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STATISTICAL DESCRIPTION OF A PAIRED NUCLEUS WITH THE INCLUSION OF ANGULAR MOMENTUM*

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Abstract

The effect of angular momentum on an excited paired nucleus has been studied. The B.C.S. Hamiltonian, modified to include the z projection of the angular momentum has been diagonalized and expressed in terms of the quasi-particle occupation numbers. The grand partition function and all the relevant thermodynamical functions as well as the level density expression have been derived for the general case of an arbitrary set of single particle levels. Furthermore, the formalism has been applied to the uniform model and, whenever possible, analytical expressions have been derived. In particular the zero temperature angular momentum dependence of the gap parameter, the critical angular momentum as well as the yrast line have been calculated. The critical temperature as a function of angular momentum, which defines the phase-transition between paired and unpaired systems, has been calculated. A new effect called the thermally assisted pairing correlation, involving an increase of pairing with increasing temperature has been predicted. The completeness of the formalism as applied to spherical or deformed nuclei has been discussed.

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1. Introduction

Improvements in the results of the statistical treatment of excited nuclei are connected with the use of more and more realistic single particle models. The original work of Bethe[1]) on level densities was based upon the uniform model (set of equally-spaced single-particle levels populated by non interacting fermions). The success of this model, modified in many ways by a number of authors[2]) is due to its simple analytical results, despite the oversimplified and unrealistic Hamiltonian it is based upon. After the validity of the shell model was established and it became possible to calculate a realistic sequence of single particle levels, such model was seldom used for evaluating the statistical nuclear properties: rather, there has been the tendency to use a mocked-up shell model level sequence, such as a set of equally spaced levels of constant degeneracy[3]), or a bunched single particle level spectrum[4,5]). Again there was a tendency to obtain simple analytical results, which, on one hand would account for some of the most relevant experimental results, and on the other would be convenient for experimentalists to use. At present the availability of high speed computing machines allows one to solve the problem of the level density calculations on the basis of an arbitrary sequence of single particle levels[6,7]). Furthermore the superconductivity theory and the B.C.S. Hamiltonian[8,9]), the success of which is dealing with the pairing effects of ground state nuclei is well recognized[10]), have also been applied in the evaluation of level densities[11,12]). In this way the prediction of the low energy behavior of level densities has been much improved. In the present paper we generalize the formalism describing the statistical nuclear properties by including the nuclear angular momentum. A preliminary account of the results has already been published[13]). More specifically, we shall evaluate all the statistical nuclear properties on the basis of an arbitrary shell model level sequence, with inclusion of pairing effects and angular momentum by means of the BCS Hamiltonian. The usual procedure in statistical calculations consists in determining the grand partition function of the system and in restricting it in such a way as to conserve energy, number of particles and, in general, any other first integral of motion. However only the first integrals that can be expressed in terms of sums over single particle states can be handled easily in this fashion. While the total angular momentum does not have such property, its z projection M does. Therefore the following calculations will be restricted to a constant angular momentum z projection M. In sec. 4 it will be shown that, in most cases, such procedure is justified and the formalism is complete. In the first part of the paper the general formalism will be derived, while in the second part actual calculations will be presented for the case of the uniform model in order to illustrate the predictions of the present formalism.

2. General Theory

2.1. THE HAMILTONIAN

The Hamiltonian of a Fermi gas with an attractive interaction can be written as follows in the second quantization form:

$$H = \sum_{\pm k} \varepsilon_k \, a_k^\dagger a_k - G \sum_{kk'} a_{-k'}^\dagger a_{k'}^\dagger a_k a_{-k} \quad , \tag{1}$$

where ε_k are the unperturbed single particle energy levels, G is the strength of the pairing interaction and $a_k^\dagger$, a_k are the single-particle creation and annihilation operators.

It is convenient to consider a new Hamiltonian of the following form:

$$H \to H - \lambda N - \gamma M \quad , \tag{2}$$

where N is the number of particles, M is the projection of the total angular momentum on a laboratory-fixed z axis or on a body-fixed z'axis, and λ and γ are two Lagrange multipliers to be determined later on.

The quantities N and M can be expressed in operator form:

$$N = \sum_{\pm k} a_k^\dagger a_k \qquad M = \sum_{k} m_k \, a_k^\dagger a_k - \sum_{-k} m_k \, a_{-k}^\dagger a_{-k} \quad , \tag{3}$$

where m_k are the single particle spin projections.

The Hamiltonian, modified as in (2) can be rewritten as:

$$H = \sum_{k} \xi_k^+ \, a_k^\dagger a_k + \sum_{-k} \xi_{-k}^- \, a_{-k}^\dagger a_{-k} - G \sum_{kk'} a_{-k'}^\dagger a_{k'}^\dagger a_k a_{-k} \quad , \tag{4}$$

where

$$\xi_k^+ = \varepsilon_k - \lambda - \gamma\, m_k ; \qquad \xi_k^- = \varepsilon_k - \lambda + \gamma\, m_k \quad . \tag{5}$$

2.2. THE BOGOLIUBOV QUASI-PARTICLE TRANSFORMATION AND THE DIAGONALIZATION OF THE HAMILTONIAN

Such Hamiltonian can be diagonalized approximately by means of the Bogoliubov procedure[9,14]. Let us define a new set of operators as a linear combination of the previously defined operators:

$$b_{-k} = u_k\, a_{-k} + v_k\, a_{+k}^{\dagger}$$

$$b_{+k} = u_k\, a_{+k} - v_k\, a_{-k}^{\dagger} \quad . \tag{6}$$

The inverse transformation is:

$$a_{+k} = u_k\, b_{+k} + v_k\, b_{-k}^{\dagger}$$

$$a_{-k} = u_k\, b_{-k} - v_k\, b_{+k}^{\dagger} \quad . \tag{7}$$

The new operators (quasi-particle operators) do obey the commutation relation:

$$b_k\, b_k^{\dagger} + b_k^{\dagger}\, b_k = 1 \quad , \tag{8}$$

which implies:

$$u_k^2 + v_k^2 = 1 \quad . \tag{9}$$

By substituting eq. (7) in eq. (4) and retaining only the diagonal terms we obtain:

$$H = \sum v_k^2(\xi_k^+ + \xi_k^-) + \sum n_k^+(\xi_k^+ u_k^2 - \xi_k^- v_k^2) + \sum n_k^-(\xi_k^- u_k^2 - \xi_k^+ v_k^2)$$

$$- G[\sum_{kk'} u_k v_k (1 - n_k^+ - n_k^-)]^2 \quad , \tag{10}$$

where $n_k^{\pm} = b_{\pm k}^{\dagger} b_{\pm k}$ are the quasi particle occupation numbers.

By minimization of eq. (10) with respect to u_k keeping n_k^+ and n_k^- constant one obtains:

$$(\xi_k^+ + \xi_k^-) u_k v_k = \Delta(u_k^2 - v_k^2) \quad , \tag{11}$$

where

$$\Delta = G \sum u_k v_k (1 - n_k^+ - n_k^-) \quad . \tag{12}$$

The quantity Δ is called the "gap parameter" and it is a measure of the pairing correlation.

From eq. (11) and eq. (9) we have:

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\mathfrak{z}_k}{\sqrt{\Delta^2 + \mathfrak{z}_k^2}}\right) ; \quad v_k^2 = \frac{1}{2}\left(1 - \frac{\mathfrak{z}_k}{\sqrt{\Delta^2 + \mathfrak{z}_k^2}}\right) \quad , \tag{13}$$

where

$$\mathfrak{z}_k = \frac{\xi_k^+ + \xi_k^-}{2} = \varepsilon_k - \lambda \quad .$$

The substitution of eq. (13) in eq. (12) yields:

$$\sum \frac{1 - n_k^+ - n_k^-}{\sqrt{\Delta^2 + \xi_k^2}} = \frac{2}{G} \quad , \tag{14}$$

which is the so called "gap equation" in its most general form.

By means of eq. (13) and eq. (14) we can rewrite the Hamiltonian (10) in the following form:

$$H = \sum v_k^2(\xi_k^+ + \xi_k^-) + \sum n_k^+(\xi_k^+ u_k^2 - \xi_k^- v_k^2) + \sum n_k^-(\xi_k^- u_k^2 - \xi_k^+ v_k^2) - \frac{\Delta^2}{G} \quad ,$$

which, after some algebra takes the final form:

$$H = \sum(\varepsilon_k - \lambda - E_k) + \sum n_k^+(E_k - \gamma\, m_k) + \sum n_k^-(E_k + \gamma\, m_k) + \frac{\Delta^2}{G} \quad , \tag{15}$$

where

$$E_k = [(\varepsilon_k - \lambda)^2 + \Delta^2]^{1/2} \quad .$$

2.3. THE GRAND PARTITION FUNCTION

In order to obtain the thermodynamical description of the system we calculate now the grand partition function, defined as:

$$e^{\Omega} = \mathrm{Tr}\ e^{-\beta H} \quad . \tag{16}$$

This is indeed the grand partition function and not the partition function, because of the modifications introduced in the Hamiltonian in eq. (2).

By means of the Hamiltonian as expressed in eq. (15) the logarithm of the grand partition function is immediately obtained:

$$\Omega = -\beta \sum(\varepsilon_k - \lambda - E_k) + \sum \ln[1 + \exp - \beta(E_k - \gamma m_k)]$$

$$+ \sum \ln[1 + \exp - \beta(E_k + \gamma m_k)] - \beta \frac{\Delta^2}{G} \quad , \tag{17}$$

where $\beta = \frac{1}{T}$ is the inverse of the statistical temperature T. The quantities Δ, λ, γ, β are related to each other through the gap equation, which now takes the form:

$$\sum \frac{1}{2E_k} [\tanh \frac{1}{2} \beta(E_k - \gamma m_k) + \tanh \frac{1}{2} \beta(E_k + \gamma m_k)] = \frac{2}{G} \quad . \tag{18}$$

2.4. THE LEVEL DENSITY AND RELATED STATISTICAL QUANTITIES

The level density of the system is the inverse Laplace transform of the grand partition function:

$$\rho(E,N,M) = (\frac{1}{2\pi i})^3 \oint d\beta \oint d\alpha \oint d\mu \; e^S \quad , \tag{19}$$

where $\alpha = \beta\lambda$, $\mu = \beta\gamma$ and

$$S = \Omega - \alpha N - \mu M + \beta E \quad . \tag{20}$$

The Darwin Fowler triple integral of eq. (19) fixes the energy, the number of particles and the angular momentum projection in the grand partition function.

