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STATISTICAL PROPERTIES OF A PAIRED NUCLEUS WITH FIXED QUASIPARTICLE NUMBER†

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The pairing Hamiltonian, diagonal in the quasiparticle space, has been used to determine the statistical and thermodynamical properties of a system with fixed number of quasiparticles. The formalism can describe the phase transition occurring at fixed energy as the system relaxes from the initial to the equilibrium quasiparticle number.

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In many cases a nuclear reaction is initiated by generating a very simple particle-hole configuration (doorway state) like the creation of one particle-one hole state in the photonuclear reactions or by the excitation of other simple particle hole states in particle induced reactions.

The initial doorway state usually relaxes by generating more and more complicated configurations involving an increasingly larger number of quasiparticles and leading eventually to the formation of the compound nucleus. The relaxation process terminates when the system reaches its most probable number of quasiparticles associated with the compound nucleus formation.

Such an entropization process is frequently described by means of the master equation and in general it requires the knowledge of the phase space associated with specified numbers of quasiparticles [1,2].

†Work performed under the auspices of the U. S. Atomic Energy Commission.

The calculations on systems with fixed quasiparticle number performed so far deal exclusively with the evaluation of the level densities and have been restricted to independent particle models ranging from the equidistant model to the shell model [1,2,3].

In the present note an attempt is made to introduce the residual interactions by means of the pairing Hamiltonian with the aim of obtaining the dependence of the pairing correlation upon energy and quasiparticle number.

The Hamiltonian used in this paper is the pairing Hamiltonian in its diagonal form in quasiparticle space:

$$H = \sum (\varepsilon_k - \lambda - E_k) + 2 \sum n_k E_k + \frac{\Delta^2}{G} \tag{1}$$

where ε_k are the doubly degenerate single particle energies, λ is the particle chemical potential, G is the pairing strength, $E_k = \sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}$ are the quasiparticle energies, n_k are the quasiparticle occupation numbers and Δ is the gap parameter which can be obtained from the gap equation:

$$\frac{2}{G} = \sum \frac{1 - 2n_k}{E_k} \tag{2}$$

The quasiparticle number $Q = 2 \sum n_k$ can be fixed in the calculation by introducing the following auxiliary Hamiltonian:

$$H' = H - \xi Q = \sum (\varepsilon_k - \lambda - E_k) + \Delta^2/G + 2 \sum n_k (E_k - \xi) \tag{3}$$

where ξ is a Lagrange multiplier which assumes the meaning of the quasiparticle chemical potential.

From the auxiliary Hamiltonian the Grand Partition Function e^{Ω} can be obtained:

$$\Omega = -\beta \sum (\varepsilon_k - \lambda - E_k) - \beta \frac{\Delta^2}{G} + 2 \sum \ln[1 + \exp - \beta(E_k - \xi)] \tag{4}$$

where $\beta = 1/T$ is the reciprocal of the temperature.

The gap equation takes the form:

$$\sum \frac{1}{E_k} \tanh \frac{1}{2} \beta (E_k - \xi) = \frac{2}{G} \tag{5}$$

The first integrals of motion can be obtained by differentiation of Ω:

$$N = \frac{1}{\beta} \frac{\partial \Omega}{\partial \lambda} = \sum [1 - \frac{\varepsilon_k - \lambda}{E_k} \tanh \frac{1}{2} \beta (E_k - \xi)] \qquad \text{particle equation} \tag{6}$$

$$Q = \frac{1}{\beta} \frac{\partial \Omega}{\partial \xi} = 2 \sum \frac{1}{1 + \exp \beta (E_k - \xi)} \qquad \text{quasiparticle equation} \tag{7}$$

$$E = - \frac{\partial \Omega}{\partial \beta} = \sum \varepsilon_k [1 - \frac{\varepsilon_k - \lambda}{E_k} \tanh \frac{1}{2} \beta (E_k - \xi)] - \frac{\Delta^2}{G} \qquad \text{energy equation.} \tag{8}$$

By fixing the value of G, N, Q and E, the above four equations can be solved for λ, ξ, β and Δ. These quantities can be used to calculate the entropy:

$$S = 2 \sum \ln [1 + \exp - \beta (E_k - \xi)] + 2\beta \sum \frac{E_k - \xi}{1 + \exp \beta (E_k - \xi)} \tag{9}$$

A great simplification in the calculation and in the interpretation of the results can be achieved by applying the formalism to the uniform model, characterized by the density of doubly degenerate single particle levels g and by the ground state gap parameter Δ_o.

