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THERMODYNAMICAL PROPERTIES OF A PAIRED NUCLEUS WITH
A FIXED NUMBER OF QUASI-PARTICLES[†]

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ABSTRACT: The general formalism for the description of the properties of a paired system with fixed number of quasi-particles has been developed. The number of quasi-particles has been introduced into the pairing Hamiltonian by means of a Lagrange multiplier. The Grand Partition Function and all the other thermodynamical functions have been derived. The formalism has been applied to the uniform model. The properties of the system in the limit of zero temperature have been obtained analytically. It has been found that for temperatures smaller than the critical temperature of the unrestricted system, a first order phase transition from the paired to the unpaired phase occurs when the quasi-particle number is increased isothermally. Above the critical temperature the transition becomes of the second order. The model also predicts that at a fixed quasi-particle number the pairing correlation increases with increasing temperature. In particular, at the highest excitation, and at small quasi-particle number, the pairing correlation is as strong as in the ground state. A rapid decrease and an eventual disappearance of pairing occurs as the system is allowed to relax towards its equilibrium number of quasi-particles.

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1. INTRODUCTION

The statistical properties of a system with a fixed number of excitations (quasi-particles) are of interest in the study of relaxation phenomena in nuclei. By far the widest use of these properties has been made in the description of pre-equilibrium emission of nucleons¹⁻⁴). However, one can forecast a multiplicity of cases where the statistical properties of a fixed quasi-particle system may be of interest. For instance, in the description of the width of a doorway state (single particle or collective in nature), the coupling of such a state with a certain class of particle-hole states needs to be considered.

The previous papers that have dealt with this problem have restricted it in two ways. On the one hand they have limited their scope to the evaluation of the level density, on the other they have limited their calculation to the independent particle model, either in the simplified form of the constant spacing model (uniform model)⁵⁻⁷) or in the more refined form of the shell model⁸⁻¹⁰). In the present paper we shall try to give a detailed presentation of the various relevant thermodynamical quantities as a function of the quasi-particle number. At the same time, the residual interaction will be introduced in the form of the pairing approximation. In systems with unrestricted quasi-particle number the residual interaction is very important only at low energy¹¹⁻¹⁴). In this paper it will be shown that, at small quasi-particle numbers, the pairing correlation is present even at very high excitation energies and that it plays a dominant role during the relaxation process leading from a small quasi-particle number to its equilibrium value.

In order to clearly identify the correlation between quasi-particle number and pairing, we shall use the uniform model which eliminates the shell effects associated with the fluctuations in the single-particle spacings.

The main thrust of this paper is in its attempt to offer a global view of the general thermodynamical properties of such systems more than in the exact numerical calculation of specific quantities like the level density. With this in mind, the saddle-point approximation has been employed even where some inaccuracy is to be expected, as in the case of small energies and/or small quasi-particle numbers. On the other hand, an effort has been made to obtain, whenever possible, simple analytical results which have the advantage of giving an in-depth view of the overall picture. In section 2 the general Hamiltonian is described without reference to any specific single-particle model. From it the Grand Partition Function is obtained and the overall formalism is derived.

In section 3 the formalism is applied to the uniform model. Section 3.a. deals with the limiting case of zero temperature. The dependence of the gap parameter and of the energy upon quasi-particle number is obtained analytically. A first-order phase transition, never observed before with this kind of Hamiltonian, is described in the general context of the discussion of phase stability. The relation between the yrast line and the E, Q dependence at $T=0$ is discussed. Section 3.b. deals with the same problems for $T > 0$. Furthermore the entropy and level densities are calculated. Section 4 contains the conclusion and a brief assessment of the general state of the field. A preliminary account of this work has been published¹⁵).

2. GENERAL FORMALISM

2.1. The Hamiltonian

In this paper we shall use the simplest form of a pairing Hamiltonian with constant pairing strength:

$$H = \sum_{\pm k} \epsilon_k a_k^\dagger a_k - G \sum_{k'} a_{k'}^\dagger a_{k'}^\dagger a_k a_k, \quad (1)$$

where ϵ_k are the single-particle energy eigenvalues; $a_k^\dagger, a_k$ are the particle creation and annihilation operators; and G is the pairing strength.

This Hamiltonian, modified to ensure the conservation of the average particle number, can be approximately diagonalized by means of the Bogoliubov quasi-particle transformation to yield the expression

$$H' = \sum (\epsilon_k - \lambda - E_k) + 2 \sum n_k E_k + \Delta^2/G, \quad (2)$$

where λ is the Lagrange multiplier introduced to fix the particle number;

$n_k = b_k^\dagger b_k$ is the quasi-particle occupation number for the level k ;

E_k are the quasi-particle energy eigenvalues, given by:

$$E_k = \sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}; \quad (3)$$

and the quantity Δ , called pairing gap, is given by the equation

$$\frac{2}{G} = \sum \frac{1 - 2n_k}{E_k}. \quad (4)$$

In order to fix the mean number of quasi-particles we introduce a new auxiliary Hamiltonian:

$$H'' = H' - \xi Q \quad (5)$$

where

$$Q = 2 \sum n_k \quad (6)$$

is the quasi-particle number and ξ is the Lagrange multiplier necessary for this particular constraint.

