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Comparison between the exact and the thermal description of the pairing interaction in ^{114}Sn

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The pairing interaction is solved exactly in the ^{114}Sn nucleus using a realistic strength parameter as well as standard energy levels for the shell seniority zero states. The same single-particle and two-body Hamiltonian is treated with finite-temperature BCS and the thermal random-phase approximation. The results obtained through these calculations are compared to obtain insight about the suitability of the thermal approach to the description of nuclear phenomena.

Since the temperature concept was introduced in nuclear physics[1] the temperature-dependent version of nuclei has been studied in great detail.[2-8] In the studies done in nuclear structure, the main assumption has been the validity of temperature-dependent mean-field approximations, such as the temperature-dependent Hartree-Fock-Bogoliubov[2,8] or thermal random-phase approximation[3,4] (RPA) descriptions. These types of approaches have been applied to both schematic[5] and realistic problems,[6] but a comparison between the results obtained using the thermal description and the exact one has only been done essentially for very simple and schematic models,[2] where the validity of the standard methods of quantum statistical mechanics has been assumed. Recently, the importance of fluctuations,[6-7,9-11] or equivalently, deviations from the mean-field behavior[12-15] of temperature-dependent properties that are expected to be important when finite systems are treated has been stressed.

The Hamiltonian which we used is

$$H=\sum_{ja}\epsilon_{ja}b^{\dagger}_{ja}b_{ja}-GP^{\dagger}P\,, \tag{1}$$

where

$$P^{\dagger}=\sum_{j,a>0}b^{\dagger}_{ja}b^{\dagger}_{j\bar{a}}=\sum_{j}A^{\dagger}_{j}\,, \tag{2}$$

$b^{\dagger}_{jm}$ being the particle creation operator in the state (jm) while $(j\bar{m})$ denotes its time-reversal state. The exact spectrum of (1) was obtained using the standard technique described in Ref. 16. For one shell the eigenstates of (1) are given, as usual, as

$$|k,v\rangle=N_{kv}(A^{\dagger}_{j})^{k}B^{v}|0\rangle\,, \tag{3}$$

where N_{kv} is a normalization constant and the operator B^{v} which creates v particles (with seniority v) satisfies the conditions

$$\begin{aligned}&A_{j}B^{v}|0\rangle=0\,,\\&\left(\sum_{j,a}b^{\dagger}_{ja}b_{ja}\right)B^{v}|0\rangle=vB^{v}|0\rangle\,.\end{aligned} \tag{4}$$

When there are many shells, the structure of the states is similar. We will only consider the states which have seniority zero in all the shells. The matrix elements of the interacting part of the Hamiltonian (1) can be written as

$$\langle k_1,\ldots,k_n+1,\ldots,k_l-1,\ldots,k_s|H_{\rm int}|k_1,\ldots,k_n,\ldots,k_l,\ldots,k_s\rangle=-G\sqrt{k_l(k_n+1)(j_l+\tfrac{3}{2}-k_l)(j_n+\tfrac{1}{2}-k_n)}\,,$$

where k_n corresponds to the number of particles in the shell k. In a similar way we can evaluate the matrix element of an operator that will be related to the two-particle transfer operator, i.e.,

$$\langle k_1,\ldots,k_n+1,\ldots,k_s|A^{\dagger}_{j_n}|k_1,\ldots,k_n,\ldots,k_s\rangle=\sqrt{(k_n+1)(j_n+\tfrac{1}{2}-k_n)}\,. \tag{5}$$

In order to perform the calculation for ^{114}Sn we choose the values for the single-particle energies shown in Table I, and we fixed the effective pairing constant in $23/A$. Both types of values are similar to those used in Ref. 17. With this Hamiltonian it is possible to obtain its energy spectra by diagonalizing it numerically, both for ^{114}Sn and ^{116}Sn, and also to evaluate the matrix element of the operator $P^{\dagger}$ between all (the 105) states of ^{114}Sn and the (110) states of ^{116}Sn.

In order to display the main features of the square of these matrix elements (which, in principle, will be proportional to the two-particle transfer), it is convenient to choose a logarithmic scale, and also to disregard the matrix elements which are too small. As the biggest matrix elements are of the order of 100, in Fig. 1 we display the logarithm of all matrix elements that are bigger than one for the first 100 states of both systems. The structure of this figure looks rather promising from the point of view of a thermal description, as there are only a very small number of states of ^{116}Sn connecting with each state of ^{114}Sn. The thermal description allows only for five nonvanishing matrix elements[6] for temperatures smaller than the critical one.

We will review now, how to perform the thermal description. The low-energy states can be described properly using a finite-temperature BCS (FTBCS) treatment,

TABLE I. Single-particle energy levels for neutrons in ^{114}Sn and ^{116}Sn.