Because of the uniformity of the spectrum, the particle chemical potential λ is a constant so that it can be set equal to zero and the particle equation can be disregarded. A particularly simple case which is amenable to a completely analytical treatment is the zero temperature limit ($\beta \to \infty$). In this limit the gap equation can be integrated analytically and gives the following relation between ξ and Δ:

$$\xi = \frac{1}{2} \sqrt{\frac{\Delta}{\Delta_o}} (\Delta_o + \Delta) \tag{10}$$

The integration of the quasiparticle equation yields the following expression:

$$Q = 4g \sqrt{\xi^2 - \Delta^2} \tag{11}$$

By combining the above two equations a relationship between Q and Δ is obtained:

$$Q = 2g\sqrt{\frac{\Delta}{\Delta_o}}(\Delta_o - \Delta) \tag{12}$$

As can be seen in fig. 1 the gap parameter initially decreases with increasing quasiparticle number. However, the $\Delta = \Delta(Q)$ function, after extending as far as $Q_{max} = \frac{4}{3\sqrt{3}} g\,\Delta_o$ at $\Delta_{max} = \frac{\Delta_o}{3}$, folds back and goes to zero at $Q = 0$. Therefore, the function $\Delta = \Delta(Q)$ is triple valued ($\Delta = 0$ is always a solution of the gap equation) in the range from $Q = 0$ to $Q = Q_{max}$.

In order to decide which of the three values is the physically stable solution one must study the dependence of the energy upon quasiparticle number. The energy equation can be integrated analytically and gives:

$$E = \begin{cases} \frac{1}{2} g(\Delta_o^2 - \Delta^2)(1 + \frac{\Delta}{\Delta_o}) & \text{for } \Delta > 0 \\ \frac{1}{2} g\,\Delta_o^2 + \frac{Q^2}{8g} & \text{for } \Delta = 0 \end{cases} \tag{13}$$

In fig. 1 such a function is shown. As Δ goes from Δ_o to 0 the E vs. Q function follows a loop which must be bypassed by the stable solution. The location of the bypass can be established by means of the condition: $E_{paired} = E_{unpaired}$, or:

$$\frac{1}{2} g(\Delta_o^2 - \Delta^2)(1 + \frac{\Delta}{\Delta_o}) = \frac{1}{2} g\,\Delta_o^2 + \frac{Q}{8g} \tag{14}$$

The values of Δ, Q, E at the bypass point are:

$$\frac{\Delta_x}{\Delta_o} = \frac{1}{2} \;;\quad Q_x = g\frac{\Delta_o}{\sqrt{2}} \;;\quad E_x = \frac{9}{8}\frac{1}{2} g\,\Delta_o^2 = \frac{9}{8} C \tag{15}$$

where C is the condensation energy.

At the bypass point, Δ/Δ_o goes abruptly from $\frac{1}{2}$ to 0. For temperatures larger than zero and smaller than the critical temperature of the unrestricted system, a similar picture appears, namely the function $\Delta = \Delta(Q)$ is triple valued over a certain range of Q. The stable solution can be obtained by considering the dependence of the Free Energy $F = -T\Omega + \xi Q$ upon Q.

This function (like the energy E at T = 0) presents a loop which must be bypassed by the stable solution. At the bypass Δ suffers a discontinuity,

dropping from a finite value to zero. At the same time Δ can reach zero continuously at a finite value of Q. The branch of the curve $\Delta = \Delta(Q)$ beyond the location of the discontinuity corresponds to an unstable solution. As the temperature increases the values of Q at which Δ vanishes continuously and discontinuously approach each other and eventually merge into each other. In fig. 2 the loci of the points where Δ vanishes continuously and discontinuously are shown in the T,Q plane.

Contrary to the $T = 0$ limit, for $T > 0$ the discontinuous vanishing of Δ characterized by $\Delta F = 0$ is associated with a jump in energy $\Delta E \neq 0$. So this transition is a first order phase transition.

The free energy can also be used to determine the most probable number of quasiparticles. The equilibrium condition is achieved when the free energy is at a minimum, which occurs for $\xi = 0$. In fig. 2 the $\xi = 0$ line, corresponding to the most probable quasiparticle number, is plotted in the T,Q plane.

In fig. 2 the lines of constant Δ are also presented. It can be seen that the pairing correlation extends well above the critical temperature of the unrestricted system, provided that the number of quasiparticles is smaller than its most probable value. Figure 2 also shows that by raising the temperature of the system at fixed quasiparticle number, the pairing correlation increases if the system is already paired, and if the system is not paired it will eventually become paired. This phenomenon, which we called elsewhere thermally assisted pairing correlation [4], is due to the fact that, as the temperature increases, the quasiparticle distance from the Fermi surface becomes larger and the blocking diminishes.

