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July 1971

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BASIC FORMULATION OF NUCLEAR LEVEL DENSITY CALCULATIONS*

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ABSTRACT

Peierls' Theorem and the Bogoliubov inequality are used to derive a variational principle for the grand partition function of a quantum mechanical system. The variational principle is applied to the case of a general non-relativistic Hamiltonian with two-body forces, under the special Bogoliubov transformation.

1. INTRODUCTION

Since the original work of Bethe[1] 35 years ago, much effort has been devoted to the calculation of level densities and other nuclear statistical properties (see in particular the review article by Ericson[2]). But only in recent years has there been any effort to obtain level densities directly starting from a realistic Hamiltonian.[3-6]

In nuclear physics, the systems considered have less than 300 particles. We cannot simply take over concepts from ordinary thermodynamics, i.e. systems with over 10^{20} particles. The concept of the grand partition function is introduced abstractly.

Consider first a system with one kind of particle A state of the system is defined by 2 constants of the motion, the number of particles N and the energy E.

The grand partition function is defined as

$$Z = \sum_{N'E'} \exp \beta(\mu N' - E') \quad , \tag{1.1}$$

where the sum is over all possible values of N' and E'. The sum over energies can be replaced by an integral if the proper weighting function is inserted; this is none other than the level density $\rho(N,E)$. Strictly speaking $\rho(N,E)$ is defined as

$$\rho(N,E) = \sum_{E'} \delta(E - E') \quad .$$

In practice the level density is considered to be a continuous function. Thus

$$Z = \sum_{N'} \int dE' \; \rho(N', E') \exp(\alpha N' - \beta E') \quad , \tag{1.2}$$

where we have written

$$\alpha = \beta\mu \quad . \tag{1.3}$$

The grand partition function is essentially a Laplace transform of the level density; the latter can be obtained by inversion. Specifically $\rho(N,E)$ is the inverse Laplace transform of the coefficient of $\exp(\alpha N)$ in the grand partition function:

$$\rho(N,E) = \left(\frac{1}{2\pi i}\right)^2 \int_{\gamma - i\infty}^{\gamma + i\infty} d\beta \int_{\gamma_n - i\pi}^{\gamma_n + i\pi} d\alpha \; e^S \quad , \tag{1.4}$$

where

$$S = \ln Z - \alpha N + \beta E \quad . \tag{1.5}$$

The integrals in Eq. (1.4) can be evaluated approximately by the method of steepest descent. The exponent S has a saddle point at

$$N = \frac{\partial \ln Z}{\partial \alpha} \qquad E = -\frac{\partial \ln Z}{\partial \beta} \quad . \tag{1.6}$$

Then the level density is given approximately by

$$\rho(N,E) = \frac{e^S}{2\pi \, D^{1/2}} \quad , \tag{1.7}$$

where

$$D = \begin{vmatrix} \frac{\partial^2 \ln Z}{\partial \alpha^2} & \frac{\partial^2 \ln Z}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \alpha \partial \beta} & \frac{\partial^2 \ln Z}{\partial \beta^2} \end{vmatrix} , \tag{1.8}$$

all evaluated at the saddle point.

The exact values of the energies E' of the nuclear states are not known. So Z will be rewritten as

$$Z = \mathrm{Tr}\ e^{-\beta(H - \mu N)} , \tag{1.9}$$

where H and N are now quantum mechanical operators. This permits the evaluation of Z in any convenient set of quantum states.

It is simple to generalize this treatment to a system with two kinds of particles, neutrons and protons. The grand partition function becomes

$$Z = \mathrm{Tr}\ \exp\left[-\beta(H - \mu_n N_n - \mu_p N_p)\right] . \tag{1.10}$$

N_n, N_p are number operators for neutrons and protons. Proceeding as before

$$\rho(N_n, N_p, E) = \frac{e^S}{(2n)^{3/2} D^{1/2}} \tag{1.11}$$

where $$S = \ln Z - \alpha_n N_n - \alpha_p N_p + \beta E , \tag{1.12}$$

$$D = \begin{vmatrix} \frac{\partial^2 \ln Z}{\partial \alpha_n^2} & \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \alpha_p} & \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \alpha_p} & \frac{\partial^2 \ln Z}{\partial \alpha_p^2} & \frac{\partial^2 \ln Z}{\partial \alpha_p \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \beta} & \frac{\partial^2 \ln Z}{\partial \alpha_p \partial \beta} & \frac{\partial^2 \ln Z}{\partial \beta^2} \end{vmatrix} , \tag{1.13}$$

all evaluated at the saddle point defined by

$$N_n = \frac{\partial \ln Z}{\partial \alpha_n} \qquad N_p = \frac{\partial \ln Z}{\partial \alpha_p} \qquad E = -\frac{\partial \ln Z}{\partial \beta} \quad . \tag{1.14}$$

