2\rangle$ in units of $\hbar^2$, for the energetically lowest-lying solutions of the CFTHF equations.

| $E_{JK}^{\mathrm{CHF}}$ (MeV) | $\Delta J^2$ for temperature $T$ (MeV) | | | | |
|---|---|---|---|---|---|
| ($T=0$ MeV) | 0.0 | 0.3 | 0.5 | 0.8 | 1.0 |
| −69.506 | 1746.29 | 1737.16 | 1674.47 | 1562.70 | 1507.49 |
| −69.476 | 1811.58 | 1807.45 | 1752.71 | 1567.08 | |
| −68.085 | 577.00 | 632.35 | 706.07 | 783.71 | 816.77 |
| −67.970 | 490.94 | | | | |
| −66.069 | 678.46 | 617.91 | 614.78 | 646.79 | 718.04 |

$\epsilon d_{5/2}=-5.00$ MeV ,

$\epsilon d_{3/2}=0.08$ MeV ,

$\epsilon s_{1/2}=-4.13$ MeV .

To solve the CFTHF equations, the HF orbitals $\psi_\nu$ were expanded in a truncated harmonic oscillator basis with expansion coefficients $\{d_\nu^i\}$. The resulting equations were then solved simultaneously via the Newton-Rhaphson method.

The thermal response of the variational energies of the lowest solutions of the CFTHF equations is given in Fig. 1. In addition, $\Delta J^2$ has been tabulated for all four solutions at a few representative temperatures (see Table I). One should compare these results with the zero temperature CHF calculations of Ref. 4. For $T=0$ the CHF results fall in two groups, the first group consisting of solutions strongly localized in angular momentum with $\Delta J^2 \lesssim 850\hbar^2$ and the second consisting of delocalized solutions with $\Delta J^2 \gtrsim 1500\hbar^2$. One should note that $\Delta J^2 \approx 600\hbar^2$ corresponds to a width of the angular

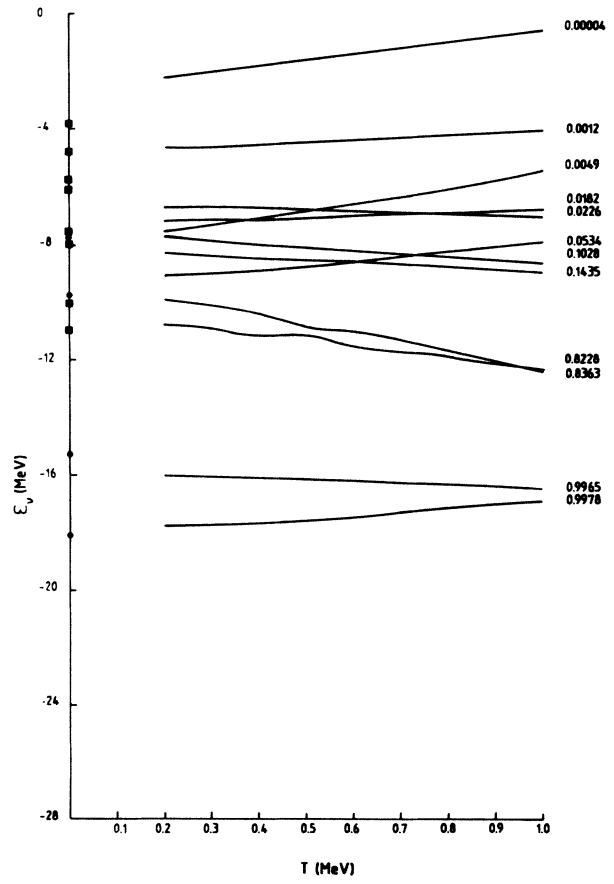


FIG. 2. The thermal excitation of the single particle levels of the lowest lying abnormal CFTHF solution. The thermal occupation probabilities of the single particle levels at $T=1$ MeV are given on the right-hand side of the figure. At $T=0$ the occupied levels are denoted by solid circles.

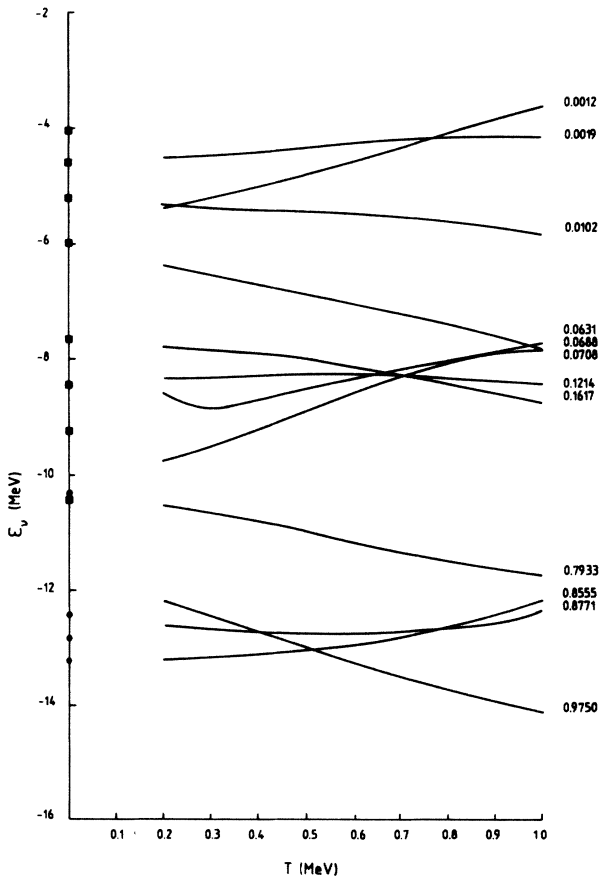


FIG. 3. The thermal excitation of the single particle levels of the higher lying abnormal CFTHF solution. The thermal occupation probabilities of the single particle levels at $T=1$ MeV are given on the right-hand side of the figure. At $T=0$ the occupied levels are denoted by solid circles.