Explicitly, the new Hamiltonian can be written as

$$H'' = \sum (\epsilon_k - \lambda - E_k) + \frac{\Delta^2}{G} + 2 \sum n_k (E_k - \xi) . \quad (7)$$

2.2. The Grand Partition Function and the Other Thermodynamical Functions

The Grand Partition Function can be immediately obtained from the Hamiltonian H'' . Remembering that

$$e^{\Omega} = \text{Tr } e^{-H''} , \quad (8)$$

one obtains:

$$\Omega = -\beta \sum (\epsilon_k - \lambda - E_k) - \beta \frac{\Delta^2}{G} + 2 \sum \ln \left[1 + \exp - \beta (E_k - \xi) \right] \quad (9)$$

From this expression, all the other thermodynamical functions can be obtained by differentiation:

- The particle number:

$$N = \frac{1}{\beta} \frac{\partial \Omega}{\partial \lambda} = \sum \left[1 - \frac{\epsilon_k - \lambda}{E_k} \tanh \frac{1}{2} \beta (E_k - \xi) \right] . \quad (10)$$

- The quasi-particle number:

$$Q = \frac{1}{\beta} \frac{\partial \Omega}{\partial \xi} = 2 \sum \frac{1}{1 + \exp \beta (E_k - \xi)} . \quad (11)$$

- The energy:

$$E = -\frac{\partial \Omega}{\partial \beta} = \sum \epsilon_k \left[1 - \frac{\epsilon_k - \lambda}{E_k} \tanh \frac{1}{2} \beta (E_k - \xi) \right] - \frac{\Delta^2}{G} . \quad (12)$$

- The gap equation:

$$\frac{\partial \Omega}{\partial \Delta} = 0 \quad \text{or} \quad \sum \frac{1}{E_k} \tanh \frac{1}{2} \beta (E_k - \xi) - \frac{2}{G} = 0 . \quad (13)$$

The last four equations can be solved simultaneously for β , λ , ξ , Δ , and these quantities can be used for the evaluation of the entropy:

$$S = 2 \sum \ln[1 + \exp - \beta(E_k - \xi)] + 2\beta \sum \frac{E_k - \xi}{1 + \exp \beta(E_k - \xi)} . \quad (14)$$

2.3. The Level Density

The level density is the inverse Laplace transform of the Grand Partition Function:

$$\rho(E, N, Q) = \iiint \exp(\Omega + \beta\lambda N + \beta\xi Q - \beta E) dE d\beta\lambda d\beta\xi . \quad (15)$$

The application of the saddle-point approximation to the evaluation of the integrals yields the following result:

$$\rho(E, N, Q) = \frac{\exp S}{(2\pi)^{3/2} D^{1/2}} , \quad (16)$$

where

$$D = \begin{vmatrix} \frac{\partial^2 \Omega}{\partial \alpha^2} & \frac{\partial^2 \Omega}{\partial \alpha \partial \mu} & \frac{\partial^2 \Omega}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \Omega}{\partial \mu \partial \alpha} & \frac{\partial^2 \Omega}{\partial \mu^2} & \frac{\partial^2 \Omega}{\partial \mu \partial \beta} \\ \frac{\partial^2 \Omega}{\partial \beta \partial \alpha} & \frac{\partial^2 \Omega}{\partial \beta \partial \mu} & \frac{\partial^2 \Omega}{\partial \beta^2} \end{vmatrix} . \quad (17)$$

In this expression $\alpha = \beta\lambda$, $\mu = \beta\xi$.

In all the quantities appearing in eq. (17), one must use the saddle point values of β , λ , ξ , Δ , namely those obtained by solving the eqs. (10, 11 12) and (13). The expressions for the second derivatives are the following:

$$\frac{\partial^2 \Omega}{\partial \mu^2} = \frac{1}{2} \sum \text{sech}^2 \frac{1}{2} \beta (E_k - \xi) - \frac{1}{2} \beta \Delta \frac{\partial \Delta}{\partial \mu} \sum E_k^{-1} \text{sech}^2 \frac{1}{2} \beta (E_k - \xi) , \quad (18)$$

$$\frac{\partial^2 \Omega}{\partial \alpha^2} = \sum (\epsilon_k - \lambda)^2 a_k + \Delta^2 \sum b_k - \beta \Delta \frac{\partial \Delta}{\partial \alpha} \sum (\epsilon_k - \lambda) (a_k - b_k) , \quad (19)$$

$$\begin{aligned} \frac{\partial^2 \Omega}{\partial \beta^2} = & \Delta^2 \sum \epsilon_k \left[\lambda b_k + (\epsilon_k - \lambda) a_k \right] + \sum \epsilon_k^2 (\epsilon_k - \lambda)^2 a_k + \\ & + \beta \Delta \frac{\partial \Delta}{\partial \beta} \left\{ \sum \epsilon_k (\epsilon_k - \lambda) (a_k - b_k) + \frac{2}{\beta G} \right\} , \end{aligned} \quad (20)$$