The angular momentum dependence of the level density can be obtained by adding another constant of the motion: M, the magnetic quantum number. The appropriate generalization of the grand partition function is

$$Z = \mathrm{Tr} \exp\left[-\beta(H - \mu_n N_n - \mu_p N_p - \gamma M)\right] \quad . \tag{1.15}$$

As before

$$\rho(N_n, N_p, M, E) = \frac{e^S}{(2\pi)^2 D^{1/2}} \tag{1.16}$$

where

$$S = \ln Z - \alpha_n N_n - \alpha_p N_p - \nu M + \beta E \quad . \tag{1.17}$$

We have put

$$\nu = \beta\gamma \quad . \tag{1.18}$$

D is, as before, a determinant of second derivatives

$$D = \begin{vmatrix} \frac{\partial^2 \ln Z}{\partial \alpha_n^2} & \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \alpha_p} & \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \nu} & \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \alpha_p} & \frac{\partial^2 \ln Z}{\partial \alpha_p^2} & \frac{\partial^2 \ln Z}{\partial \alpha_p \partial \nu} & \frac{\partial^2 \ln Z}{\partial \alpha_p \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \nu} & \frac{\partial^2 \ln Z}{\partial \alpha_p \partial \nu} & \frac{\partial^2 \ln Z}{\partial \nu^2} & \frac{\partial^2 \ln Z}{\partial \nu \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \alpha_n \partial \beta} & \frac{\partial^2 \ln Z}{\partial \alpha_p \partial \beta} & \frac{\partial^2 \ln Z}{\partial \nu \partial \beta} & \frac{\partial^2 \ln Z}{\partial \beta^2} \end{vmatrix} . \tag{1.19}$$

All these quantities are evaluated at the saddle point defined by

$$N_n = \frac{\partial \ln Z}{\partial \alpha_n} \qquad N_p = \frac{\partial \ln Z}{\partial \alpha_p}$$

$$M = \frac{\partial \ln Z}{\partial \nu} \qquad E = -\frac{\partial \ln Z}{\partial \beta} . \tag{1.20}$$

The J-dependence of the level density is obtained by a procedure due to Bethe[1]

$$\rho(N_n, N_p, J, E) = \rho(N_n, N_p, M, E)\Big|_{M=J} - \rho(N_n, N_p, M, E)\Big|_{M=J+1} . \tag{1.21}$$

The theory of level densities bears close resemblance to ordinary thermodynamics. μ is the Fermi energy, β is the inverse temperature, S is the entropy; the saddle-point equations (1.6), (1.14), or (1.20) are the same as in thermodynamics.

What is different is the presence of the term $D^{1/2}$ in the denominator of the level density expression. In ordinary thermodynamics S is overwhelmingly greater than 1/2 $\ln D$; we simply identify S with $\ln \rho$. In the nuclear case this approximation is more questionable, and certainly should not be made in an accurate calculation.

In the past, calculations of the grand partition function and other statistical quantities were based on a set of independent single-particle states with occupation numbers n_i and energy ε_i. Then

$$N = \sum_i n_i$$

$$E = \sum_i n_i \varepsilon_i \quad , \tag{1.22}$$

and the grand partition function becomes

$$Z = \sum_i \{1 + e^{-\beta(\varepsilon_i - \mu)}\} \quad .$$

No effort was made to relate the ε_i to a realistic Hamiltonian.

Recently, Sano and Yamasaki[3] and others[4-6] have taken the first steps in this direction. Their level density calculations are based on a Hamiltonian which includes a simple version of the pairing interaction (between nucleons in states differing only by the sign of the magnetic quantum number).

In this paper we will develop a variational principle for the grand partition function which is suitable for a more general Hamiltonian. The principle is based on Peierls' theorem and the Bogoliubov inequality. An application will be made to the case of a Hamiltonian with two-body forces.

2. VARIATIONAL PRINCIPLE FOR THE GRAND PARTITION FUNCTION

A well-known variational principle states that the ground-state energy of a quantum mechanical system is less than or equal to the expectation value of the Hamiltonian with an arbitrary wavefunction. Given a trial wavefunction with adjustable parameters, the best values of the parameters are those which minimize the expectation value of the Hamiltonian.