A most relevant diagram is the map of the entropy in the E,Q plane shown in fig. 3. This figure is important because the variation in entropy due to the

increase in Q <u>at constant energy</u> can be read out directly. Relaxation phenomena occur indeed at constant energy and stop when the entropy of the system is at a maximum. In the figure the position of the maximum in entropy is shown by a dotted line. The boundary of the paired phase is also shown, together with the forbidden region in the E,Q plane due to the first order phase transition.

In conclusion, the present description, limited to the uniform model should be able to provide at least a qualitative picture of the relevant statistical quantities of the problem. More sophisticated calculations are being performed on the basis of the shell model.

References

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Figure Captions

Fig. 1. Dependence of the gap parameter Δ and of the energy E upon quasiparticle number Q at T = 0. The unstable solutions are represented by means of thin, dashed lines. The gap parameter is expressed in units of the ground state gap parameter Δ_o, the quasiparticle number in units of the most probable quasiparticle number Q_{cr} at the critical temperature, the energy in units of the condensation energy $C = \frac{1}{2} g \Delta_o^2$.

Fig. 2. Lines of constant Δ (thin lines) in the T,Q plane. The lines are plotted at .1 Δ_o intervals. The thick solid line corresponds to the boundary between the paired and the unpaired region. The dotted line corresponds to $\xi = 0$ and gives the value of the most probable quasiparticle number. The dotted line with small and large dots represents the region where the unstable solution leads to $\Delta = 0$.

Fig. 3. Lines of constant entropy in the E,Q plane. The lines are plotted at intervals of 0.1 S_{cr} where S_{cr} is the entropy at the critical temperature. The thick solid line represents the region of maximum possible quasiparticle number at constant energy. The dotted line at the left corresponds to the most probable quasiparticle number ($\xi = 0$). The two dotted lines on the right define the discontinuity in energy associated with the first-order phase transition.