$$\frac{\partial^2 \Omega}{\partial \alpha \partial \beta} = -\Delta^2 \sum \left\{ \lambda b_k + (\epsilon_k - \lambda) a_k \right\} - \sum \epsilon_k (\epsilon_k - \lambda)^2 a_k - \beta \Delta \frac{\partial \Delta}{\partial \beta} \sum (\epsilon_k - \lambda) (a_k - b_k) , \quad (21)$$

$$\frac{\partial^2 \Omega}{\partial \mu \partial \alpha} = \frac{1}{2} \sum \frac{(\epsilon_k - \lambda)}{E_k} \text{sech}^2 \frac{1}{2} \beta (E_k - \xi) - \frac{1}{2} \beta \Delta \frac{\partial \Delta}{\partial \alpha} \sum E_k^{-1} \text{sech}^2 \frac{1}{2} \beta (E_k - \xi) , \quad (22)$$

$$\begin{aligned} \frac{\partial^2 \Omega}{\partial \mu \partial \beta} = & -\frac{1}{2} \sum \left[\text{sech}^2 \frac{1}{2} \beta (E_k - \lambda) \right] \left[E_k + \frac{\lambda (\epsilon_k - \lambda)}{E_k} \right] \\ & - \frac{1}{2} \beta \Delta \frac{\partial \Delta}{\partial \beta} \sum E_k^{-1} \text{sech}^2 \frac{1}{2} \beta (E_k - \xi) . \end{aligned} \quad (23)$$

The derivatives of Δ with respect to the three Lagrange multipliers are given by:

$$\frac{\partial \Delta}{\partial \beta} = - \frac{\Delta^2 \sum a_k + \sum a_k \epsilon_k (\epsilon_k - \lambda) - \lambda \sum b_k (\epsilon_k - \lambda)}{\beta \Delta \sum (a_k - b_k)} , \quad (24)$$

$$\frac{\partial \Delta}{\partial \mu} = \frac{1}{2} \frac{\sum E_k^{-1} \operatorname{sech}^2 \frac{1}{2} \beta (E_k - \xi)}{\beta \Delta \sum (a_k - b_k)} , \quad (25)$$

$$\frac{\partial \Delta}{\partial \alpha} = \frac{\sum (\epsilon_k - \lambda) (a_k - b_k)}{\beta \Delta \sum (a_k - b_k)} . \quad (26)$$

These derivatives must be set equal to zero when $\Delta = 0$. In all the above expressions we have set:

$$\begin{aligned} a_k &= \frac{1}{2} E_k^{-2} \operatorname{sech}^2 \frac{1}{2} \beta (E_k - \xi) , \\ b_k &= \beta^{-1} E_k^{-3} \tanh \frac{1}{2} \beta (E_k - \xi) . \end{aligned} \quad (27)$$

These expressions provide a complete formalism for the description of the statistical properties of paired systems with fixed quasi-particle number.

3. APPLICATION OF THE FORMALISM TO THE UNIFORM MODEL

The pairing properties inherent to the above formalism can be explored best by applying it to the uniform model. In such a model the doubly degenerate single-particle levels are equidistant so that the single-particle spectrum can be characterized by the single-particle level density g . The lack of shell structure allows one to identify unambiguously the effect of the number of quasi-particles on the pairing correlation.

The model is completely described by the single-particle level density g , which defines the independent particle aspect of the problem and by the ground state gap parameter Δ_0 , which defines the pairing residual interaction. A great advantage of this model is the fact that the particle chemical potential

λ is a constant due to the symmetry of the single-particle spectrum. Thus one can set $\lambda = 0$ and disregard the particle equation.

In what follows, the limiting properties of the system as the temperature tends to zero will be considered first. The study will then be extended to the case of $T > 0$. In the graphs presented from here on, the gap parameter will be expressed in terms of the ground state gap parameter Δ_0 ; the energy and free energy in units of the condensation energy $C = \frac{1}{2}g\Delta_0^2$; the temperature in terms of the critical temperature $T_{cr} = 2\Delta_0/3.5$; the quasi-particle number in terms of the most probable quasi-particle number at the critical temperature $Q_{cr} = 4g T_{cr} \ln 2$; the entropy in terms of the entropy at the critical point $S_{cr} = 2(\pi^2/3)g T_{cr}$.

3.a. Limiting Properties for $T=0$ ($\beta \rightarrow \infty$)

3.a.1. The Gap Equation

The gap equation in the uniform model can be rewritten as follows:

$$2g \int_0^S \frac{\tanh \frac{1}{2} \beta (E - \xi)}{E} d\epsilon = \frac{2}{G} = 2g \int_0^S \frac{\tanh \frac{1}{2} \beta E}{E} d\epsilon, \quad (28)$$

where $\pm S$ is the range over which the pairing interaction extends, $E = \sqrt{\epsilon^2 + \Delta^2}$ is the quasi-particle energy and ξ is the quasi-particle chemical potential.