In this work we will derive a variational principle for the grand partition function which is a thermal extension of the variational principle for the ground state. A joint application of Peierls' theorem[7] and the Bogoliubov inequality[8,9] leads to a strict lower bound for the grand partition function. The variational principle consists in adjusting the available parameters so as to maximize this lower bound.

Peierls' theorem[7] says that

$$Z = \mathrm{Tr}\, e^{-\beta H} \geqslant \sum_k e^{-\beta \langle k|H|k \rangle} , \tag{2.1}$$

where $|k\rangle$ is an arbitrary set of orthonormal states (see Appendix B for proof).

In other words, if H_d is the diagonal part of the Hamiltonian in some representation, then

$$\mathrm{Tr}\, e^{-\beta H} \geqslant \mathrm{Tr}\, e^{-\beta H_d} . \tag{2.2}$$

If any Hamiltonian operator is written as $H = H_0 + H_1$, we can make use of the Bogoliubov inequality[8,9] (see Appendix C for proof):

$$\ln \mathrm{Tr}\, e^{-\beta(H_0 + H_1)} \geqslant \ln \mathrm{Tr}\, e^{-\beta H_0} - \beta \frac{\mathrm{Tr}(H_1 e^{-\beta H_0})}{\mathrm{Tr}\, e^{-\beta H_0}} . \tag{2.3}$$

Once a representation is chosen to pick out H_d, the diagonal terms of H, and H_d is suitable expressed as $H_0 + H_1$, then the right-hand side of (2.3) is a strict lower bound for the grand partition function.

Adjustable parameters can be introduced both in the choice of representation for H_d and in the form of H_0 and H_1. The parameters are then varied to maximize the lower bound of the grand partition function.

The Hamiltonian of a nonrelativistic system of identical Fermions interacting by 2-body interactions is

$$H = \sum_{\alpha\gamma} T_{\alpha\gamma}\, c_\alpha^+ c_\gamma + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}\, c_\alpha^+ c_\beta^+ c_\delta c_\gamma \quad . \tag{2.4}$$

The c_α^+, c_α are single-particle creation and annihilation operators satisfying the usual anticommutation relations

$$[c_\alpha^+, c_\beta^+]_+ = [c_\alpha, c_\beta]_+ = 0$$

$$[c_\alpha^+, c_\beta]_+ = \delta_{\alpha\beta} \quad . \tag{2.5}$$

The $T_{\alpha\gamma}$ are single-particle matrix elements of the kinetic energy and any overall field; the $V_{\alpha\beta\gamma\delta}$ are antisymmetrized interaction matrix elements. They have a number of symmetry properties:

$$T_{\gamma\alpha} = T_{\alpha\gamma}^*$$

$$V_{\gamma\delta\alpha\beta} = V_{\alpha\beta\gamma\delta}^* \quad , \tag{2.6}$$

since the T and V operators are Hermitian;

$$V_{\beta\alpha\gamma\delta} = V_{\alpha\beta\delta\gamma} = - V_{\alpha\beta\gamma\delta} \quad , \tag{2.7}$$

by the definition of antisymmetric matrix elements.

Let us introduce a new set of creation and annihilation operators a_α^+, a_α, by a linear transformation of the c_α^+, c_α. We can use Wick's theorem to rewrite the Hamiltonian in terms of the new operators.

The transformed Hamiltonian consists of 3 terms:

$$H = U + H_2 + H_4 \quad . \tag{2.8}$$

Fully contracted terms:

$$U = \sum_{\alpha\gamma} T_{\alpha\gamma} \langle c_\alpha^+ c_\gamma \rangle + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \langle c_\alpha^+ c_\gamma \rangle \langle c_\beta^+ c_\delta \rangle$$

$$+ \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \langle c_\alpha^+ c_\beta^+ \rangle \langle c_\delta c_\gamma \rangle \quad . \tag{2.9}$$

Terms with 2 uncontracted operators:

$$H_2 = \sum_{\alpha\gamma} T_{\alpha\gamma} : c_\alpha^+ c_\alpha : + \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \langle c_\beta^+ c_\delta \rangle : c_\alpha^+ c_\gamma :$$

$$+ \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} [\langle c_\alpha^+ c_\beta^+ \rangle : c_\delta c_\gamma : + : c_\alpha^+ c_\beta^+ : \langle c_\delta c_\gamma \rangle] \quad . \tag{2.10}$$

Terms with 4 uncontracted operators:

$$H_4 = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} : c_\alpha^+ c_\beta^+ c_\delta c_\gamma : \quad . \tag{2.11}$$

The symbol : : is for normal order. It is understood that the normal ordering refers to the a's, not the c's. $\langle c_\alpha^+ c_\gamma \rangle$ is the expectation value of $c_\alpha^+ c_\gamma$ in the vacuum state of the new operators a_α^+, a_α.