Such an integral can be evaluated with good approximation by means of the saddle point method. The exponent S has a saddle point at:

$$N = \frac{\partial\Omega}{\partial\alpha} \; ; \quad M = \frac{\partial\Omega}{\partial\mu} \; ; \quad E = -\frac{\partial\Omega}{\partial\beta} \quad . \tag{21}$$

The level density is:

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

where

$$D = \begin{vmatrix} \frac{\partial^2\Omega}{\partial\alpha^2} & \frac{\partial^2\Omega}{\partial\alpha\partial\mu} & \frac{\partial^2\Omega}{\partial\alpha\partial\beta} \\ \frac{\partial^2\Omega}{\partial\mu\partial\alpha} & \frac{\partial^2\Omega}{\partial\mu^2} & \frac{\partial^2\Omega}{\partial\mu\partial\beta} \\ \frac{\partial^2\Omega}{\partial\beta\partial\alpha} & \frac{\partial^2\Omega}{\partial\beta\partial\mu} & \frac{\partial^2\Omega}{\partial\beta^2} \end{vmatrix} \quad . \tag{22}$$

Both S and D must be evaluated at the saddle point. It can be noticed that eqs. (21) which give the saddle-point conditions also define the first integrals of the system. They can be calculated explicitly:

$$N = \sum [1 - \frac{\varepsilon_k - \lambda}{2E_k} \{\tanh \tfrac{1}{2}\beta(E_k - \gamma\, m_k) + \tanh \tfrac{1}{2}\beta(E_k + \gamma\, m_k)\}] \quad , \tag{23}$$

$$M = \sum m_k [\frac{1}{1 + \exp \beta(E_k - \gamma\, m_k)} - \frac{1}{1 + \exp \beta(E_k + \gamma\, m_k)}] \quad , \tag{24}$$

$$E = \sum \varepsilon_k [1 - \frac{\varepsilon_k - \lambda}{2E_k} \{\tanh \frac{1}{2} \beta(E_k - \gamma m_k) + \tanh \frac{1}{2} \beta(E_k + \gamma m_k)\}] - \frac{\Delta^2}{G} \quad . \qquad (25)$$

The system of eqs. (18), (23), (24), and (25) defines the saddle point values of Δ, λ, γ, and β. At first sight, it may seem strange that in eqs. (23), (24), and (25) there are no terms containing the partial derivatives of Δ with respect to β, λ and γ. As a matter of fact, considering for instance the derivation of eq. (23), the full result is:

$$N = \sum [1 - \frac{\varepsilon_k - \lambda}{2E_k} \{\tanh \frac{1}{2} \beta(E_k - \gamma m_k) + \tanh \frac{1}{2} \beta(E_k + \gamma m_k)\}]$$

$$+ \Delta \frac{\partial \Delta}{\partial \lambda} [- \frac{2}{G} + \sum \frac{1}{2E_k} \{\tanh \frac{1}{2} \beta(E_k - \gamma m_k) + \tanh \frac{1}{2} \beta(E_k + \gamma m_k)\}] \quad ; \qquad (26)$$

however, by virtue of eq. (18) the coefficient of $\Delta \frac{\partial \Delta}{\partial \lambda}$ is equal to zero. A similar situation arises for the other first integrals (24) and (25) which indeed turn out to be independent of the partial derivatives of Δ.

By means of eq. (20) where we substitute eqs. (23), (24), and (25), after some simplifications we can obtain the expression for the entropy:

$$S = \sum \ln[1 + \exp -\beta(E_k - \gamma m_k)] + \sum \ln[1 + \exp -\beta(E_k + \gamma m_k)]$$

$$+ \beta \sum \frac{E_k - \gamma m_k}{1 + \exp \beta(E_k - \gamma m_k)} + \beta \sum \frac{E_k + \gamma m_k}{1 + \exp \beta(E_k + \gamma m_k)} \quad . \qquad (27)$$

In order to complete the formalism, we need the second derivatives of Ω which enter in the denominator of the level density expression:

$$\frac{\partial^2\Omega}{\partial\mu^2} = \frac{1}{4} \sum m_k^2[\text{sech}^2 \tfrac{1}{2} \beta(E_k - \gamma m_k) + \text{sech}^2 \tfrac{1}{2} \beta(E_k + \gamma m_k)]$$

$$- \beta\Delta \frac{\partial\Delta}{\partial\mu} \sum \frac{m_k}{4E_k} [\text{sech}^2 \tfrac{1}{2} \beta(E_k - \gamma m_k) - \text{sech}^2 \tfrac{1}{2} \beta(E_k + \gamma m_k)] \quad (28)$$

$$\frac{\partial^2\Omega}{\partial\alpha^2} = \sum (\varepsilon_k - \lambda)^2 a_k + \Delta^2 \sum b_k - \beta\Delta \frac{\partial\Delta}{\partial\alpha} \sum (\varepsilon_k - \lambda)(a_k - b_k) \quad (29)$$

$$\frac{\partial^2\Omega}{\partial\beta^2} = \lambda \Delta^2 \sum \varepsilon_k b_k + \Delta^2 \sum \varepsilon_k(\varepsilon_k - \lambda) a_k + \sum \varepsilon_k^2(\varepsilon_k - \lambda)^2 a_k$$

$$+ \beta\Delta \frac{\partial\Delta}{\partial\beta} [\sum \varepsilon_k(\varepsilon_k - \lambda)(a_k - b_k) + \frac{2}{\beta G}] \quad (30)$$

$$\frac{\partial^2\Omega}{\partial\mu\partial\alpha} = \frac{1}{4} \sum \frac{(\varepsilon_k - \lambda)}{E_k} m_k[\text{sech}^2 \tfrac{1}{2} \beta(E_k - \gamma m_k) - \text{sech}^2 \tfrac{1}{2} \beta(E_k + \gamma m_k)]$$

$$+ \beta\Delta \frac{\partial\Delta}{\partial\alpha} \frac{1}{4} \sum \frac{m_k}{E_k} [\text{sech}^2 \tfrac{1}{2} \beta(E_k + \gamma m_k) - \text{sech}^2 \tfrac{1}{2} \beta(E_k - \gamma m_k)] \quad (31)$$

$$\frac{\partial^2\Omega}{\partial\mu\partial\beta} = \frac{1}{4} \sum \frac{m_k}{E_k} \{(\varepsilon_k - \lambda) \varepsilon_k + \Delta^2\}[\text{sech}^2 \tfrac{1}{2} \beta(E_k + \gamma m_k) - \text{sech}^2 \tfrac{1}{2} \beta(E_k - \gamma m_k)]$$

$$+ \beta\Delta \frac{\partial\Delta}{\partial\beta} \sum \frac{m_k}{4E_k} [\text{sech}^2 \tfrac{1}{2} \beta(E_k + \gamma m_k) - \text{sech}^2 \tfrac{1}{2} \beta(E_k - \gamma m_k)] \quad (32)$$

$$\frac{\partial^2\Omega}{\partial\alpha\partial\beta} = - \lambda\Delta^2 \sum b_k - \sum \varepsilon_k(\varepsilon_k - \lambda)^2 a_k - \Delta^2 \sum (\varepsilon_k - \lambda) a_k$$

$$- \beta\Delta \frac{\partial\Delta}{\partial\beta} \sum (\varepsilon_k - \lambda)(a_k - b_k) \quad . \quad (33)$$

In all of these expressions we have used the quantities:

$$a_k = \frac{1}{4}\frac{1}{E_k^2}\,[\mathrm{sech}^2\,\frac{1}{2}\,\beta(E_k - \gamma\, m_k) + \mathrm{sech}^2\,\frac{1}{2}\,\beta(E_k + \gamma\, m_k)] \quad , \tag{34}$$

$$b_k = \frac{1}{2\beta E_k^3}\,[\tanh\frac{1}{2}\,\beta(E_k - \gamma\, m_k) + \tanh\frac{1}{2}\,\beta(E_k + \gamma\, m_k)] \quad . \tag{35}$$

2.5. THE DERIVATIVES OF Δ WITH RESPECT TO THE LAGRANGE MULTIPLIERS

In eq. (28) through eq. (33) the derivatives of Δ with respect to β, α, μ are contained, in contrast with the expressions for the first integrals. We proceed now to the calculation of such derivatives.

The gap equation (18) defines Δ as an implicit function of β, α, μ. Formally we can write:

$$f(\Delta,\beta,\alpha,\mu) = 0 \quad .$$

The total differential is:

$$df = (\frac{\partial f}{\partial\beta} + \frac{\partial f}{\partial\Delta}\;\frac{\partial\Delta}{\partial\beta})\,d\beta + (\frac{\partial f}{\partial\alpha} + \frac{\partial f}{\partial\Delta}\;\frac{\partial\Delta}{\partial\alpha})\,d\alpha + (\frac{\partial f}{\partial\mu} + \frac{\partial f}{\partial\Delta}\;\frac{\partial\Delta}{\partial\mu})\,d\mu = 0 \quad .$$

The above relation is satisfied if and only if the quantities in parentheses are simultaneously equal to zero. Thus we obtain:

$$\frac{\partial\Delta}{\partial\beta} = -\frac{\frac{\partial f}{\partial\beta}}{\frac{\partial f}{\partial\Delta}}\;;\quad \frac{\partial\Delta}{\partial\alpha} = -\frac{\frac{\partial f}{\partial\alpha}}{\frac{\partial f}{\partial\Delta}}\;;\quad \frac{\partial\Delta}{\partial\mu} = -\frac{\frac{\partial f}{\partial\mu}}{\frac{\partial f}{\partial\Delta}} \quad . \tag{36}$$

Explicitly we have:

$$\frac{\partial\Delta}{\partial\beta} = - \frac{\Delta^2 \sum a_k + \sum a_k \varepsilon_k(\varepsilon_k - \lambda) - \lambda \sum b_k(\varepsilon_k - \lambda)}{\beta\Delta \sum (a_k - b_k)} \qquad (37)$$

$$\frac{\partial\Delta}{\partial\mu} = - \frac{\frac{1}{4} \sum \frac{1}{E_k} m_k[\text{sech}^2 \frac{1}{2} \beta(E_k + \gamma m_k) - \text{sech}^2 \frac{1}{2} \beta(E_k - \gamma m_k)]}{\beta\Delta \sum (a_k - b_k)} \qquad (38)$$

$$\frac{\partial\Delta}{\partial\alpha} = - \frac{\sum (\varepsilon_k - \lambda)(b_k - a_k)}{\beta\Delta \sum (a_k - b_k)} \quad . \qquad (39)$$

Such derivatives should be set equal to zero whenever $\Delta = 0$. In this way we have a general formalism which allows one to determine the statistical properties of a paired nucleus as a function of its excitation energy E and its angular momentum projection M.

2.6. GENERALIZATION TO THE CASE OF TWO KINDS OF PARTICLES

So far we have treated the system as being composed of a single kind of particles: actually a nucleus is composed of neutrons and protons. The whole theory is immediately generalized: it is sufficient to introduce a new Lagrange multiplier for the new kind of particles. The thermodynamical quantities can be obtained by recalling that the logarithm of the grand partition function, the energy and the entropy are additive quantities:

$$\Omega = \Omega_1 + \Omega_2 \; ; \qquad E = E_1 + E_2 \; ; \qquad S = S_1 + S_2 \quad . \qquad (40)$$

Furthermore it should be noticed that the level density expression must be written as:

$$\rho = \frac{\exp S}{(2\pi)^2 D^{1/2}} \quad . \tag{41}$$

The quantity D is now a determinant of the second derivatives of Ω with respect to the four Lagrange multipliers: it is therefore a 4×4 determinant instead of the 3×3 determinant of eq. (22).

By putting $\gamma = 0$ everywhere, the formalism reduces to the case of $M = 0$: such case has been treated already by Sano and Yamasaki[11]) and Decowski et al.[12]). It is worthwhile to point out that in the case of Sano and Yamasaki the saddle point was searched only with respect to β, which implies a difference in the denominator of the level density expression; in the case of Decowski et al. there is a discrepancy in the derivatives of Δ with respect to β and α.

Finally we observe that the present formalism can be used to calculate the level densities starting from any set of neutron and proton single particle levels obtained from shell model calculations. Although such computations turn out to be rather complex, they can be handled adequately by means of the high speed computers available at present. However, in order to gain a better insight in the theory, let us consider its application to the uniform model which allows one to simplify the calculations and, to a certain extent, to obtain rather simple analytical expressions for the relevant thermodynamical quantities.