In the limit of $\beta \rightarrow \infty$ the above expression can be integrated explicitly:

$$2g \left(\operatorname{arcsinh} \frac{S}{\Delta} - 2 \operatorname{arcsinh} \frac{\sqrt{\xi^2 - \Delta^2}}{\Delta} \right) = 2g \operatorname{arcsinh} \frac{S}{\Delta_0}. \quad (29)$$

By using the logarithmic expressions for the $\operatorname{arcsinh}$ one obtains:

$$\frac{\Delta_0}{\Delta} \frac{\left[1 + \left(1 + \frac{\Delta^2}{S^2} \right)^{\frac{1}{2}} \right]}{\left[1 + \left(1 + \frac{\Delta_0^2}{S^2} \right)^{\frac{1}{2}} \right]} = \left[\frac{\sqrt{\xi^2 - \Delta^2}}{\Delta} + \left(\frac{\xi^2 - \Delta^2}{\Delta^2} + 1 \right)^{\frac{1}{2}} \right]^2 \quad (30)$$

Because of the arbitrariness of the choice of S , provided that the pairing strength G is suitably renormalized, one can choose $S \gg \Delta_0$ so that in the above expression all the terms of order Δ_0^2/S^2 and higher can be dropped.

With a little algebra the following expression for the quasi-particle chemical potential is obtained in terms of Δ :

$$\xi = \frac{1}{2} \sqrt{\frac{\Delta}{\Delta_0}} (\Delta + \Delta_0) . \quad (31)$$

3.a.2. The Quasi-Particle Equation

Similarly the quasi-particle number equation can be written as:

$$Q = 4g \int_0^\infty \frac{d\varepsilon}{1 + \exp \beta(E - \xi)} . \quad (32)$$

In the limit of $\beta \rightarrow \infty$ one obtains the following analytic result:

$$Q = 4g \sqrt{\xi^2 - \Delta^2} \quad (33)$$

Equation (31) and Eq. (33) can be combined to give a relation between Q and Δ :

$$Q = 2g \sqrt{\frac{\Delta}{\Delta_0}} (\Delta_0 - \Delta) . \quad (34)$$

3.a.3. Discussion on the Phase Stability

Contrary to the regular dependences of Δ on both temperature and angular momentum (both related to the quasi-particle number), observed in previous studies¹⁶⁻¹⁸, the dependence of Δ upon Q is anomalous. Figure 1 shows that Δ is a triple valued function of Q (one trivial and two non-trivial solutions) in the interval $0 \leq Q \leq Q_{cr}$, where $Q_{cr} = \frac{4}{3\sqrt{3}} g\Delta_0$, and it is single-valued ($\Delta = 0$) for $Q > Q_{cr}$.

The larger solution starts at $\Delta = \Delta_0$ when $Q = 0$; it decreases as expected from this value down to $1/3 \Delta_0$ at $Q = Q_{cr}$. Similarly the smaller nontrivial solution starts at $\Delta = 0$ for $Q = 0$ and increases with increasing Q until it merges into the larger solution at $Q = Q_{cr}$.

This peculiar state of affairs must be resolved by deciding which of the three solutions is the stable one.

An immediate test on the two nontrivial solutions can be made by checking the sign of $\partial^2 H'' / \partial \Delta^2$. One may recall that the gap equation, expressed by $\partial H'' / \partial \Delta = 0$ represents the requirement that the Hamiltonian be stationary with respect to Δ . If $\partial^2 H'' / \partial \Delta^2$ is positive, then one has indeed a minimum, while a negative sign implies that the solution is a maximum.

The second derivative calculated at the equilibrium value of Δ , $\partial H'' / \partial \Delta = 0$ is given by the following expression¹⁶⁾:

$$\frac{\partial^2 H''}{\partial \Delta^2} = \Delta^2 \sum \frac{1 - 2n_k}{E_k^3} - \Delta^4 \frac{G}{2} \left[\sum \frac{1 - 2n_k}{E_k^3} \right]^2. \quad (35)$$

By substituting n_k with its thermal average and considering the uniform model one obtains:

$$\frac{\partial^2 H''}{\partial \Delta^2} = 2g\Delta^2 \int_0^S \frac{\tanh \frac{1}{2} \beta(E - \xi) d\xi}{E^3} - g G \Delta^4 \left[\int_0^S \frac{\tanh \frac{1}{2} \beta(E - \xi) d\xi}{E^3} \right]^2. \quad (36)$$

If one chooses S to be a very large number, the gap equation forces G to be very small for a given value of Δ_0 . Consequently, the second term of the above equation can be dropped.

By integrating the first term and considering the limits $\Delta_0/S \ll 1$ and $\beta \rightarrow \infty$ one obtains:

$$\frac{\partial^2 H''}{\partial \Delta^2} = 2g \left(1 - 2 \frac{\sqrt{\xi^2 - \Delta^2}}{\xi} \right). \quad (37)$$

By substituting ξ with its expression in terms of Δ [eq. (31)] one finally obtains:

$$\frac{\partial^2 H''}{\partial \Delta^2} = 2g \left(1 - 2 \frac{\Delta_0 - \Delta}{\Delta_0 + \Delta} \right) \quad (38)$$

This expression vanishes for $\Delta = \Delta_0/3$, which is the value of Δ to which the larger and the smaller solutions converge. For values of Δ larger than $\Delta_0/3$ the second derivative is positive, thus indicating a stable solution. For values of Δ smaller than $\Delta_0/3$, the second derivative is negative and the solution is unstable.