A linear transformation connects the single-particle operators c_α^+, c_α to a set of quasi-particle operators a_α^+, a_α. To apply Peierls' theorem we must pick out of H_2 and H_4 the terms diagonal in the a_α^+, a_α representation.

The diagonal terms must create the same quasiparticles they destroy. This means the only combinations of a, a^+ operators we can get in the diagonal terms of H_2 and H_4 are products like $a_\alpha^+ a_\alpha$ and $a_\alpha^+ a_\gamma^+ a_\gamma a_\alpha$. Introducing the number operators

$$n_\alpha \equiv a_\alpha^+ a_\alpha$$

we can write the diagonal terms of the transformed Hamiltonian under any linear transformation of the original representation as:

$$H_d = U + \sum_\alpha W_\alpha n_\alpha + \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} n_\alpha n_\gamma \quad . \tag{2.12}$$

The exact form of U, W_α and $W_{\alpha\gamma}$ depends on the choice of linear transformation.

To apply the Bogoliubov inequality H_d must be decomposed into $H_0 + H_1$. Following the lead of Bogoliubov[8] and others[9,10] we choose

$$H_1 = \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} (n_\alpha - f_\alpha)(n_\gamma - f_\alpha) \quad . \tag{2.13}$$

Then

$$H_0 = U - \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} f_\alpha f_\gamma + \sum_\alpha E_\alpha n_\alpha \quad , \tag{2.14}$$

where

$$E_\alpha = W_\alpha + \sum_\alpha W_{\alpha\gamma} f_\gamma \quad . \tag{2.15}$$

The f_α are variational parameters.

The physical significance of this decomposition is that the "interaction term" H_1 involves only products of fluctuations $n_\alpha - f_\alpha$, provided that f_α is a thermal average of n_α.

Bogoliubov <u>et al</u>.[8,9] have shown that with this decomposition the Bogoliubov inequality is in fact an equality with a remainder term of order V^{-1} compared to the leading terms, V being the volume of the system. In the nuclear case V^{-1} is equivalent to A^{-1}, where A is the number of nucleons.

The Bogoliubov inequality says that $\ell n\ Z$ is a lower bound to the grand partition function, where

$$\ell n\ Z_1 \equiv \mathrm{Tr}\ e^{-\beta H_0} - \beta \frac{\mathrm{Tr}(H_1 e^{-\beta H_0})}{\mathrm{Tr}\ e^{-\beta H_0}} \quad . \tag{2.16}$$

Substituting in (2.14):

$$\mathrm{Tr}\ e^{-\beta H_0} = \exp - \beta[U - \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} f_\alpha f_\gamma] \quad \mathrm{Tr} \left[e^{-\beta \sum_\alpha E_\alpha n_\alpha} \right] . \tag{2.17}$$

If the trace is calculated in the quasi-particle representation the n_α operators are diagonal, and have eigenvalues 0 or 1. So

$$\mathrm{Tr}\, e^{-\beta H_0} = \exp - \beta[U - \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma}\, f_\alpha\, f_\gamma] \prod_\alpha (1 + e^{-\beta E_\alpha}) \quad . \tag{2.18}$$

Substituting (2.13) and (2.18) into (2.16):

$$\ln Z_1 = -\beta\, U + \sum_\alpha \ln(1 + e^{-\beta E_\alpha}) - \frac{\beta}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} \frac{\mathrm{Tr}(n_\alpha n_\gamma\, e^{-\beta H_0})}{\mathrm{Tr}\, e^{-\beta H_0}}$$

$$+ \beta \sum_{\alpha\gamma} W_{\alpha\gamma}\, f_\alpha \frac{\mathrm{Tr}(n_\alpha\, e^{-\beta H_0})}{\mathrm{Tr}\, e^{-\beta H_0}} \quad . \tag{2.19}$$