3. Applications of the Theory to the Uniform Model

3.1. THE SINGLE PARTICLE MODEL

We assume a set of equally-spaced doubly-degenerate single-particle levels (Nilsson-like levels) with density g and with constant angular momentum projection $m_k = m$. For symmetry reasons the energy scale can be displaced in such a way as to make the chemical potential λ equal to zero at all temperatures (in the general case, the chemical potential λ varies with the temperature). In some of the calculations which will be presented, mostly in the case where we are dealing with energy as a variable, the uniform model has been employed with the following parameters: $g = 7\ \text{MeV}^{-1}$ $\Delta_o = 1.0$ MeV; $m = 2\hbar$. Such values have been chosen with the purpose of simulating a nucleus in the region of heavy rare earths.

3.2. DEPENDENCE OF THE GAP PARAMETER Δ UPON M AT ZERO TEMPERATURE ($\beta = \infty$)

From here on we assume that the pairing correlation extends over an energy interval $\pm\omega$ above and below the Fermi surface. Therefore all the summations over the single particle levels can be transformed into integrals within the limits $\pm\omega$.

For T = 0 and M = 0 the gap equation (18) yields the zero-temperature zero-angular momentum gap parameter:

$$\Delta_o = \frac{\omega}{\sinh 1/gG} \simeq 2\omega \exp(-1/gG) \quad . \tag{42}$$

The approximation holds when $gG \ll 1$. In order to obtain the dependence of Δ upon M for T = 0 let us first integrate eq. (24):

$$M = 2mg \left[\int_0^\infty \frac{d\varepsilon}{1 + \exp \beta(E - \gamma m)} - \int_0^\infty \frac{d\varepsilon}{1 + \exp \beta(E + \gamma m)} \right] . \quad (43)$$

For $\beta \to \infty$ the integrand in the second integral is zero in the whole range of integration, while in the first integral the integrand is equal to unity up to $E = \gamma m$ or $\varepsilon = [(\gamma m)^2 - \Delta^2]^{1/2}$ and is equal to zero for larger values of ε. We obtain then:

$$M = 2mg\ [(\gamma m)^2 - \Delta^2]^{1/2} . \quad (44)$$

Also for $\beta \to \infty$ the gap equation (18) for M = 0 and M = M can be written as:

$$f(\Delta_o) = \frac{2}{G} ; \quad f(\Delta,\gamma) = \frac{2}{G} , \quad (45)$$

or

$$f(\Delta_o) = f(\Delta,\gamma) . \quad (46)$$

After integration we obtain:

$$\frac{1}{2} [2 \operatorname{arcsinh} \frac{\omega}{\Delta} - 2 \operatorname{arcsinh} (\frac{(\gamma m)^2 - \Delta^2}{\Delta^2})] = \operatorname{arcsinh} \frac{\omega}{\Delta_o} . \quad (47)$$

After some manipulations we can write:

$$\frac{\omega}{\Delta_o} [(\Delta_o^2 + \omega^2)^{1/2} - (\Delta^2 + \omega^2)^{1/2}] = [(\gamma m)^2 - \Delta^2]^{1/2} . \quad (48)$$

If $\omega >> \Delta_o$, as we can always choose, we obtain with a good approximation:

$$\frac{\omega^2}{\Delta_o}\left[1 + \frac{1}{2}\frac{\Delta_o^2}{\omega^2} - 1 - \frac{1}{2}\frac{\Delta^2}{\omega^2}\right] = \left[(\gamma m)^2 - \Delta^2\right]^{1/2} , \quad (49)$$

or

$$\frac{1}{2}\frac{\Delta_o^2 - \Delta^2}{\Delta_o} = [(\gamma m)^2 - \Delta^2]^{1/2} = \frac{M}{2mg} . \quad (50)$$

We finally end-up with the very simple expression:

$$\Delta = \Delta_o \left(1 - \frac{M}{M_c}\right)^{1/2} , \quad (51)$$

where

$$M_c = gm\,\Delta_o \quad ; \quad (52)$$

the following expressions are immediately derived:

$$\left(\frac{d\Delta}{dM}\right)_{M=0} = \frac{-1}{2gm} \; ; \quad \lim_{M \to M_c} \frac{d\Delta}{dM} = -\infty . \quad (53)$$

The dependence of Δ upon M, expressed by eq. (51) is shown in fig. 1. It is seen that the gap parameter, and thus the pairing correlation, decreases with M, until, at a critical value M_c, given by eq. (52) the pairing correlation vanishes.

Equations (53) express the slopes of $\Delta = \Delta(M)$ for $M = 0$ and $M = M_c$. The qualitative meaning of such results can be easily understood by considering the Hamiltonian as in eq. (1). The second term of such a Hamiltonian says that, whenever a pair of particles can be transferred from a filled level to an empty one, there is an energy gain G. The first term, of course, means that, in order to transfer a pair of particles from a level k to a level k' one has to invest an amount of energy equal to $2(\varepsilon_{k'} - \varepsilon_k)$. This means that only the levels close to the Fermi surface are the most affected by the pairing interaction. In order to generate angular momentum, we must break some of the pairs: the excitations which arise in this way (quasi particles) occupy single particle levels which become unavailable (blocked) to the scattered pairs. Thus the pairing correlation decreases and, when the angular momentum is sufficiently large, the crowding of quasi-particles around the Fermi levels makes the pairing correlation energetically unfavored (fig. 2).

3.3. DEPENDENCE OF THE GAP PARAMETER UPON ANGULAR MOMENTUM AND EXCITATION ENERGY

Let us consider first the case of $M = 0$. Again the gap equation (18) gives the dependence of Δ upon T. In fig. 3 such dependence is presented: the increase in temperature produces a decrease in the pairing correlation until, at and above a critical temperature T_c, $\Delta = 0$ and the pairing correlation disappears altogether. The critical temperature is given by the relation[11]:

$$T_c = 1.14\ \omega \exp(-1/gG) \quad . \tag{54}$$

By application of the eq. (41) we obtain the well known relation[11]:

$$\frac{2\ \Delta_o}{T_c} = 3.50 \quad . \tag{55}$$

Again the decrease of the pairing correlation with increasing temperature is due to the fact that the excitation energy breaks pairs of particles which generate quasi particles blocking single-particle levels close to the Fermi surface. In fig. 4 the dependence of Δ upon the excitation energy is presented.

Since we have seen that both energy and angular momentum tend to decrease the pairing correlation, it is interesting to see their combined effect. This can be done by determining the dependence of the critical temperature upon the angular momentum projection M. Such a function which defines the boundaries between the superconducting and the normal phase in the M - T plane is shown in fig. 5. For $0 \leqslant M < M_c$ the gap equation (18) yields a single solution for the critical temperature, which decreases with M as expected. However, for $M \geqslant M_c$, the gap equation yields two critical temperatures; the upper critical temperature is the continuation of the curve obtained for $M < M_c$, while the lower critical temperature starts from zero at $M = M_c$ and merges into the upper critical temperature for $M \simeq 1.22\ M_c$. It is very important to note that for $M > M_c$ the system is normal in the temperature range between zero and the lower critical temperature, it is a superconductor in the temperature range between the lower and the upper critical temperatures, and it is normal again for temperature values above the upper critical temperature. We are dealing here with an unexpected effect, namely for $M > M_c$ a system in the normal phase can become a superconductor by increasing its temperature or excitation energy. This in contrast with the known case for M = 0 (fig. 3 and fig. 4) where an increase in temperature tends to destroy the pairing correlation. Such an effect could be called "anomalous pairing" or "thermally assisted pairing correlation" because it is sustained by an increase in temperature.

Let us attempt to gain a qualitative insight into such phenomenon. As stated above, angular momentum is generated by breaking pairs of particles, by putting the quasi particles generated in this way into the single particle levels close to the Fermi surface, and by polarizing their spins. If the angular momentum is sufficiently high and the temperature is equal to zero, a large number of quasi particles do completely occupy the closest levels above and below the Fermi surface. Such a complete blocking of single particle levels makes the pairing correlation energetically unfavorable (fig. 6a). An increase in temperature tends to relax the tight packing of quasi-particles by spreading them farther and farther away from the Fermi surface: in this way some single particle levels become partially unoccupied and thus become available for pairs scattered by the pairing interaction (fig. 6b). At a temperature equal to the lower critical temperature, such a spreading out of quasi particles is just sufficient to make the pairing correlation energetically favored. A further increase of the temperature will eventually produce the normal pairing breakdown by generating an increasingly large number of quasi-particles.

Such a remarkable effect persists also for values of M smaller than M_c. This can be shown clearly by calculating the dependence of the gap parameter Δ upon the temperature and the angular momentum projection. In order to do that, we must solve the system formed by eq. (18) and eq. (24). In fig. 7 the T - M plane is again divided into two regions, one where the system is paired, the other where the system is normal. In the paired regions lines have been drawn which correspond to a constant Δ value, from Δ = 0.95 MeV to Δ = 0.1 MeV in 0.05 MeV steps. It appears that for a constant M value, below M_c, Δ begins to increase with increasing temperature, reaches a maximum, finally decreases, and vanishes at the critical temperature. For $M > M_c$ the gap parameter Δ stays equal to zero from T = 0 up to the lower critical temperature, in the paired region Δ

increases, goes through a maximum, decreases again and vanishes at the upper critical temperature. It can be noticed that Δ goes through a maximum with increasing temperature for any non-zero value of M. Since this initial increase in Δ with increasing temperature can also be called "thermally assisted pairing correlation", it follows that such effect can hardly be called anomalous: actually the effect for M = 0 could be called anomalous because only in such a case Δ decreases monotonously with increasing temperature.

3.4. PASSAGE FROM THE TEMPERATURE SCALE TO THE ENERGY SCALE

Although the concept of temperature in a nucleus may be useful, it is more common to speak of nuclei in terms of energy: indeed, for the great majority of purposes, excited nuclei are considered with a fixed excitation energy rather than with fixed temperature.