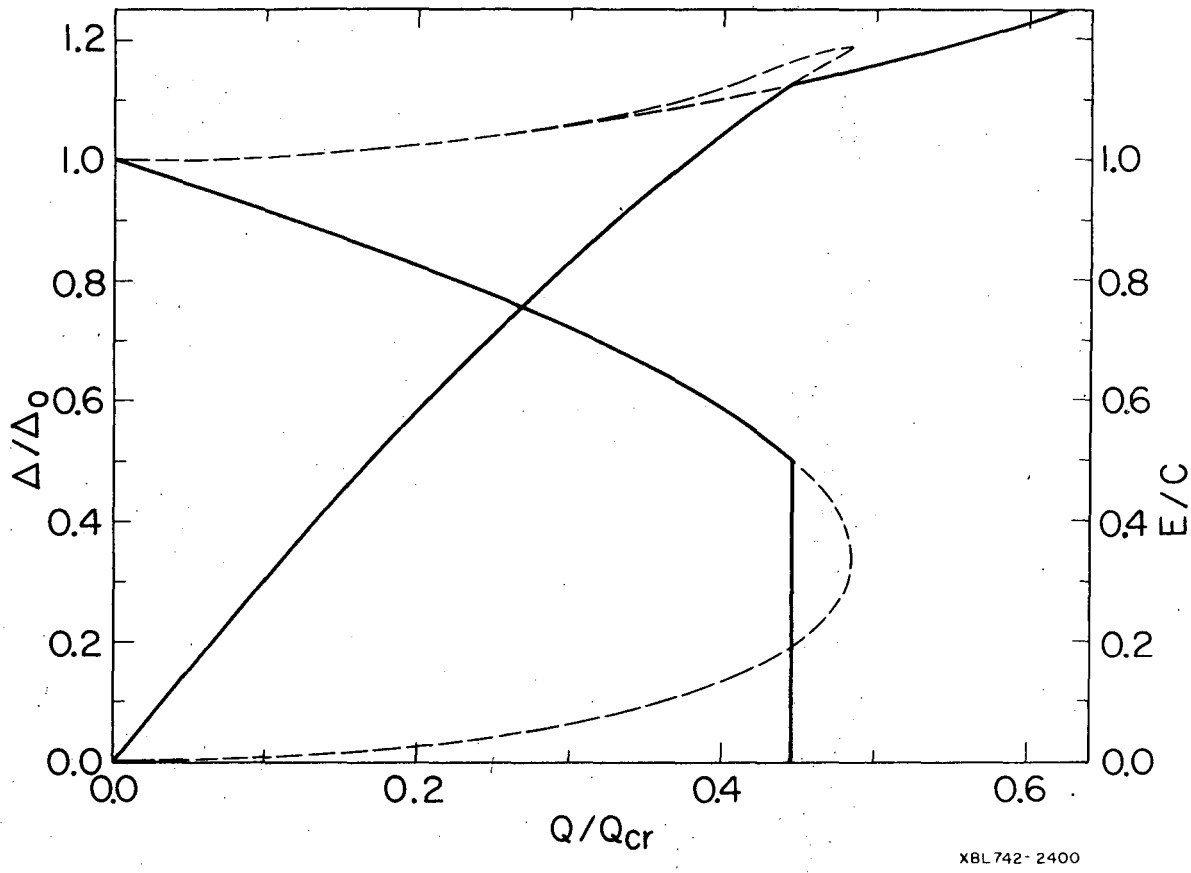

Fig. 1

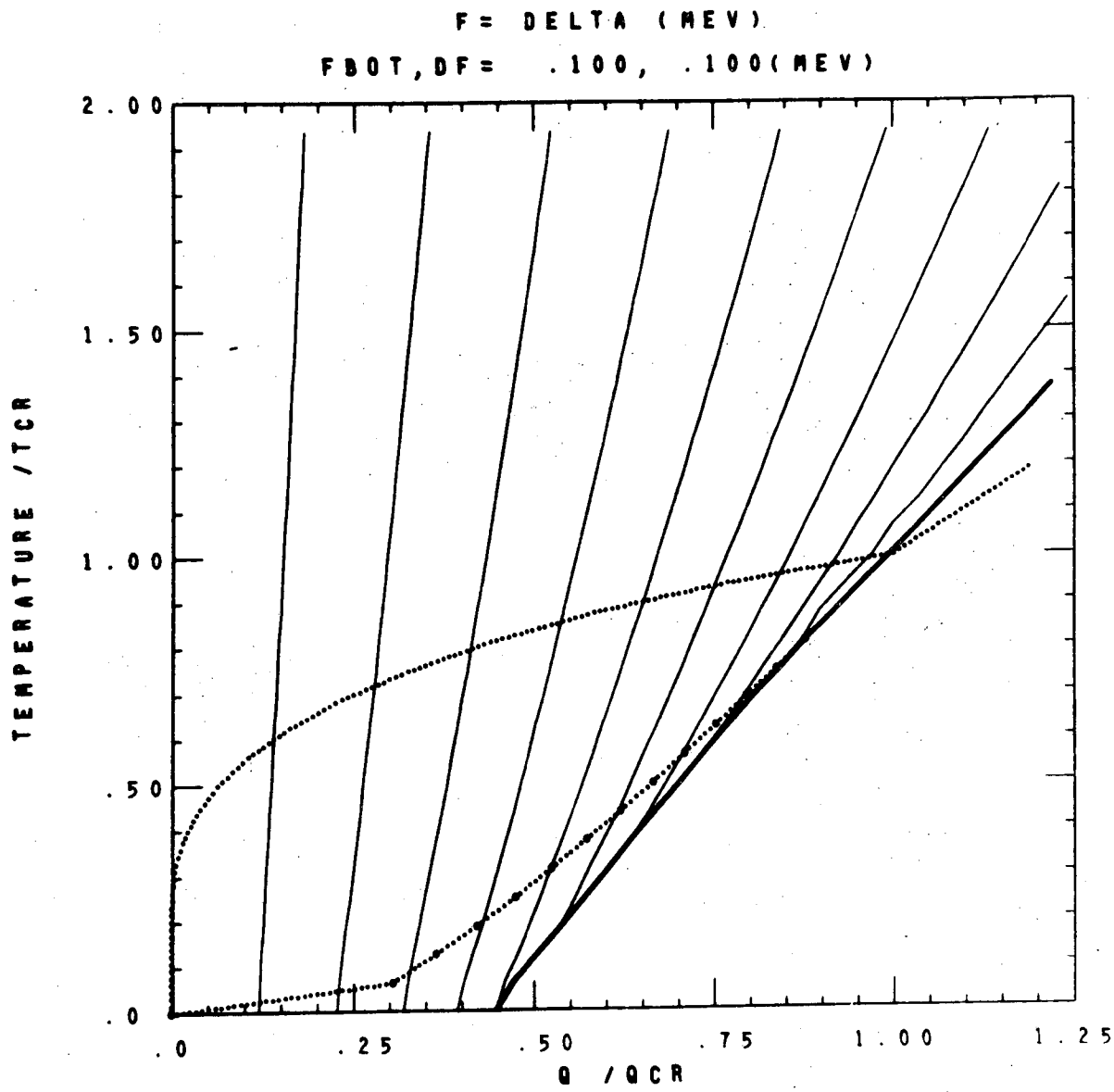

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Fig. 2