3.a.4. The Energy Equation

At this point one must decide on which of the two remaining solutions, the paired or the trivial one ($\Delta = 0$), is the stable solution. In order to determine such a point, one must inspect the energy equation.

In the limit of $\beta \rightarrow \infty$ and for the uniform model, the energy equation becomes

$$E = g \int_{-S}^{+S} \epsilon \, d\epsilon - 2g \left[\int_{\sqrt{\xi^2 - \Delta^2}}^S \frac{\epsilon^2}{E} \, d\epsilon - \int_0^{\sqrt{\xi^2 - \Delta^2}} \frac{\epsilon^2}{E} \, d\epsilon \right] - \frac{\Delta^2}{G}. \quad (39)$$

After one integration one obtains:

$$E = -gS^2 - \frac{1}{2} g\Delta^2 + 2g\xi \sqrt{\xi^2 - \Delta^2}. \quad (40)$$

The quantity of interest is the excitation energy. By subtracting the ground state energy:

$$E_0 = -gS^2 - \frac{1}{2} g\Delta_0^2 \quad (41)$$

and by substituting ξ with its own expression, one obtains:

$$\begin{aligned} E^* &= \frac{1}{2} g \left(\Delta_0^2 - \Delta^2 \right) \left(1 + \frac{\Delta}{\Delta_0} \right) && \text{for } \Delta > 0, \\ E^* &= \frac{1}{2} g\Delta_0^2 + \frac{Q^2}{8g} && \text{for } \Delta = 0. \end{aligned} \quad (42)$$

This last equation has been obtained by using the expression:

$$\xi = \frac{Q}{4g} \quad \text{for } \Delta = 0.$$

3.a.5. The Existence of a First-Order Phase Transition

In fig. 1 the excitation energy is plotted as a function of the quasi-particle number. As the gap parameter Δ goes from Δ_0 to 0, the energy follows a loop. The stable solution is the one with the least energy. Therefore the loop must be bypassed. At the bypass point the curves for the paired and the unpaired energies cross. Thus the bypass coordinates can be obtained by equating these two energies:

$$\begin{aligned} E_{\text{paired}} &= E_{\text{unpaired}} && \text{or} \\ \frac{1}{2} g \left(\Delta_0^2 - \Delta^2 \right) \left(1 + \frac{\Delta}{\Delta_0} \right) &= \frac{1}{2} g\Delta_0^2 + \frac{Q^2}{8g} \end{aligned} \quad (43)$$

This equation together with eq. (34) gives

$$\frac{\Delta_x}{\Delta_0} = \frac{1}{2}; \quad Q_x = g \frac{\Delta_0}{\sqrt{2}} \quad (44)$$

where Δ_x and Q_x are the values of Δ and Q at the crossing.

The excitation energy at the crossing is:

$$E_x = \frac{9}{8} \frac{1}{2} g \Delta_0^2 = \frac{9}{8} C, \quad (45)$$

where C is the pairing condensation energy.

In conclusion, for values of $Q < Q_x$ the paired solution is the stable one. At $Q = Q_x$, Δ goes abruptly from the value $\Delta_0/2$ to zero and it remains zero for any value of $Q > Q_x$.

This phase transition is much sharper than the one occurring at the critical angular momentum, where Δ goes continuously to zero but where the first derivative of Δ suffers a discontinuity.

3.a.6. On the Stability of the Aligned Configuration

A simple inspection of the equations indicates that for $T=0$ the quasi-particles occupy the single-particle levels pairwise with opposite spin projections. One may wonder whether a configuration with one quasi-particle per level, like that occurring in the yrast line (aligned configuration), is more stable than the configuration described above (normal configuration). The answer is not immediate, because while the aligned configuration has a higher single-particle energy, it also has a larger pairing which depresses the energy. The former point concerning the single-particle energy is obvious. The latter, concerning the pairing, can be seen in what follows.

The relation between Q and Δ in the aligned scheme can be easily obtained in analogy with the evaluation of the paired yrast line¹⁶⁻¹⁸):

$$Q_{\text{aligned}} = g \Delta_0 \left[1 - \left(\frac{\Delta}{\Delta_0} \right)^2 \right]. \quad (46)$$

The ratio between the number of quasi-particles necessary to give the same gap parameter in the two configurations is:

$$\frac{Q_{\text{aligned}}}{Q_{\text{normal}}} = \frac{1}{2} \left[\sqrt{\frac{\Delta_0}{\Delta}} + \sqrt{\frac{\Delta}{\Delta_0}} \right]. \quad (47)$$

This ratio is always slightly larger than one in the interval $1 > \Delta/\Delta_0 \geq 0.5$, thus indicating that more quasi-particles are needed by the aligned configuration in order to obtain a given value of Δ .