The last two terms in the above equation can be evaluated by taking derivatives of (2.17) with respect to E_α:

$$\frac{\mathrm{Tr}(n_\alpha\, e^{-\beta H_0})}{\mathrm{Tr}\, e^{-\beta H_0}} = \frac{1}{e^{\beta E_\alpha} + 1} \tag{2.20}$$

$$\frac{\mathrm{Tr}(n_\alpha n_\gamma\, e^{-\beta H_0})}{\mathrm{Tr}\, e^{-\beta H_0}} = \frac{\delta_{\alpha\gamma}\, e^{\beta E_\alpha}}{(e^{\beta E_\alpha} + 1)^2} + \frac{1}{(e^{\beta E_\alpha} + 1)(e^{\beta E_\alpha} + 1)} \quad . \tag{2.21}$$

Substituting back into (2.19):

$$\ln Z_1 = -\beta\, U + \sum_\alpha \ln(1 + e^{-\beta E_\alpha}) - \frac{\beta}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} \frac{1}{(e^{\beta E_\alpha} + 1)(e^{\beta E_\alpha} + 1)}$$

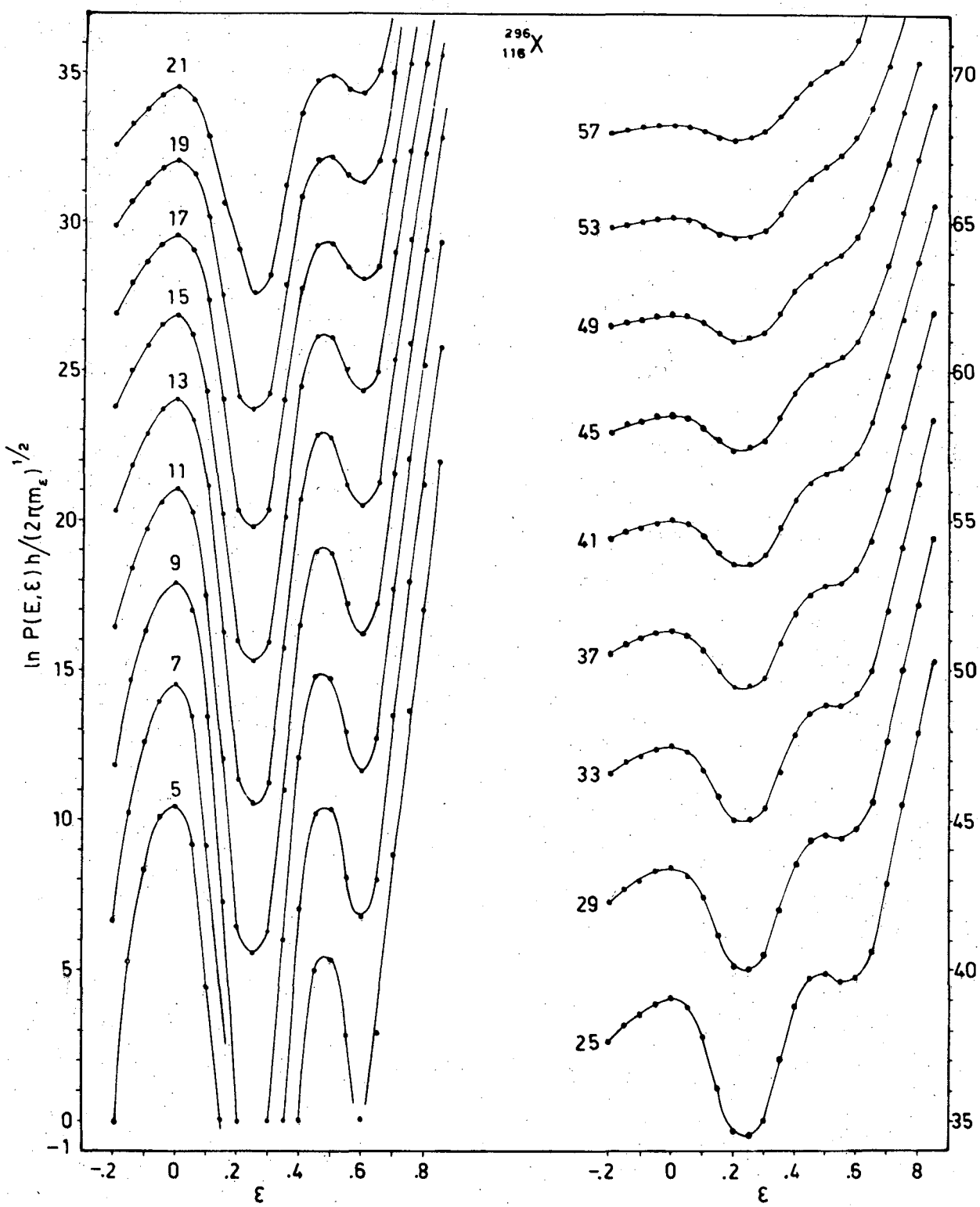
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Fig. 15