Such fact should also lead to the use of the microcanonical ensemble instead of the canonical ensemble in statistical calculations. The canonical ensemble has been used here because of the more advanced algorithms which have been developed: therefore the calculations presented so far should be understood to hold for fixed temperature. Nonetheless it is possible to calculate the average energy associated with such a temperature. The main effect of such approximation is that of introducing some smoothing of the statistical quantities with respect to energy. First, let us calculate the energy of the system for T = 0 as a function of M. Such function is usually called yrast line and it is usually defined in a somewhat different fashion (like the function giving the highest angular momentum for a given energy of alternatively giving the lowest possible energy for a given angular momentum). For the uniform model, eq. (25) becomes:

$$E = g \int_{-\omega}^{+\omega} \varepsilon\left(1 - \frac{\varepsilon}{2E}\left\{\tanh \frac{1}{2}\beta(E - \gamma m) + \tanh \frac{1}{2}\beta(E + \gamma m)\right\}\right) d\varepsilon - \frac{\Delta^2}{G} \quad . \qquad (56)$$

For $T = 0$ or $\beta \to \infty$ such expression reduces to the following:

$$E = g \int_{-\omega}^{+\omega} \varepsilon \, d\varepsilon - g \int_{-\omega}^{-M/2mg} \frac{\varepsilon^2}{E} d\varepsilon - g \int_{M/2mg}^{+\omega} \frac{\varepsilon^2}{E} d\varepsilon - \frac{\Delta^2}{G} \quad . \qquad (57)$$

By assuming $\omega >> \Delta$ and by using eq. (42) and eq. (51) we obtain:

$$E = - g\omega^2 - \frac{1}{2} g\Delta^2 + \frac{M}{2m} \left(\frac{M^2}{4m^2 g^2} + \Delta^2\right)^{1/2} \quad . \qquad (58)$$

The ground state energy ($T = 0$, $M = 0$) is:

$$E_o = - g\omega^2 - \frac{1}{2} g \Delta_o^2 \quad . \qquad (59)$$

The equation of the yrast line can be written as follows:

$$E - E_o = \frac{1}{2} g(\Delta_o^2 - \Delta^2) + \frac{M}{2m} \left(\frac{M^2}{4m^2 g^2} + \Delta^2\right)^{1/2} \quad , \qquad (60)$$

or in a simpler form:

$$E - E_o = \frac{1}{2} g \Delta_o^2 \frac{M}{M_c} \left(2 - \frac{M}{2M_c}\right) \text{ for } M < M_c \qquad (61)$$

$$E - E_o = \frac{1}{2} g \Delta_o^2 + \frac{M^2}{4m^2 g} \text{ for } M > M_c \quad . \qquad (62)$$

In fig. 8 the yrast line is shown (lower line) together with the critical energy as a function of M (upper line). These two curves, which join smoothly at M_c, define the region of the superconducting phase. The dashed line is the continuation of the yrast line given by eq. (62) for M values lower than M_c; it represents the yrast line corresponding to an uncorrelated Fermi gas. Such a line intersects the energy axis, for M = 0 at an energy equal to $\frac{1}{2} g \Delta_o^2$, which represents the condensation energy from the normal to the superconducting phase for M = 0 and T = 0. The difference between the dashed line and the lower line represents the T = 0 condensation energy as a function of M. As could be expected, such a condensation energy reduces to zero for $M = M_c$ because of the disappearance of the pairing correlation. A generalization of the calculation is shown in fig. 9. Here the energy of the system is calculated as a function of M for equally spaced constant temperature values: the yrast line is obviously a part of such a family of curves, being that characterized by T = 0. In fact for the lower temperatures the curves tend to follow the yrast line, while for the higher temperatures the curves become more parabola-like and similar to the dashed curve corresponding to the yrast line for an uncorrelated Fermi gas. This is due to the decrease in correlation and therefore in Δ associated with the temperature increase.

As a final example of the change from temperature to energy scale, fig. 10, which corresponds to fig. 7, shows the lines of equal Δ value in the E/M plane. The superconducting region is bounded by the yrast line and by the critical energy line: the inner lines, of equal Δ value go from Δ = 1 MeV to Δ = 0 MeV in steps of 0.1 MeV.

3.5. THE ENTROPY

The pairing effects are very relevant in the entropy expression also. In fig. 11 the entropy has been calculated as a function of M for a set of increasing values of temperature. In absence of pairing and in particular for M and T above their critical values, the entropy, at fixed temperature does not depend upon M. This appears clearly in the right side of the figure where the curves reduce to equally spaced straight lines parallel to the M axis. Within the paired region there is a general depression in the entropy values, the larger the lower the temperature. For the very lowest temperature values the entropy goes through a maximum.

3.6. THE LEVEL DENSITY DENOMINATOR

As it was already observed the case of the pairing correlation for $M = 0$[11]), the denominator of the level density goes through a discontinuity whenever the critical temperature is crossed: in particular, for $M > M_c$ two discontinuities should exist in correspondence with the two values of the critical temperatures (corresponding to exceedingly small excitation energies) the saddle point approximation is not to be trusted.

3.7. STATISTICAL QUANTITIES OUTSIDE THE PAIRED REGION

As far as the general case is concerned, the formalism described here holds also beyond the paired region, provided that Δ and its derivatives with respect to the Lagrange multipliers are set equal to zero.

In the case of the uniform model, the expressions for the statistical quantities can be easily integrated, so that analytical expressions can be obtained. They are given as follows:

$$N = 2\lambda g \quad ;$$

$$M = 2\gamma m^2 g \quad ;$$

$$E - E_o = \frac{1}{2} g \Delta_o^2 + \frac{M^2}{4m^2 g} + \frac{\pi^2}{3} \frac{g}{\beta^2}$$

$$S = \frac{2}{3} \pi^2 \frac{g}{\beta}$$

$$\frac{\partial^2 \Omega}{\partial \alpha^2} = \frac{2g}{\beta} \quad ;$$

$$\frac{\partial^2 \Omega}{\partial \mu^2} = \frac{2m^2 g}{\beta} \quad ;$$

$$\frac{\partial^2 \Omega}{\partial \beta^2} = \frac{2\lambda^2 g + 2\gamma^2 m^2 g}{\beta} + \frac{2}{3} \frac{\pi^2}{\beta^2} g \quad ;$$

$$\frac{\partial^2 \Omega}{\partial \alpha \partial \beta} = - \frac{2\lambda g}{\beta} \quad ;$$

$$\frac{\partial^2 \Omega}{\partial \mu \partial \beta} = - \frac{2\gamma m^2 g}{\beta} \quad ;$$

$$\frac{\partial^2 \Omega}{\partial \alpha \partial \mu} = 0 \quad . \tag{63}$$

4. Completeness of the Formalism with Respect to Angular Momentum

It has been anticipated in the introduction that in the present formalism only those first integrals can be easily handled which can be expressed in terms of a sum over single particle levels. The energy, the particle number, and the projection of the total angular momentum, do satisfy such a requirement. However, the total angular momentum does not present such good features and therefore it has not been included in the present calculation. Thus the question arises whether such a calculation ought to be considered complete. An apparent lack of completeness could be found for example in the dependence of Δ upon M for $T = 0$ (fig. 1). In fact, since the choice of the z axis is arbitrary, so will be the M projection on such an axis. Therefore it may not be clear how an intrinsic property of the system, like the pairing correlation, can depend upon the arbitrary choice of the z axis. However it can be shown that the formalism is essentially complete, at least for a spherical nucleus. It is quite obvious that if the total momentum is not aligned with the z axis, the present formalism accounts only for a part of the overall angular momentum effect. But, if the angular momentum is indeed aligned with the z axis, (and this can always be the case, if a suitable choice of the z axis is made), then there is no angular momentum component left out which may affect the intrinsic properties of the system. It follows that we can substitute the total angular momentum in place of M in all the expressions concerning the intrinsic properties of the system. Such is the case for the expression giving Δ as a function of M and T, for the yrast line expression, for the energy expression and so on. Instead, for the evaluation of the level density for a given angular momentum I, the problem is slightly more complicated. We can make the usual observation[1]):

$$\rho(E, I) = \rho(E, M = I) - \rho(E, M = I + 1) \quad , \tag{64}$$

or

$$\rho(E, I) \simeq - \left(\frac{d}{dM} \rho(E,M)\right)_{M=I + \frac{1}{2}} \quad . \tag{65}$$

In taking such a derivative, one must keep not only E and N constant but also Δ, this last quantity being evaluated at $M = I + \frac{1}{2}$. In any case the evaluation of such a derivative is not so simple. Perhaps an easier way to handle such a problem is as follows. Let us assume that the following relation holds in a small interval of M:

$$\rho(E, M) \simeq f(E)\, e^{-\frac{M^2}{2\sigma^2}} \quad , \tag{66}$$

where

$$\sigma^2 = \frac{1}{2} \sum \frac{m_k^2}{\operatorname{sech}^2 \frac{1}{2} \beta\, E_k} \quad , \tag{67}$$

and where Δ assumes the value associated to I. Such a relation introduces the concept of the spin cutoff parameter σ^2 which has been avoided up to this point. However this is not so important. In fact now we can perform the derivative:

$$\rho(E, I) = \frac{(2I + 1)}{2\sigma^2} f(E) \cdot e^{-(I + \frac{1}{2})^2/2\sigma^2} \quad , \tag{68}$$

or

$$\rho(E, I) = \frac{2I + 1}{2\sigma^2} \rho(E, M = I + \frac{1}{2}) \quad . \tag{69}$$

So, the spin cutoff parameter has been used only for the approximate evaluation of the derivative.

In the case of a non-spherical nucleus and specifically in the case of an axially symmetric nucleus, the spin projections Ω_k and the angular momentum projection K on the symmetry axis are good quantum numbers. Therefore in the present formalism one should identify M with K and m_k with Ω_k. Indeed now the formalism is not complete because it is not possible to handle the angular momentum component perpendicular to the symmetry axis. In order to do that, one should perhaps utilize the cranking model which could provide also an alternative way to solve the overall problem[15]). However it can be pointed out that axial symmetry and K conservation hold for the very lowest temperatures only. For excitation energies where the level density begins to be high, the levels should become strongly K mixed and the axial symmetry will be compromised. Furthermore the statistical washing out of the shells will tend to make all of the nuclei spherical on the average.

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Figure Captions

Fig. 1. Dependence of the gap parameter Δ upon the angular momentum M at zero temperature. Δ_o is the gap parameter for T = 0, M = 0, and M_c is the critical angular momentum above which $\Delta = 0$.

Fig. 2. Schematic illustration of the effect of angular momentum on the pairing correlation. On the left the system has zero angular momentum. The black full circles represent the particles which occupy the doubly degenerate levels up to the Fermi level E_F. Pairing smears out the Fermi surface as indicated in the diagram on the outer left, where the occupation numbers are shown as a function of the single particle energy. On the right, the system has a non-zero angular momentum, obtained by breaking pairs and by polarizing the resulting quasi particles (open circles with arrow). The quasi particles block single particle levels which become unavailable for the pairing correlation.

Fig. 3. Dependence of the gap parameters Δ upon the temperature T at zero angular momentum. T_c is the critical temperature above which $\Delta = 0$.

Fig. 4. Dependence of the gap parameter upon the excitation energy at zero angular momentum. The parameters used in the calculation are: $\Delta_o = 1$ MeV, $g = 7$ MeV^{-1}, $m = 2\hbar$.

Fig. 5. Dependence of the critical temperature upon angular momentum. The parameters are the same as in fig. 4.

Fig. 6. Explanation of the thermally assisted pairing correlation. a) On the left, the temperature is zero and the angular momentum is generated by quasi particles which are tightly packed around the Fermi surface: the pairing interaction finds the most effective levels blocked by quasi particles. b) On

the right, a non-zero temperature spreads out the distribution of quasi particles making more levels available for the pairing interaction. The result is a tendency of the gap parameter to increase with temperature for non-zero angular momentum.

Fig. 7. Contour map of the gap parameter as a function both of temperature and and angular momentum. The spacing in Δ between two successive lines is 0.05 MeV from $\Delta = 1.0$ MeV to $\Delta = 0.1$ MeV. The outer line corresponds to $\Delta = 0$ MeV.

Fig. 8. Critical energy (upper line) and yrast line (lower line) as a function of angular momentum. The dashed line, which merges into the yrast line at $M = M_c$ is the yrast line for the unpaired system. The difference in energy between the dashed line and the lower solid line represents the condensation energy due to pairing.

Fig. 9. Same as in fig. 8. The lines in the paired region correspond to the energy as a function of angular momentum at constant temperatures from $T = 0.09$ MeV to $T = 0.54$ MeV in 0.03 MeV steps.

Fig. 10. Same as in fig. 8. The contour lines in the paired region correspond to the regions of equal Δ from $\Delta = 1$ MeV to $\Delta = 0$ MeV in steps of 0.1 MeV.

Fig. 11. Entropy as a function of angular momentum for a set of equally spaced temperatures.

Fig. 12. Level density denominator as a function of temperature for different values of angular momentum (number marked on each line).