Similarly, one can obtain the energy associated with the aligned configuration:

$$E_{\text{aligned}} = \frac{1}{4} g \Delta_0^2 \left(1 - \frac{\Delta^2}{\Delta_0^2} \right) \left(3 + \frac{\Delta^2}{\Delta_0^2} \right). \quad (48)$$

The ratio of the energies for a fixed value of Δ is:

$$\frac{E_{\text{aligned}}}{E_{\text{normal}}} = \frac{1}{2} \frac{3\Delta_0^2 + \Delta^2}{\Delta_0(\Delta_0 + \Delta)}. \quad (49)$$

This ratio is also slightly larger than one for $1 > \Delta/\Delta_0 \geq 0.5$. The ratio of the energies at fixed Q is also larger than one in the same interval, thus proving that the aligned configuration never has the lowest energy at fixed Q . However, in the range $1 > \Delta/\Delta_0 \geq 0.5$, the two configurations are so close in energy that one might expect real nuclei to assume either one, depending upon the details of their single-particle structure.

3.b Properties of the System for $T > 0$

3.b.1. Solution of the Gap Equation

The dependence of the gap parameter Δ upon the quasi-particle number Q at various temperatures can be determined by solving simultaneously the gap equation (13) and the quasi-particle equation (11) numerically. Such a dependence is illustrated graphically in fig. 2. For temperatures smaller than the

critical temperature T_{cr} two paired solutions exist. For temperatures above the critical temperature, only one paired solution exists. The stability of the various solutions will be discussed in the next subsection. Aside from the bending over of the isotherms with $T > T_{cr}$, (not shown in the figure, but similar to that in fig. 1) it appears that the gap parameter at fixed number of quasi-particles actually increases with increasing temperatures. This is another example of what we have called before the thermally assisted pairing correlation¹⁷). An increase in temperature has the effect of pushing the quasi-particles farther and farther away from the particle Fermi surface. The blocking due to the quasi-particles becomes less effective and the pairing correlation is enhanced. It follows that, for a fixed quasi-particle number, the pairing correlation is not confined to temperatures smaller than the critical temperature, but it actually extends to indefinitely high temperatures.

3.b.2. Free Energy and Phase Stability

In the region of temperatures below T_{cr} , two paired solutions (plus the usual unpaired solutions) appear. In order to determine which of the solutions corresponds to a stable system, the Free Energy F must be investigated. The Free Energy can be obtained from the Grand Partition Function as follows:

$$F = -T\Omega + \xi Q \quad (50)$$

An example of the dependence of the Free Energy upon Q at a temperature $T < T_{cr}$ is given in fig. 3. As in the case of $T = 0$, a loop can be observed which must be bypassed by the stable solution. This produces a discontinuous jump from the paired configuration with larger Δ to the unpaired configuration. This isothermal transition is accompanied by an energy change $\Delta E = T\Delta S$, which indicates that indeed one is dealing with a true first-order phase transition.

A general view of Free Energy isotherms is available in fig. 4. All of these isotherms present a minimum which corresponds to the equilibrium value of Q if no restriction is set upon the system. Such a minimum satisfies the condition

$$\frac{\partial F}{\partial Q} = \xi = 0$$

In other words, when the number of quasi-particles is not restricted but is allowed to attain its equilibrium value, the quasi-particle chemical potential is identically zero. In the same figure the location of the phase transition is shown on each isotherm. Below the critical temperature, the phase transition (first order) occurs for values of Q larger than the equilibrium value; above the critical temperature, the phase transition (now second order) occurs for values of Q smaller than the equilibrium value.

3.b.3. The T, Q Phase Diagram and the Plots of Various Thermodynamical Functions

The above information can be used to generate a T, Q diagram. Such a diagram is shown in fig. 5. The boundary between the paired and the unpaired region defined by the vanishing of the gap parameter Δ is shown. Below the critical temperature such a boundary branches into two lines. The leftmost line corresponds to the continuous vanishing of Δ and it does not correspond to any stable system. The rightmost line corresponds to the discontinuous vanishing of Δ and has physical significance. The line characterized by $\xi = 0$, corresponding to the equilibrium number of quasi-particles is also shown. It starts at the origin of the diagram and stays into the paired region up to the critical temperature, when it exits into the unpaired region. It is along this line that previous pairing calculations have been made^{11-14,16-18}).

It is useful now to project various quantities on this basic diagram.

In fig. 6 lines of constant gap parameter Δ are projected in such a fashion. It is possible to appreciate two facts already pointed out before. Firstly, the gap parameter at fixed Q actually increases and tends to go to its ground state value as T tends to infinity. Secondly, even for those values of Q for which $\Delta = 0$ at $T = 0$, an increase in temperature eventually leads to the onset of pairing and to its increase towards the ground state value as an asymptotic limit. These effects are completely understood in terms of the thermally assisted pairing correlation¹⁶⁻¹⁸).