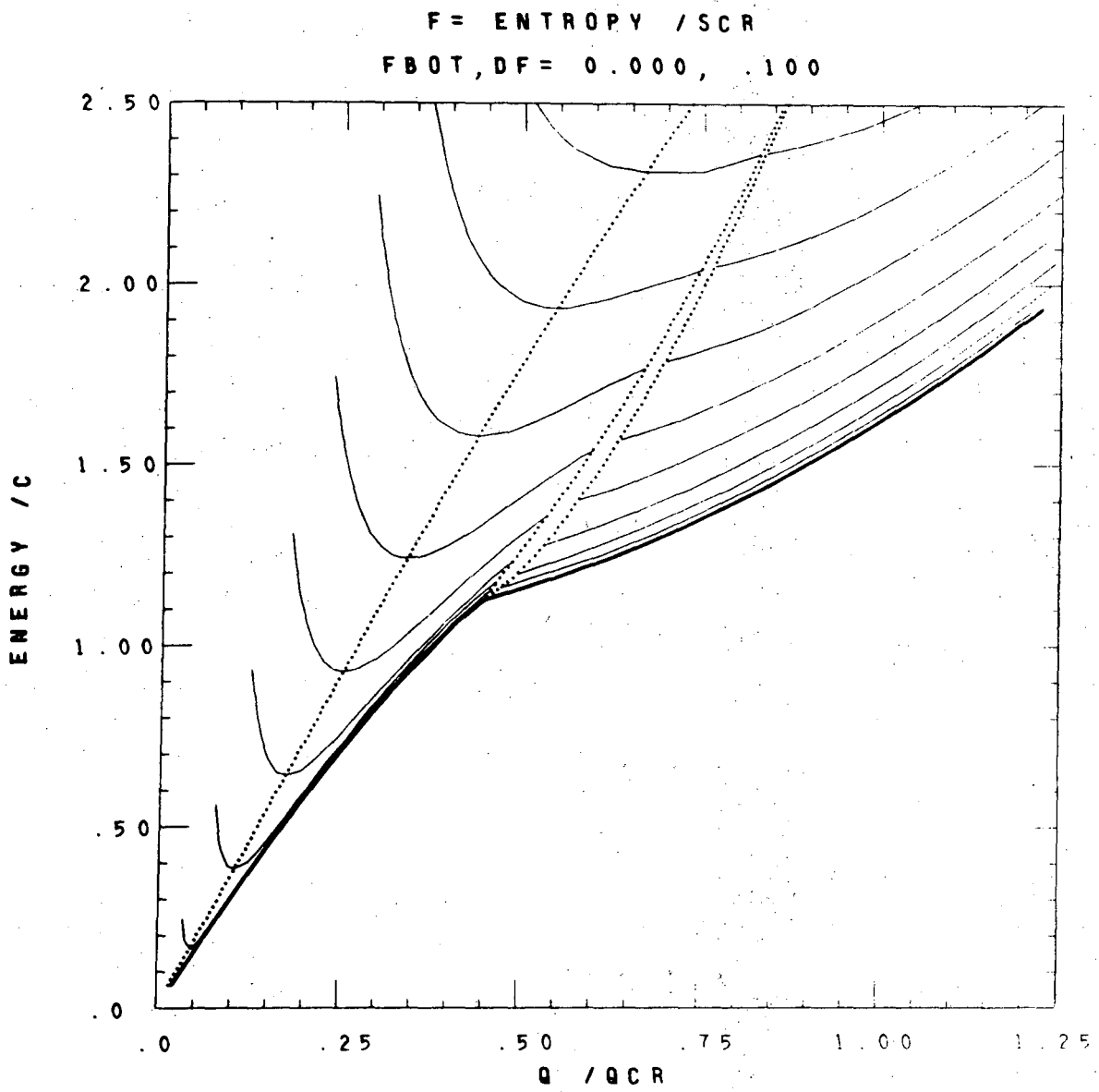

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Fig. 3

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