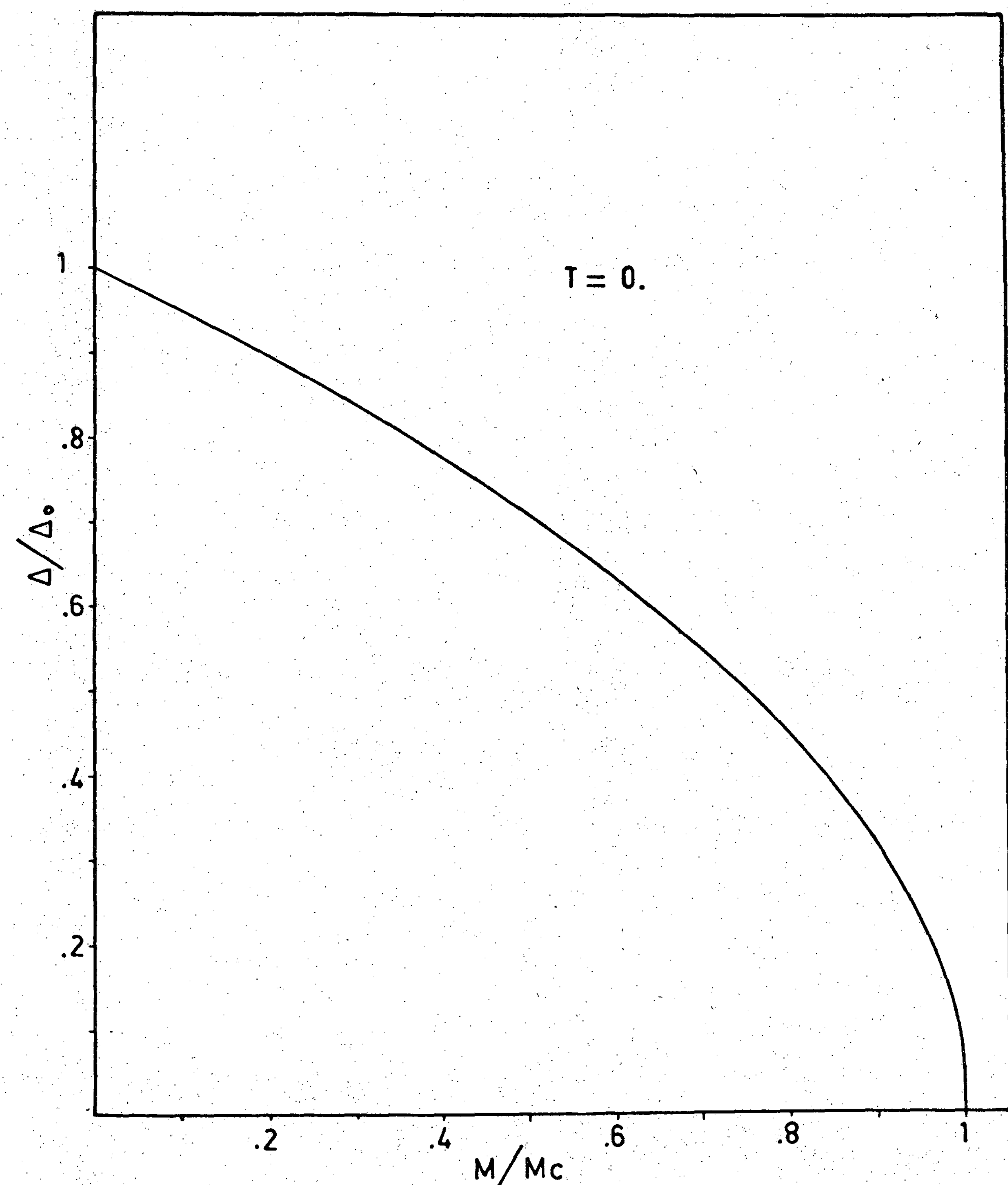

Fig. 1

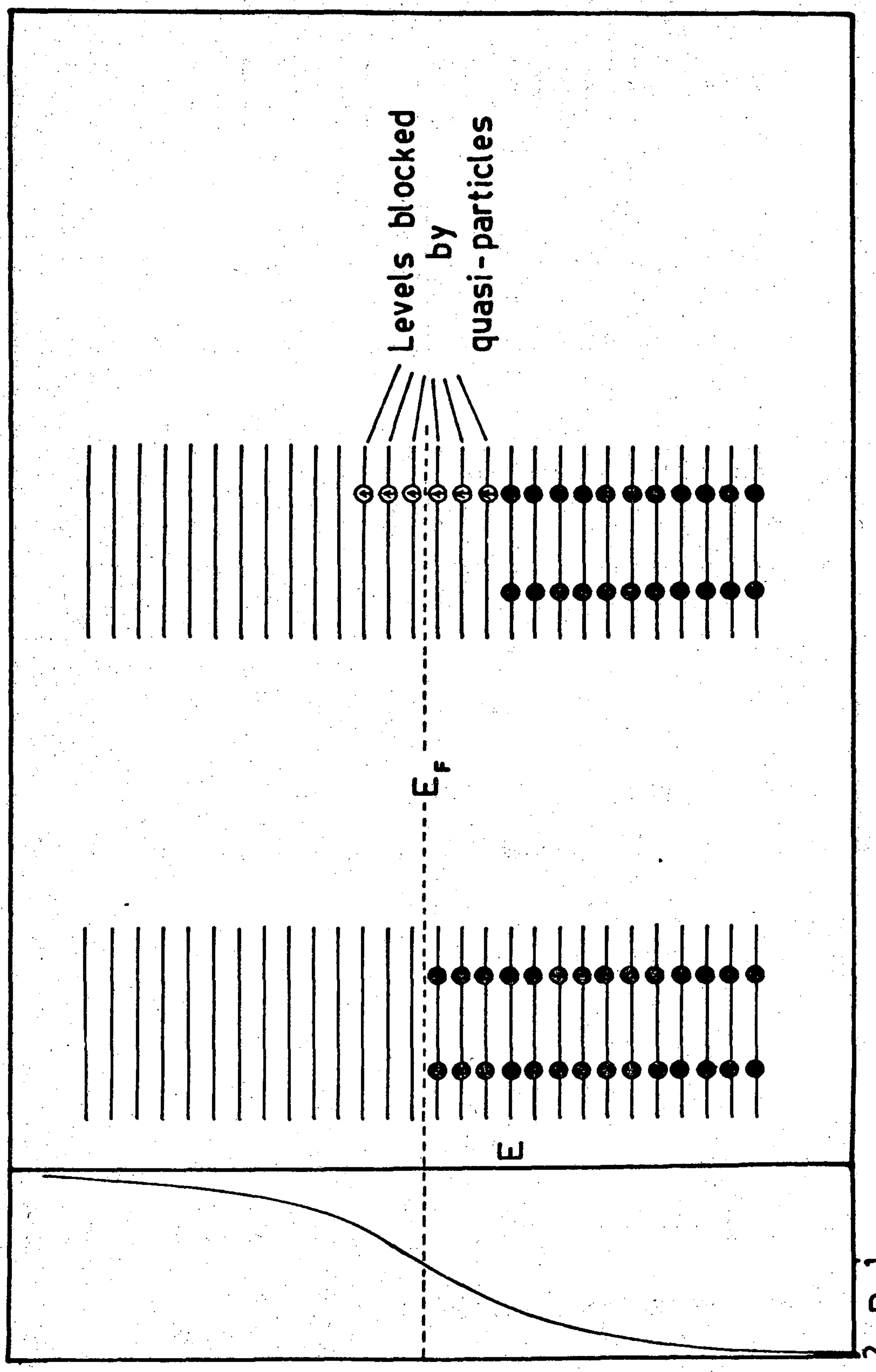

Fig. 2

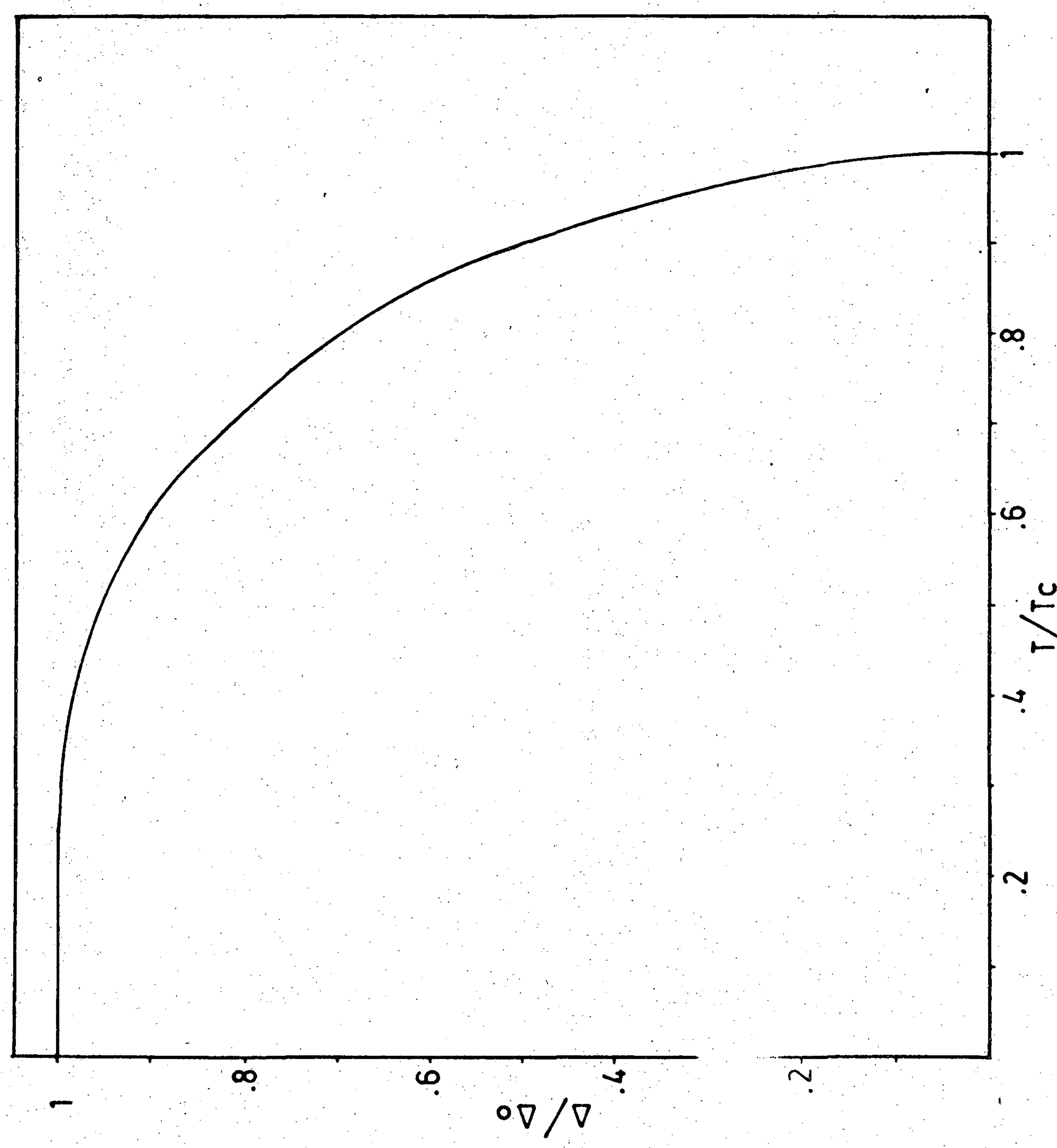

Fig. 3