TABLE II. The mass quadrupole moment $Q_0^2$ in units of $\nu^{-1}$, where $\nu^{-1}=\hbar/m\omega$ for the energetically lowest-lying solutions of the CFTHF equations.

| $E_{HF}^{CHF}$ (MeV) | $Q_0^2(\nu^{-1})$ for temperature $T$ (MeV) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ($T=0$ MeV) | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
| −69.506 | −9.112 | −9.112 | −9.113 | −9.125 | −9.147 | −9.155 | −9.129 | −9.072 | −8.984 | −8.863 | −8.687 |
| −69.476 | −8.780 | −8.780 | −8.781 | −8.785 | −8.794 | −8.808 | −8.837 | −8.894 | −8.823 | | |
| −68.085 | 11.931 | | 11.934 | 11.986 | 12.043 | 12.070 | 12.064 | 12.032 | 11.983 | 11.921 | 11.844 |
| −67.970 | 11.858 | | | | | | | | | | |
| −66.069 | −1.172 | | −0.511 | −0.532 | −0.570 | −0.616 | −0.653 | −0.666 | −0.641 | −0.572 | −0.453 |

momentum distribution of $1-2\hbar$. At zero temperature the two lowest-lying solutions are delocalized and therefore fall into the second group. The next three CHF solutions are localized and in terms of their excitation spectrum have been identified with the results obtained from an exact diagonalization. Of these solutions only the three localized solutions have an abnormal structure.

Unfortunately, at finite temperature we are unable to obtain the thermal response of the second CHF solution in the higher-lying doublet. This is undoubtedly a consequence of the similar structure of the two CHF solutions and the discontinuity resulting from their abnormal structure at zero temperature.

In the case of the lowest lying discontinuous solution of the CFTHF equation, the internal energy, $E_{HF}$, initially decreases with increasing temperature. This decrease is a feature of the approximate nature of the present calculations and we do not expect it to occur in exact calculations. The zero and finite temperature solutions only represent upper bounds to exact results. At zero temperature the corresponding exact eigenenergy lies at −74.328 MeV (Ref. 4), which is well below the value of the internal energy at low temperatures.

For the second lowest CFTHF solution, convergent solutions of the CFTHF were obtained only for temperatures $\lesssim 0.8$ MeV. Similar behavior was observed for the other solutions, but at higher temperatures. At higher temperatures the unconstrained deformed FTHF solutions undergo a "phase transition" and become spherical in shape. Attempting to avoid this "phase transition" by the use of the angular momentum constraints given in the present work does not appear to be possible. Eventually, at higher temperature, we cannot satisfy the equations of constraint, and therefore convergent solutions of the CFTHF equations are no longer obtainable. At low temperatures ($T \lesssim 0.1$ MeV) numerical difficulties are encountered in obtaining CFTHF solutions for the states of abnormal occupation.

Although the values of $\Delta J^2$ change with temperature, one can still unambiguously divide the solutions into two groups. As for the CHF solutions, the two energetically lowest-lying CFTHF solutions are delocalized, while the rest of the solutions remain localized in the distribution of their angular momentum. One should note the different thermal response of the two groups of solutions. The value of $\Delta J^2$ for the solutions that are localized at $T=0$ does not increase significantly with increasing temperature, which leads us to believe that they remain states of approximately good angular momentum. It should be noted that the thermal response of the two solutions that remain localized is similar only at lower temperatures ($T \lesssim 0.6$ MeV). One should also note the discontinuity in the thermal response of the variational energy between the zero and finite temperature results for these two solutions. This is due to their abnormal structure at zero temperature.

The thermal excitation of the single particle levels of the two abnormal CFTHF solutions [see Eq. (6)] are given in Figs. 2 and 3. In the present calculation for $T \leq 1$ MeV our choice of the model space appears to be adequate since the thermal occupation probability of the highest level does not exceed $2\times 10^{-3}$. Furthermore, the gaps between the single particle levels with highest occupation probability and the higher lying single particle levels increase with increasing temperature. This may well indicate that the CFTHF approximation is better at higher temperatures.

In Table II we give the mass quadrupole moment for the CFTHF solutions as a function of the absolute temperature. Firstly one notes that the quadrupole moment is essentially independent of temperature. This implies that the constraint on $\hat{J}^2$ leads to a constant quadrupole deformation, as might be expected. Secondly, at least in the case of the lower three solutions, there is no apparent discontinuity in the quadrupole moment obtained from the zero and finite temperature solutions. This is particularly surprising in the case of the third solution in light of the marked discontinuity in the variational energy.

In the present work we have demonstrated the feasibility of calculating the thermal response of different states of the same angular momentum in the CFTHF approximation. For states that at $T=0$ do not have the lowest single particle states occupied there is a discontinuity between the zero and finite temperature solutions. Here it is of interest to note that this discontinuity could occur in the thermal excitation of any abnormal HF state.[15,16]

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