In fig. 7, the lines of constant energies are projected on the same basic graph. The temperature, for each line of constant energy, drops dramatically as the quasi-particle number increases. This is due to the larger number of degrees of freedom available to the system with increasing Q . At high temperatures one observes a nearly hyperbolic behavior typical of the Boltzmann limit. The change in the second derivative visible at low temperature in the unpaired region is due to the onset of the strong degeneracy limit (see also section 3.b.6.). Similar considerations hold for the entropy plot shown in fig. 8. In particular one can appreciate how difficult it is, at low Q values, to increase the entropy even with a very sizable increase in temperature.

3.b.4. E, Q Diagrams and the Plots of Various Thermodynamical Quantities

The relevance of constant energy processes in nuclei makes it desirable to use the energy itself as an independent variable. The transformation can be done by means of the energy versus quasi-particle number isotherm plot shown in fig. 9. In this graph a parabolic dependence is seen in the low temperature unpaired region. The first-order phase transition produces a discontinuity responsible for a gap in the E, Q plane. The origin of such a gap can be understood best by following

any given isotherm below the critical temperature. As the system, moving along a given isotherm, reaches the region of the phase transition from the left (paired region), it experiences a sudden drop in energy at constant Q as it enters the unpaired region.

The map shown in fig. 10 gives the lines of constant Δ in the E, Q plane. In such a map one can appreciate directly the evolution in pairing of a constant energy system as it moves from a very low initial quasi-particle number to its equilibrium value. In all the cases of physical interest, the system starts off with a very large pairing gap, close to its ground state value. As the number of quasi-particles increases, the pairing correlation experiences a rapid drop which, above the critical energy, actually ends up with its complete disappearance.

In fig. 11 the lines of constant entropy are plotted in the E, Q plane. This graph is perhaps the most significant insofar as it provides information on the driving force along the path towards equilibrium at constant energy.

The entropy is small at very small quasi-particle numbers; it increases with increasing quasi-particle numbers and reaches a maximum at the $\xi = 0$ line; a further increase in quasi-particle number leads to a decrease in entropy.

The maximum entropy at constant energy obviously represents the equilibrium condition.

3.b.5. The Level Density

In order to calculate the level density, one needs to evaluate the determinant in eq. (17).

The value of the determinant as a function of Q for various temperatures is shown in fig. 12. It can be seen that some isotherms become negative in a certain Q interval. This means that the saddle-point method for the evalua-

tion of the inverse Laplace transform of the Grand Partition Function leading to the calculation of the level density fails.

This failure is associated with the anomalous dependence of ξ versus Q . Whenever $\partial\xi/\partial Q < 0$ the determinant is negative. [See fig. 13.]

In fig. 14, the end result of the calculation can be seen. The constant level density lines for a system characterized by $g = 7 \text{ MeV}^{-1}$, $\Delta_0 = 1 \text{ MeV}$ can be seen in an E, Q plot. The pattern is very similar to that of the entropy plot in the E, Q plane and the same comments apply.

A larger gap in the plot is visible due to the failure of the saddle-point method close to the region of phase transition.

3.b.6. Miscellaneous Analytical Expressions for $\Delta = 0$

- The quasi-particle equation and the line of most probable quasi-particle number

The quasi-particle equation for $\Delta = 0$ can be written as follows:

$$\begin{aligned} Q &= 4g \int_0^\infty \frac{d\varepsilon}{1 + \exp \beta(\varepsilon - \xi)} \\ &= 4gT \ln(1 + e^{\xi/T}) \end{aligned} \quad (51)$$

By setting $\xi = 0$ in the above equation one obtains the line of most probable value of Q , $\hat{Q}$ as a function of T :

$$\hat{Q} = 4gT \ln 2 \quad \text{or} \quad \frac{\hat{Q}}{Q_{\text{cr}}} = \frac{T}{T_{\text{cr}}} \quad (52)$$

The energy equation evaluated along this line gives

$$E = \frac{1}{2} g \Delta_0^2 + \frac{\pi^2}{3} g T^2 \quad (53)$$

● Limit of large positive and large negative ratios for ξ/T

For $\xi/T \gg 0$ (extreme degeneracy) one has

$$Q = 4g\xi \quad (54)$$

In the same limit the energy equation yields

$$E = \frac{1}{2} g\Delta_0^2 + 2g\xi^2 + \frac{2}{3} \pi^2 gT^2 \quad (55)$$

or

$$E = \frac{1}{2} g\Delta_0^2 + \frac{Q^2}{8g} + \frac{2}{3} \pi^2 gT^2 \quad (56)$$

For $\xi/T \ll 0$ (Boltzmann limit) one obtains

$$Q = 4gTe^{\xi/T} \quad (57)$$

In the same limit one has

$$E = \frac{1}{2} g\Delta_0^2 + 4gT^2 e^{\xi/T} = \frac{1}{2} g\Delta_0^2 + QT \quad (58)$$

4. CONCLUSION

The present paper has tried to accomplish two points: a) the introduction of the residual interaction in the pairing approximation, and b) the complete description of all of the thermodynamical aspects of the problem. An immediate extension of this work to a realistic shell-model is in progress.