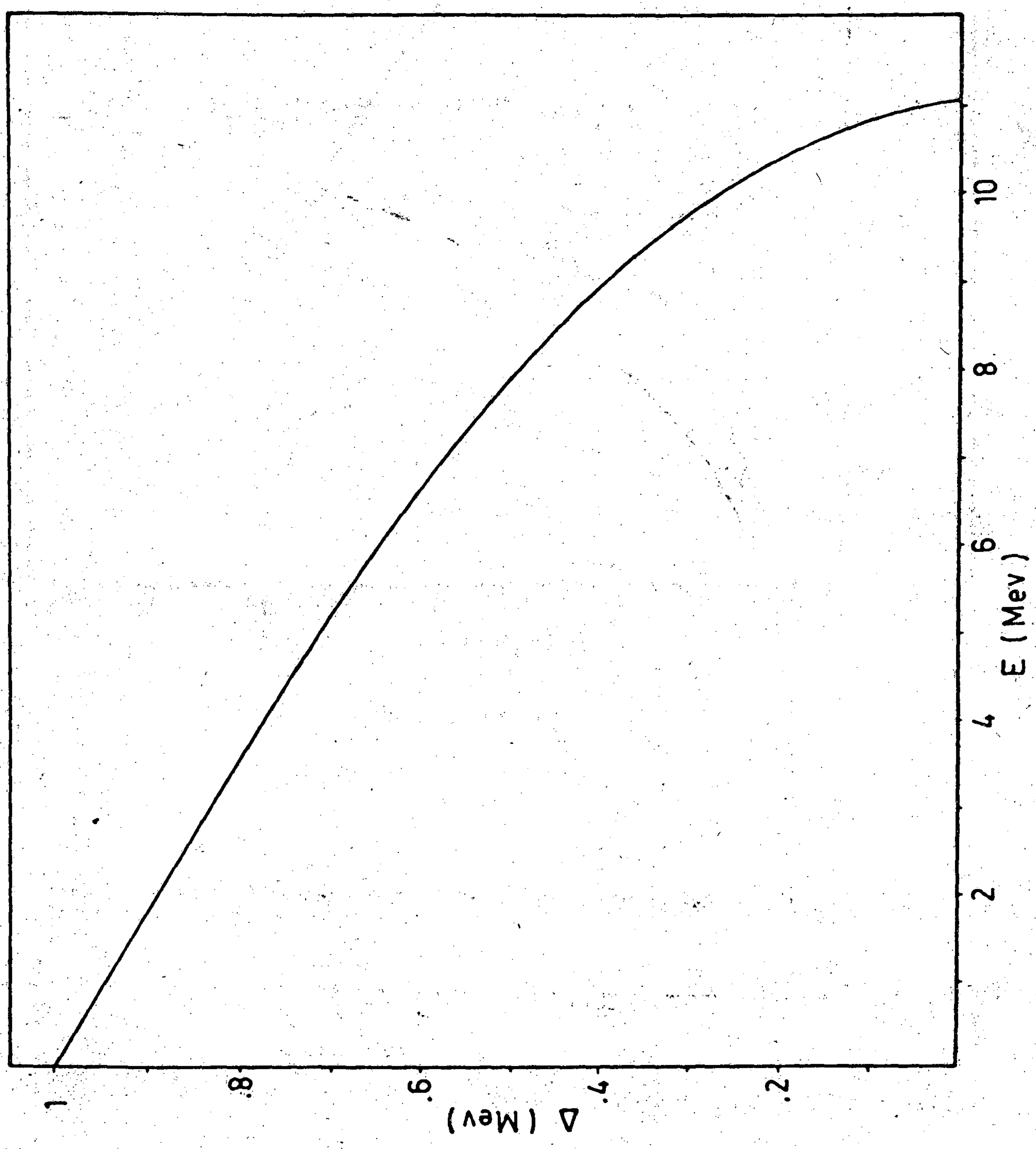

Fig. 4

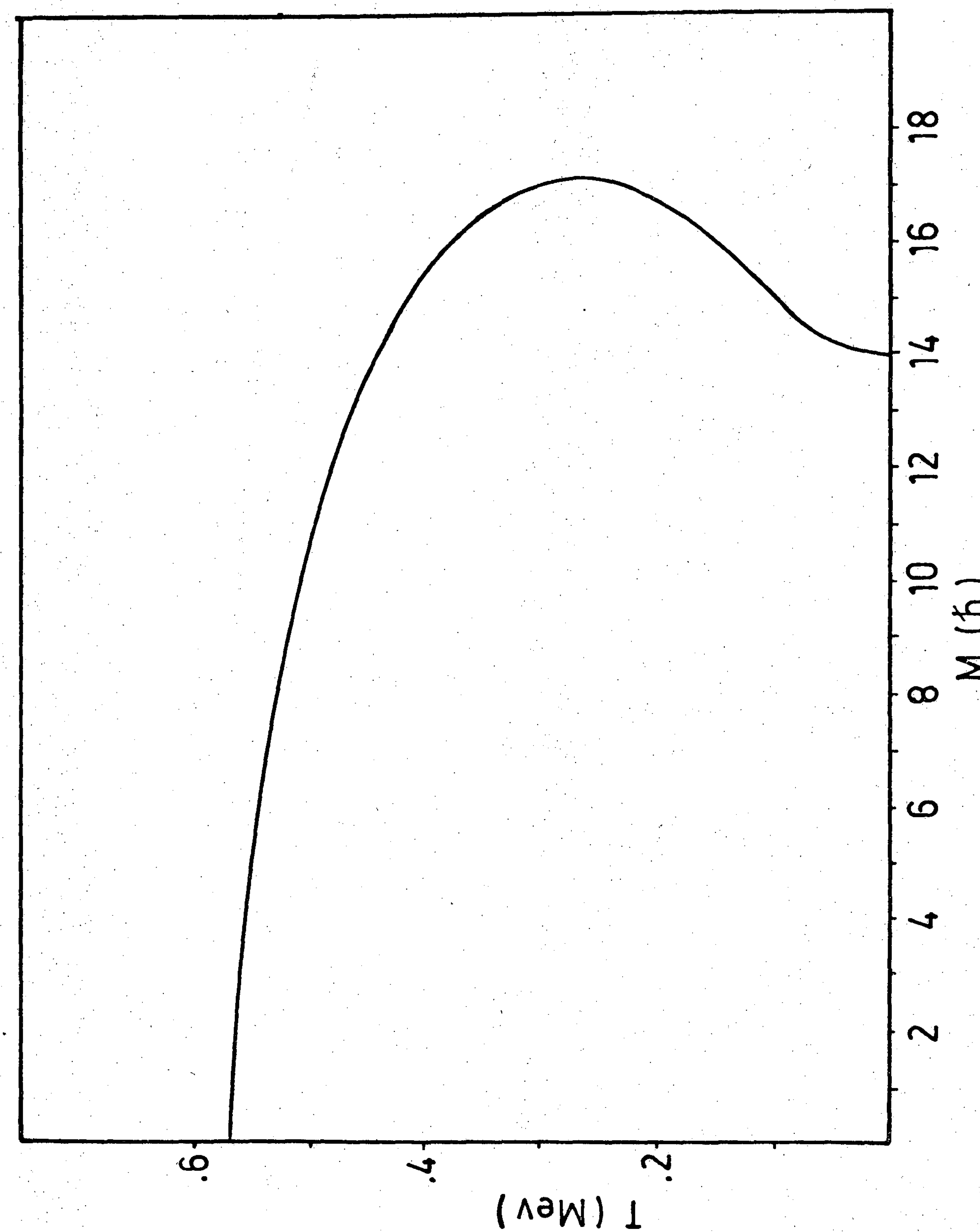

Fig. 5

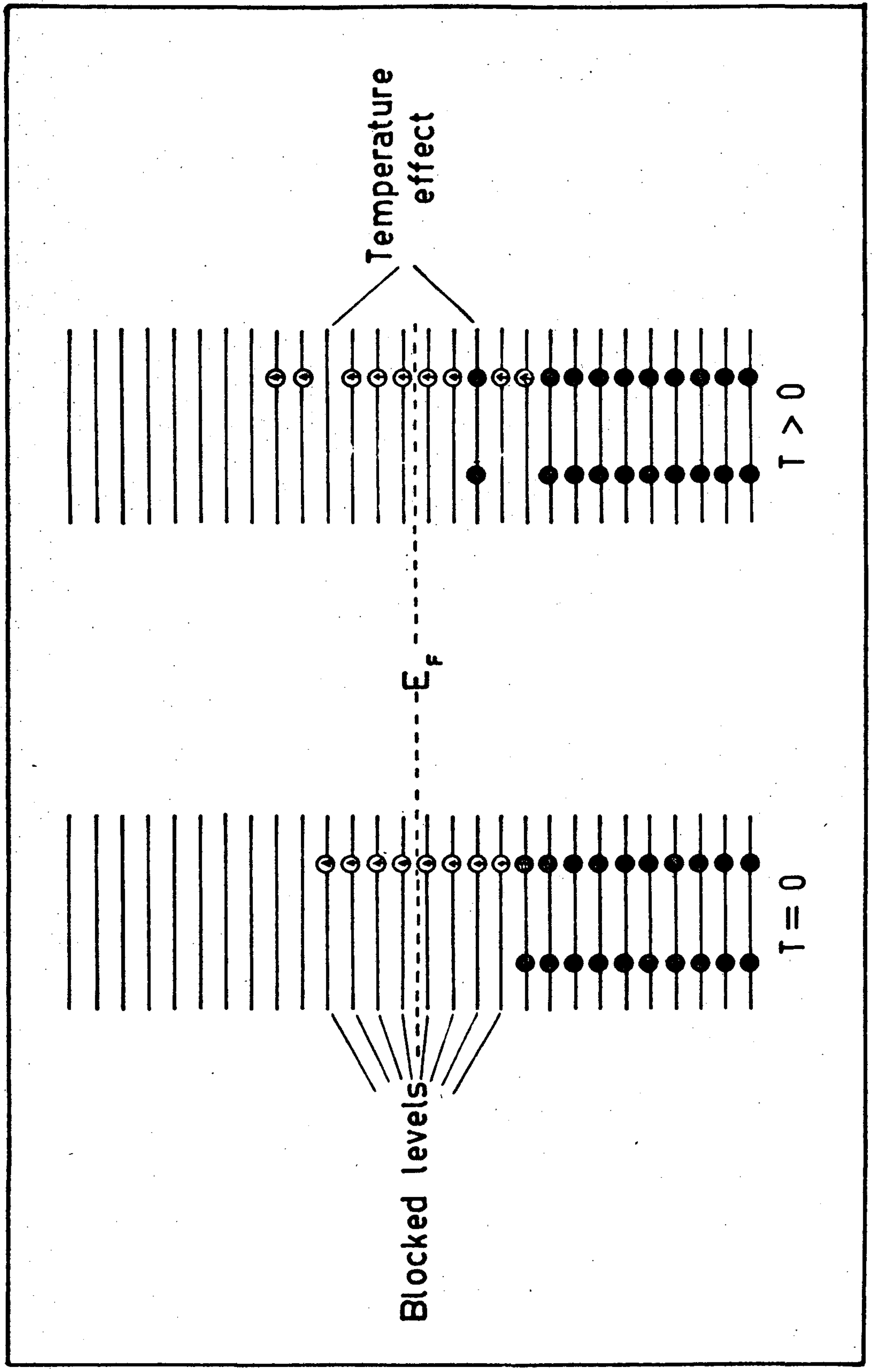

Fig. 6

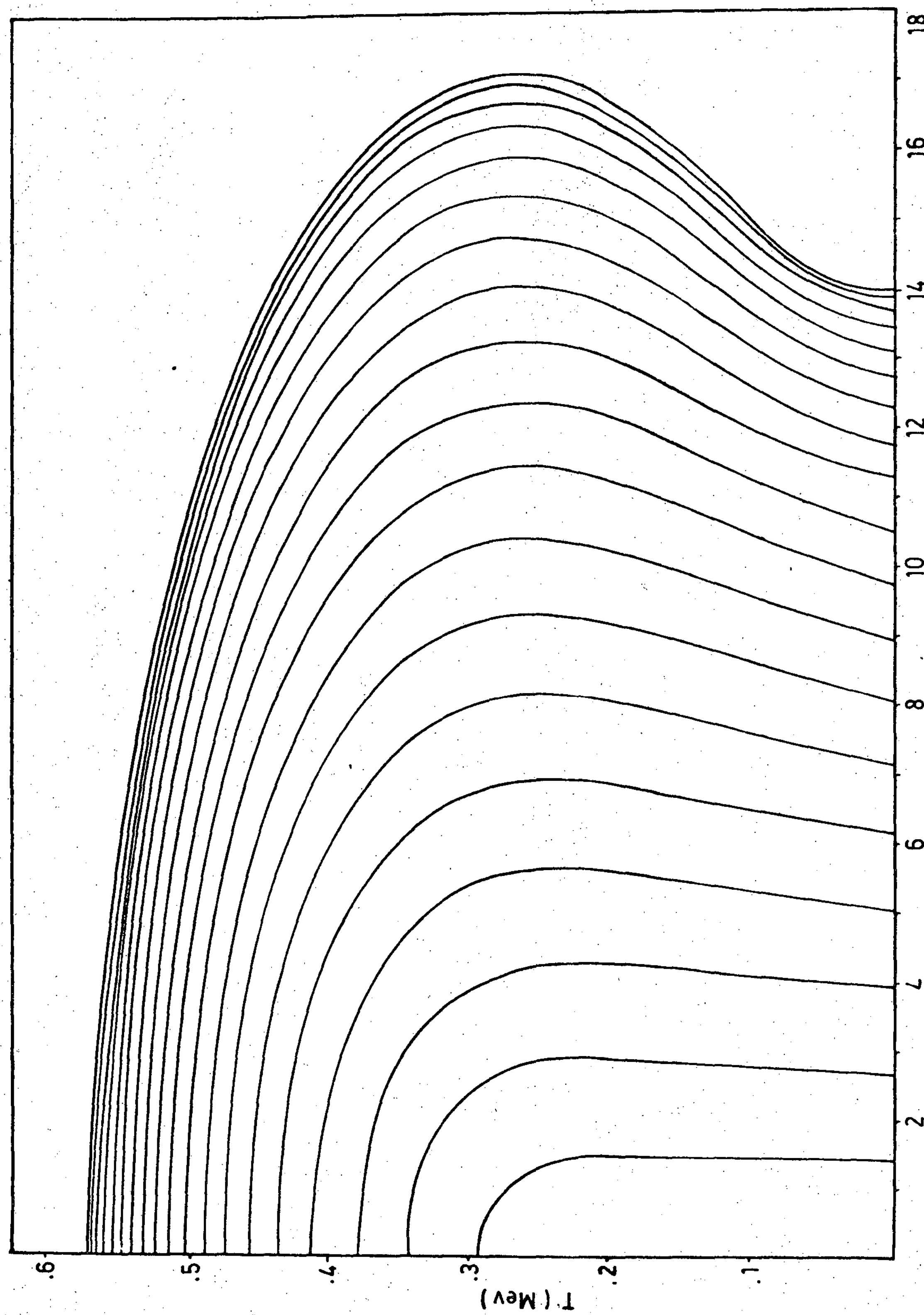