Level	Energy (MeV)
$0g\frac{7}{2}$	0.80
$1d\frac{5}{2}$	0.00
$2s\frac{1}{2}$	1.40
$1d\frac{3}{2}$	2.80
$0h\frac{11}{2}$	2.50

already discussed in Ref. 2 and which is similar to the calculations done in Ref. 6, the only difference being the strength parameter. In this case we perform the BCS procedure, transforming (1) to the quasiparticle basis. The vacuum is replaced by a reference state characterized by this temperature. The expectation values of the quasiparticle operators $\alpha_k^\dagger$ on the reference state have the value

$$\langle a_k^\dagger a_k\rangle = f_k\,, \tag{6}$$

where f_k is the thermal occupation number, i.e.,

$$f_k = \frac{1}{1+e^{E_k/k_BT}}\,, \tag{7}$$

where E_k is the corresponding quasiparticle energy. The energy of the reference state is given by

$$E_0 = -\frac{\Delta^2(T)}{G} + \sum_k (\epsilon_k - \lambda)[V_k^2(1-f_k) + U_k^2 f_k]\,, \tag{8}$$

where $\Delta(T)$ is the gap, λ is the Fermi energy, and U_k and V_k are the usual quasiparticle amplitudes

$$U_k^2 = \frac{1}{2}\left[1+\frac{\epsilon_k-\lambda}{E_k}\right],\quad V_k^2 = \frac{1}{2}\left[1-\frac{\epsilon_k-\lambda}{E_k}\right]. \tag{9}$$

Equation (8) gives a relation between the excitation energy and the temperature. As usual, one obtains the gap and the Fermi energy through the gap and number equations, which are satisfied at each temperature until a critical temperature $T_c[\simeq \frac{1}{2}\Delta(T=0)]$, where the gap vanishes. For temperatures higher than this T_c one must study the thermal pairing vibrations. As in the $T=0$ case[18] one defines two pairing vibrations, one addition mode $\Gamma_a^\dagger$ and a removal one $\Gamma_r^\dagger$. In the particular case of ^{114}Sn the levels $1d\frac{5}{2}$ and $0g\frac{7}{2}$ will be in zero order completely full, while the remaining levels ($1d\frac{3}{2}$, $2s\frac{1}{2}$, and $0h\frac{11}{2}$) will be empty. We will denote by the letter i the levels which are full and by k the empty levels. With this convention, we can write

$$\Gamma_a^\dagger = \sum_{k>0} X_{ka} A_k^\dagger - \sum_{i>0} Y_{ia} A_i^\dagger\,, \tag{10}$$

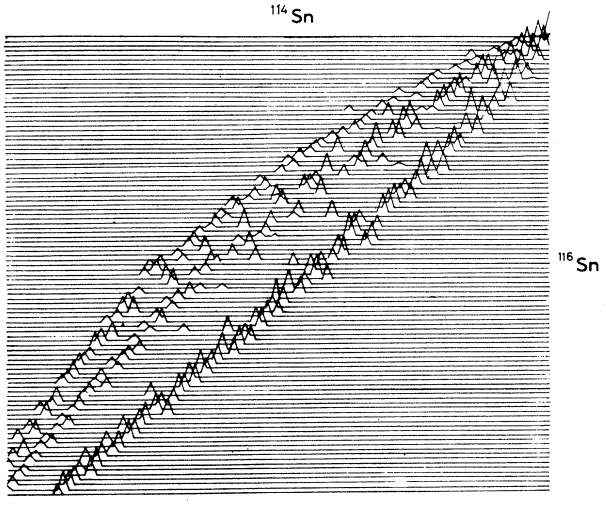

FIG. 1. The logarithm of the square of the matrix elements of the two-particle transfer operator between the first 100 states of ^{114}Sn and the same number in ^{116}Sn. The matrix elements are shown only when they are bigger than one. The upper right corner relates both ground states.

and

$$\Gamma_r^\dagger = \sum_{i>0} X_{ir} A_i - \sum_{k>0} Y_{kr} A_k\,, \tag{11}$$

and they satisfy as usual the normalization conditions

$$[\Gamma_a, \Gamma_a^\dagger] = \sum_{k>0} X_{ka}^2(1-2f_k) - \sum_{i>0} Y_{ia}^2(1-2f_i) = 1\,, \tag{12}$$

$$[\Gamma_r, \Gamma_r^\dagger] = \sum_{i>0} X_{ir}^2(1-2f_i) - \sum_{k>0} Y_{kr}^2(1-2f_k) = 1\,,$$

as well as the orthogonality ones

$$[\Gamma_r^\dagger, \Gamma_a^\dagger] = [\Gamma_r, \Gamma_a^\dagger] = 0\,. \tag{13}$$

The inverse transformation can be written as

$$\begin{aligned} A_k^\dagger &= (1-2f_k)\left(\sum_a X_{ka}\Gamma_a^\dagger + \sum_r Y_{kr}\Gamma_r\right), \\ A_i^\dagger &= (1-2f_i)\left(\sum_r X_{ir}\Gamma_r + \sum_a Y_{ia}\Gamma_a^\dagger\right), \end{aligned} \tag{14}$$

which takes into account the fact that now (for $T\neq 0$) the expectation value of the conmutation relation on the reference state has the value

$$\begin{aligned} \langle 0|[A_k, A_k^\dagger]|0\rangle &= (1-2f_k)\,, \\ \langle 0|[A_i, A_i^\dagger]|0\rangle &= -(1-2f_i)\,. \end{aligned} \tag{15}$$