Unfortunately there are many shortcomings which cannot be easily overcome. One of the difficulties lies in the elimination of spurious states associated with the pairing Hamiltonian. This problem is, of course, not restricted to systems with constant quasi-particle number, but extends to all the statistical calculations with the pairing Hamiltonian [eq. (2)] and has not

received any attention as yet. A second problem is the lack of precision of the saddle-point approximation of very small values of Q . While one can do away with the saddle-point approximation in the pure shell-model limit, this is not so simple to achieve when the pairing Hamiltonian is introduced. And yet the simplicity introduced by the saddle-point method and the ability of the formalism to give a complete, though occasionally somewhat inaccurate view of the system properties, appeared to us to be of some significance.

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FIGURE CAPTIONS

Fig. 1. Dependence of the gap parameter Δ and of the energy E upon quasi-particle number Q at $T=0$. The dashed lines correspond to the unstable solutions.

Fig. 2. Dependence of the gap parameter upon quasi-particle number at various temperatures. The inner isotherm corresponds to $T/T_{cr} = 0.00$; the successive isotherms are spaced at intervals of $0.2 T/T_{cr}$. The onset of the first-order phase transition is indicated by an open circle, the unstable solution at the same temperature is indicated by a solid point.

Fig. 3. Example of an isothermal Free Energy loop.

Fig. 4. Dependence of the Free Energy upon quasi-particle number at various temperatures. The upper line corresponds to $T/T_{cr} = 0.00$. The following lines are spaced at intervals of $0.1 T/T_{cr}$. The open circles represent the region of the first-order phase transition. The bypassed loops are not shown.

Fig. 5. Phase diagram in the T, Q plane. The solid line corresponds to the phase transition (first-order for $T/T_{cr} < 1$, second-order for $T/T_{cr} > 1$) from the paired region (left-hand side) to the unpaired region (right-hand side). The dotted line corresponds to the paired unstable solution. The line with small and large dots corresponds to the most probable value of Q ($\xi = 0$).

Fig. 6. Lines of constant gap parameter in the T, Q plane. The solid line corresponds to $\Delta = 0$; the lines to the left correspond to increasing values of Δ in steps of $0.05 \Delta/\Delta_0$.

Fig. 7. Lines of constant energy in the T, Q plane. The leftmost line corresponds to $E/C = 0.5$. The lines to the right are spaced in steps of $0.5 E/C$. Notice the mismatch of the lines in the region of the first-order phase transition.

Fig. 8. Lines of constant entropy in the T, Q plane. The leftmost line corresponds to $S/S_{cr} = 0.2$. The lines to the right are spaced in steps of $S/S_{cr} = 0.2$. Notice the mismatch of the lines in the region of the first-order phase transition.

Fig. 9. Energy quasi-particle number isotherms. The lowest line for $T=0$ is the same as in fig. 1. The higher isotherms are spaced in steps of $0.2 T/T_{cr}$. The forbidden region, defined by the two dotted lines, originates at the phase transition for $T=0$ and terminates at $T=T_{cr}, Q=Q_{cr}$. The boundaries of this region converge into a single line for $T>T_{cr}$. The locus of most probable Q is shown by the small and large dot line.

Fig. 10. Lines of constant gap parameter Δ in the E, Q plane. The leftmost line corresponds to $\Delta/\Delta_0 = 0.05$ and the lines to the right are plotted in intervals of $0.05 \Delta/\Delta_0$.

Fig. 11. Lines of constant entropy in the E, Q plane. The thick solid line corresponds to $S/S_{crit} = 0$. The lines above it are plotted in intervals of $0.125 S/S_{crit}$.

Fig. 12. Values of the determinant in the level density denominator as a function of Q at constant temperatures. The lowest line corresponds to $T/T_{cr} = 0.2$. The lines above it are spaced in intervals of $0.2 T/T_{cr}$. The value of the determinant is expressed in units of the square of the condensation energy.

Fig. 13. Dependence of the Lagrange multiplier ξ upon quasi-particle number at various temperatures. The upper curve corresponds to $T/T_{cr} = 0.0$.

The lower curves are plotted in steps of $0.2 T/T_{cr}$.

Fig. 14. Lines of constant level densities in the E, Q plane. The calculation refers specifically to a nucleus with $g = 7.0 \text{ MeV}^{-1}$ and with $\Delta_0 = 1.0 \text{ MeV}$.

The lowest level density line has a value $\ln p = 2.0$. The higher lines are plotted in steps of $3.0 \ln p$.

XBL 742-2400

Fig. 1

XBL 7411-8555

Fig. 2

XBL 7411-8556

Fig. 3

XBL 7411-8557

Fig. 4

XBL 7411-8558

Fig. 5

XBL 7411-8559

Fig. 6

XBL 7411-8560

Fig. 7

XBL 7411-8561

Fig. 8

XBL 7411-8562

Fig. 9

XBL 7411-8563

Fig. 10

XBL 7411-8564

Fig. 11

XBL 7411-8566

Fig. 12

XBL 7411-8565

Fig. 13

F = LOG(LEVEL DENSITY)

FBOT, DF = 2.000, 3.000

XBL 7411-8567

Fig. 14

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