Fig. 7

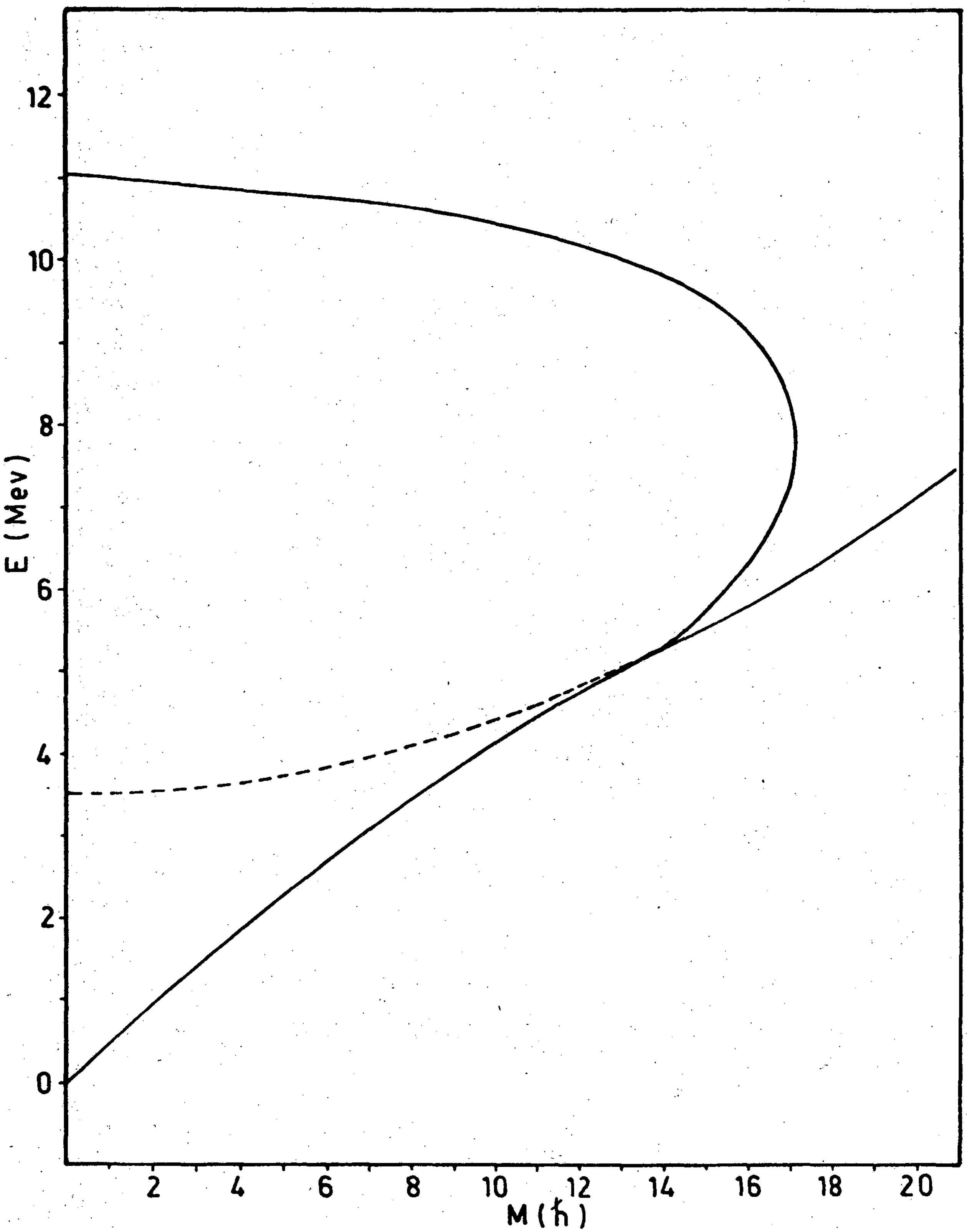

Fig. 8

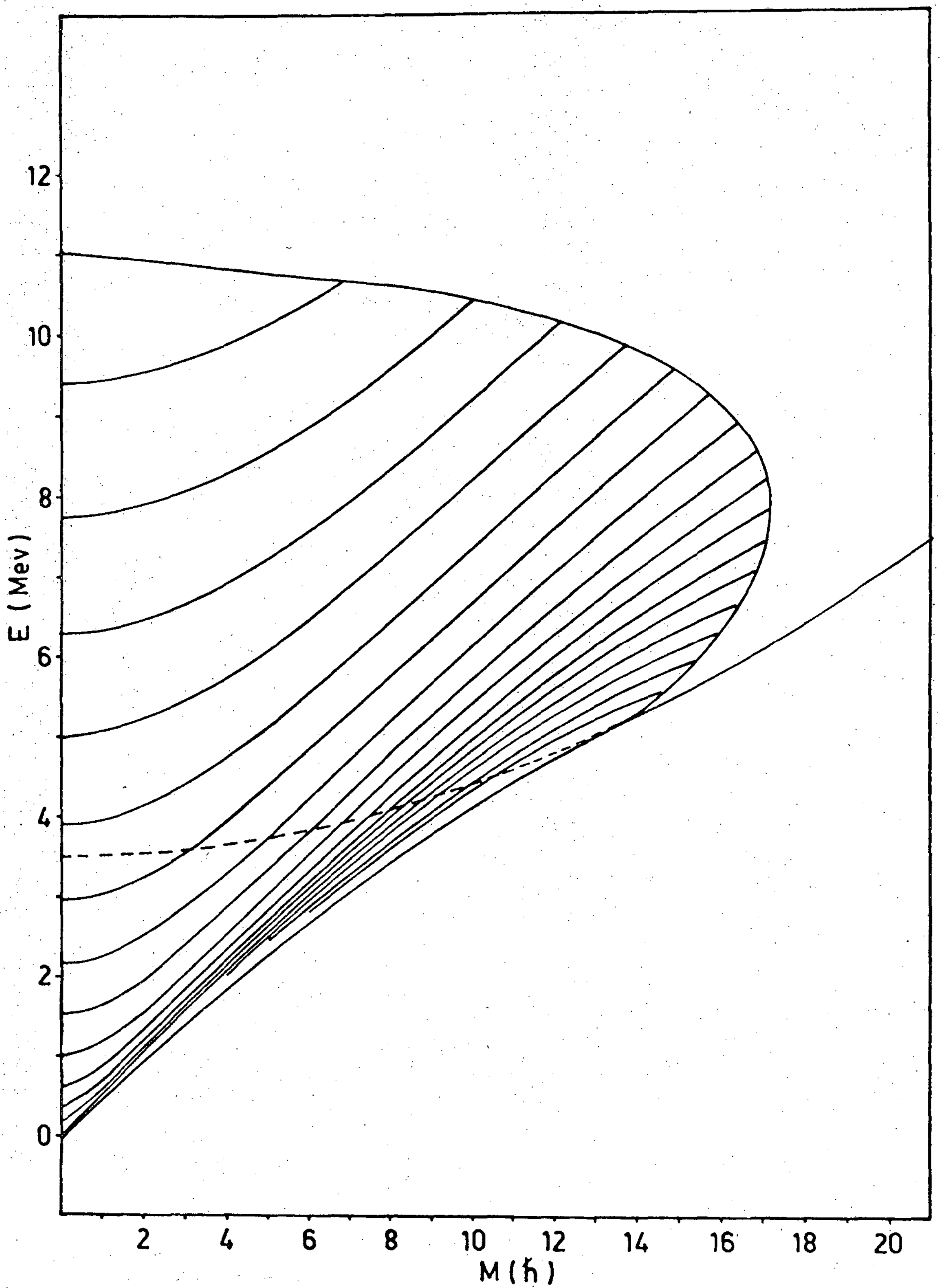

Fig. 9

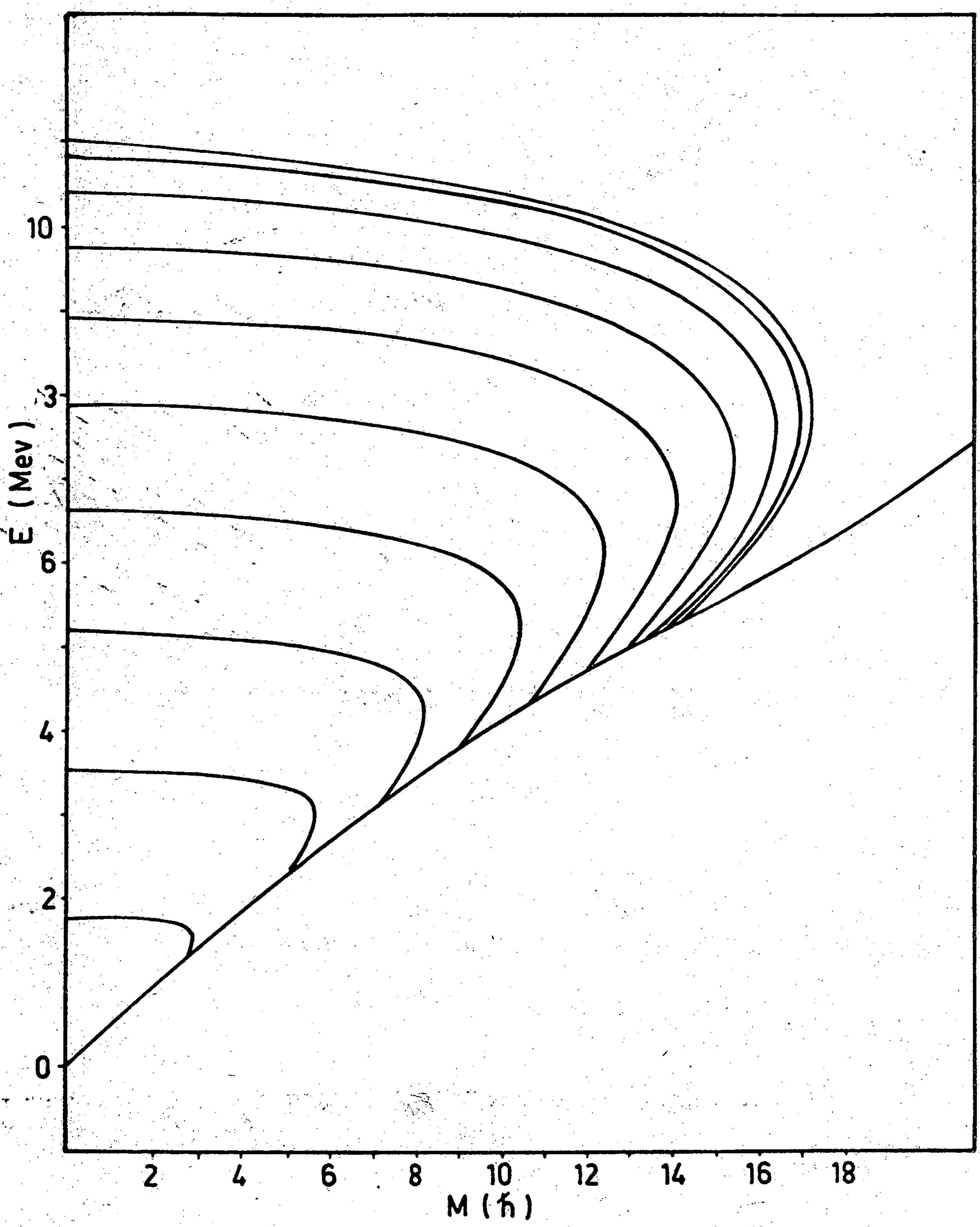