One can then write the Hamiltonian in terms of this pairing modes and one can obtain the reference state energy as

$$E_0 = 2\left[\sum_k (\epsilon_k-\lambda)(1-2f_k)\sum_r Y_{kr}^2 - \sum_i (\epsilon_i-\lambda)(1-2f_i)\sum_a Y_{ia}^2\right] - G\left[\sum_i X_{ir}(1-2f_i) + \sum_k Y_{kr}(1-2f_k)\right]^2, \tag{16}$$

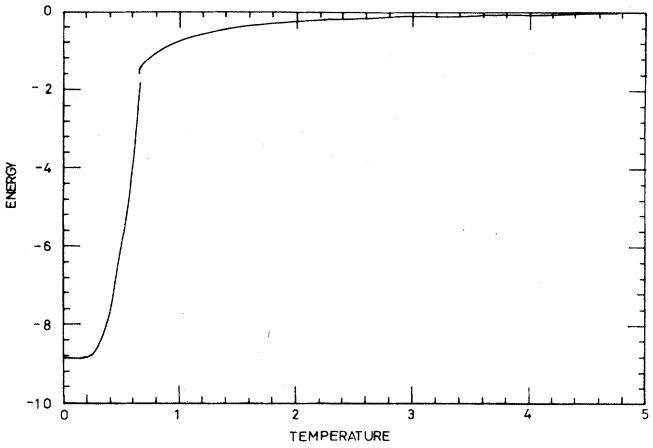

FIG. 2. Relation between the excitation energy and the temperature obtained through the FTBCS and the thermal RPA procedures.

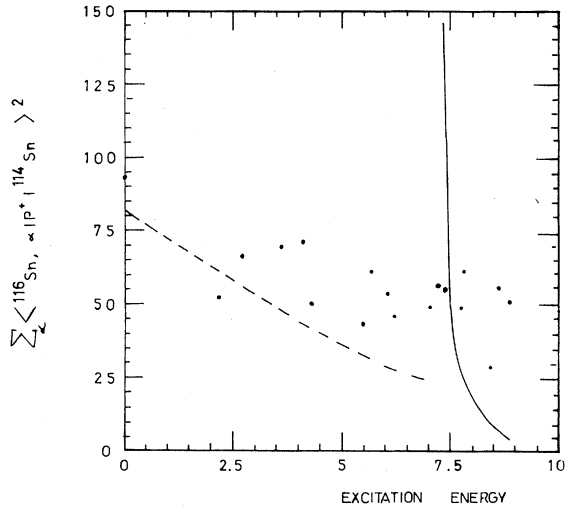

FIG. 3. The sum of the squares of the matrix elements of the operator leading from a state in ^{114}Sn to all the states in ^{116}Sn. The dots corresponds to the results obtained in the exact calculations, while the dashed line corresponds to the FTBCS ones, and the solid line corresponds to thermal RPA.

which provides us with a relation between the excitation energy and the temperatures after the phase transition (from superconductive to normal). In Fig. 2 we show the relation between the excitation energy and the temperature for all positive temperatures, obtained through the FTBCS and thermal RPA procedures. A feature which must be remembered is that when one makes a thermal description of a system having a maximum attainable energy (as happens when one cuts the Hilbert space) one cannot obtain with a thermal description the higher excited states if one restricts oneself to positive temperatures.

We want to compare the results obtained for the $P^\dagger$ operator in the exact and the thermal description. As in the exact calculation sometimes the strength of $P^\dagger$ fragments between two or three states, we decided to compare the thermal results with the sum of all the squares of the matrix elements which connects one state of ^{114}Sn with all the states of ^{116}Sn obtained in the exact calculations. When the gap is nonzero it will correspond to the matrix element of the two-particle transfer operator between the reference states in both tin isotopes. When the gap is null, after the critical temperature, one must evaluate the matrix element as in the case of the pairing vibrations. One therefore obtains for these transitions between ^{114}Sn and ^{116}Sn

$$\sum_a \left(\sum_k (1-2f_k) X_{ka} + \sum_i (1-2f_i) Y_{ia} \right)^2 . \qquad (17)$$

In Fig. 3 the dots show the exact results corresponding to the sum of the square of the matrix elements for the two-particle transfer operator starting in each of the ^{114}Sn states (up to the maximum energy that can be obtained thermally). The dashed line shows the corresponding value obtained in the superconductive description (FTBCS), while the solid line shows the results obtained in the thermal RPA description. It must be noted that while the FTBCS description is just a mean-field one, the thermal RPA takes into account the more important part of the fluctuations, and therefore the disagreement between the exact results and the thermal description is more significant.

Fluctuations, which are of the order $1/\sqrt{N}$, N being the number of active particles, are very important and are necessary when using thermal descriptions. It must be noted that in the normal region (for T larger than T_c) the value predicted by the mean-field description for the operator $P^\dagger$ is zero.

We can conclude that even for a system such as the tin isotopes, where the BCS description is known to work nicely, the thermal treatment does not give an appropriate description of the behavior of the system in the superconductive region as well as when one takes into account the thermal fluctuations through the thermal RPA in the normal region.

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