Fig. 10

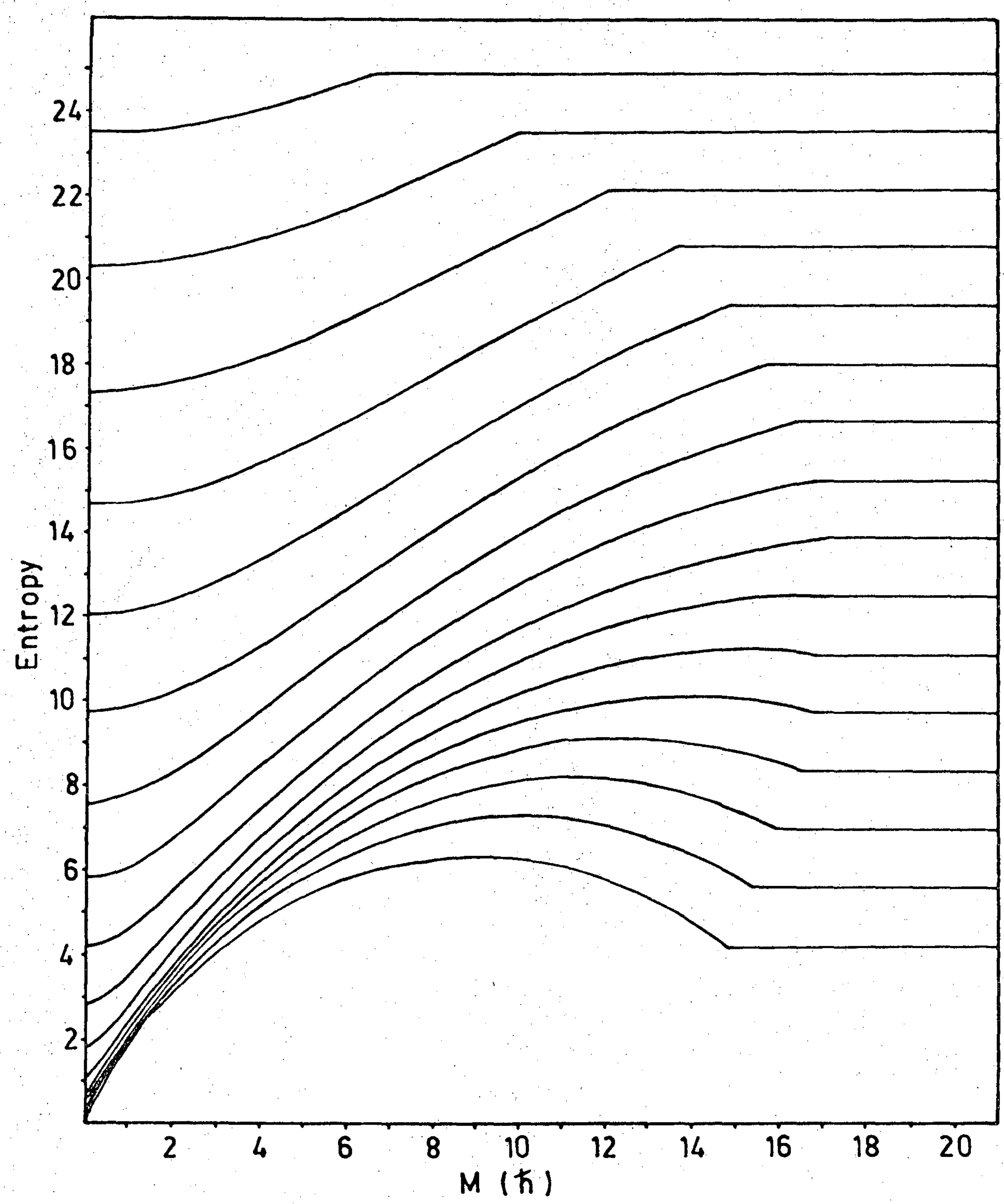

Fig. 11

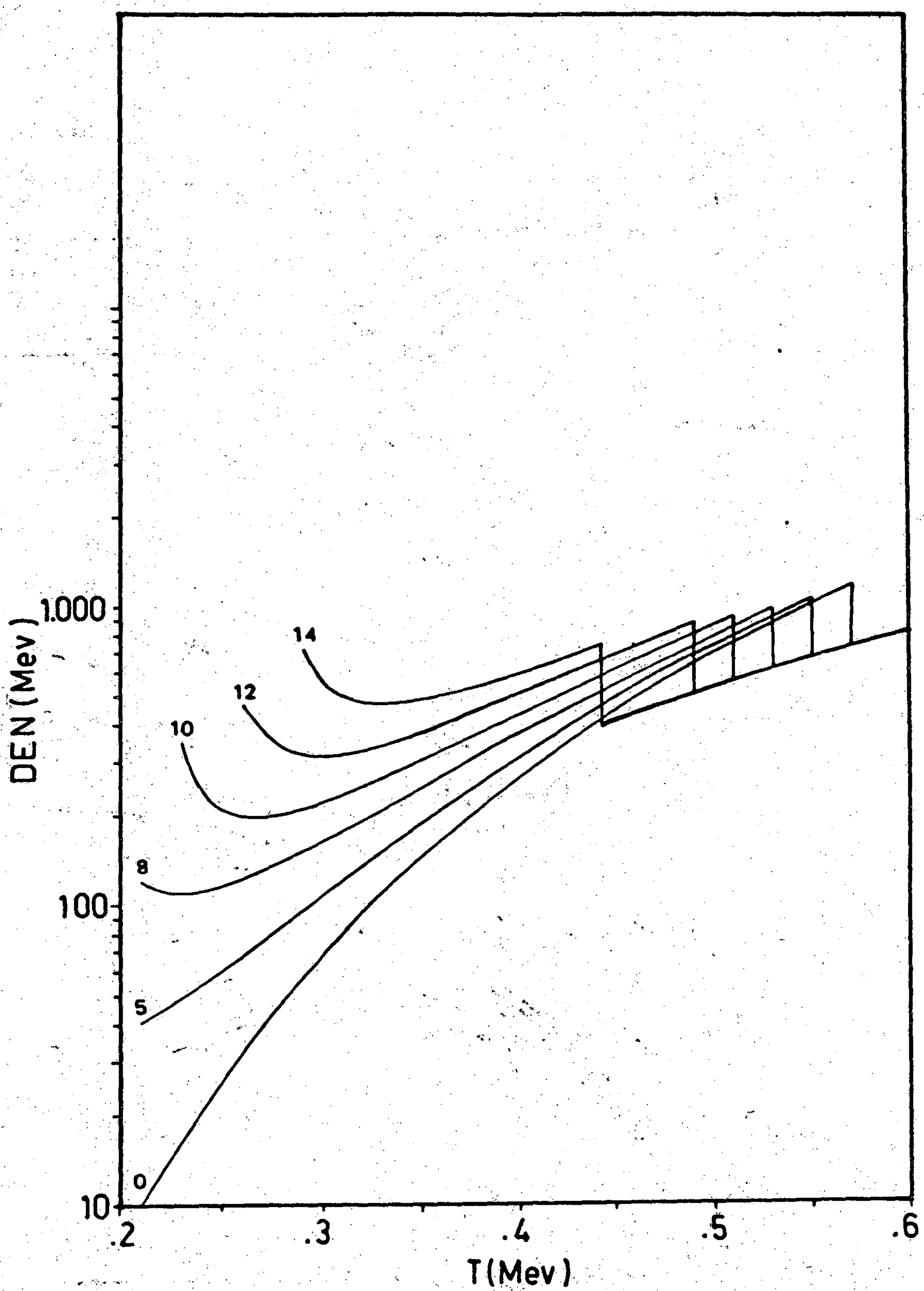

Fig. 12

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