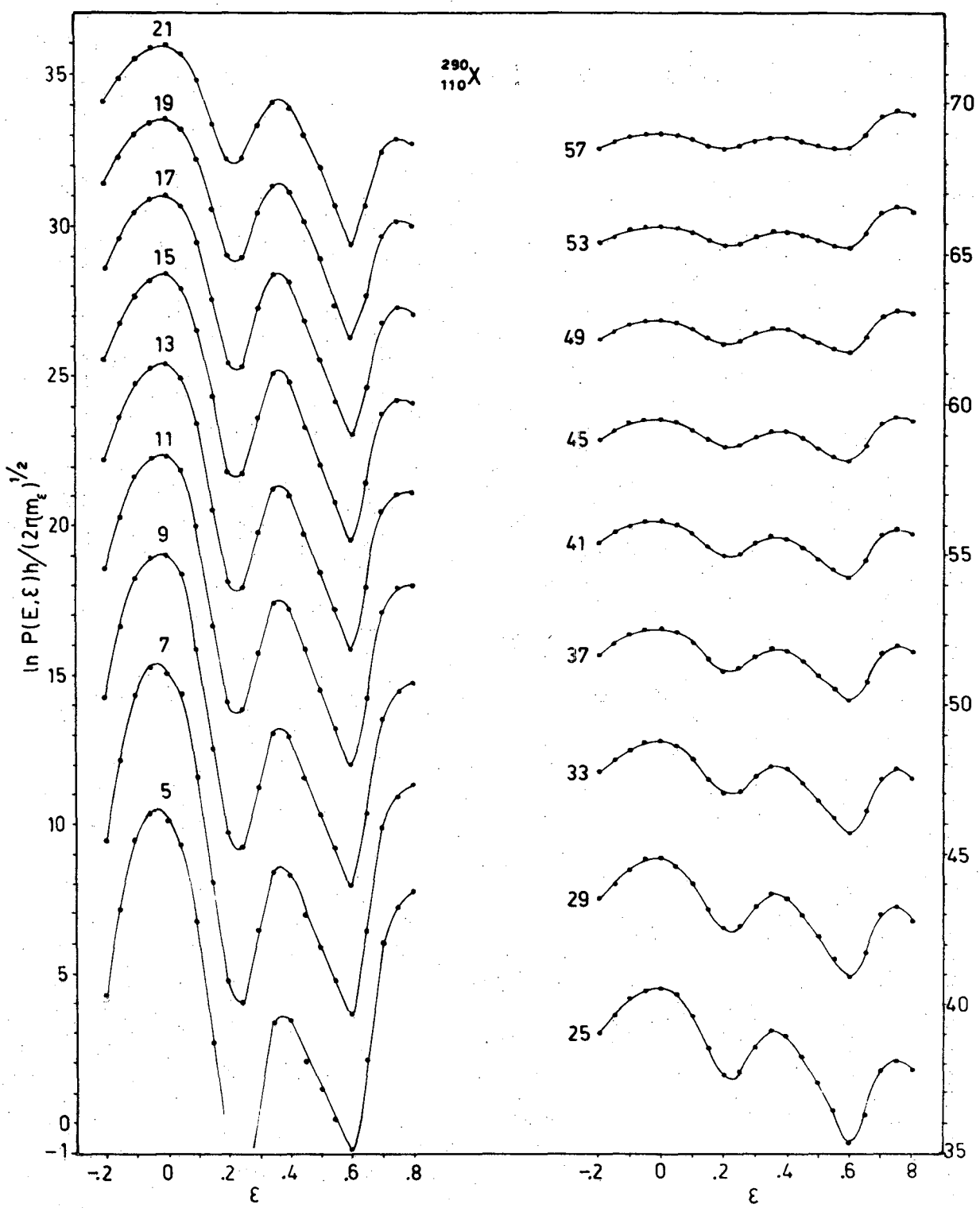
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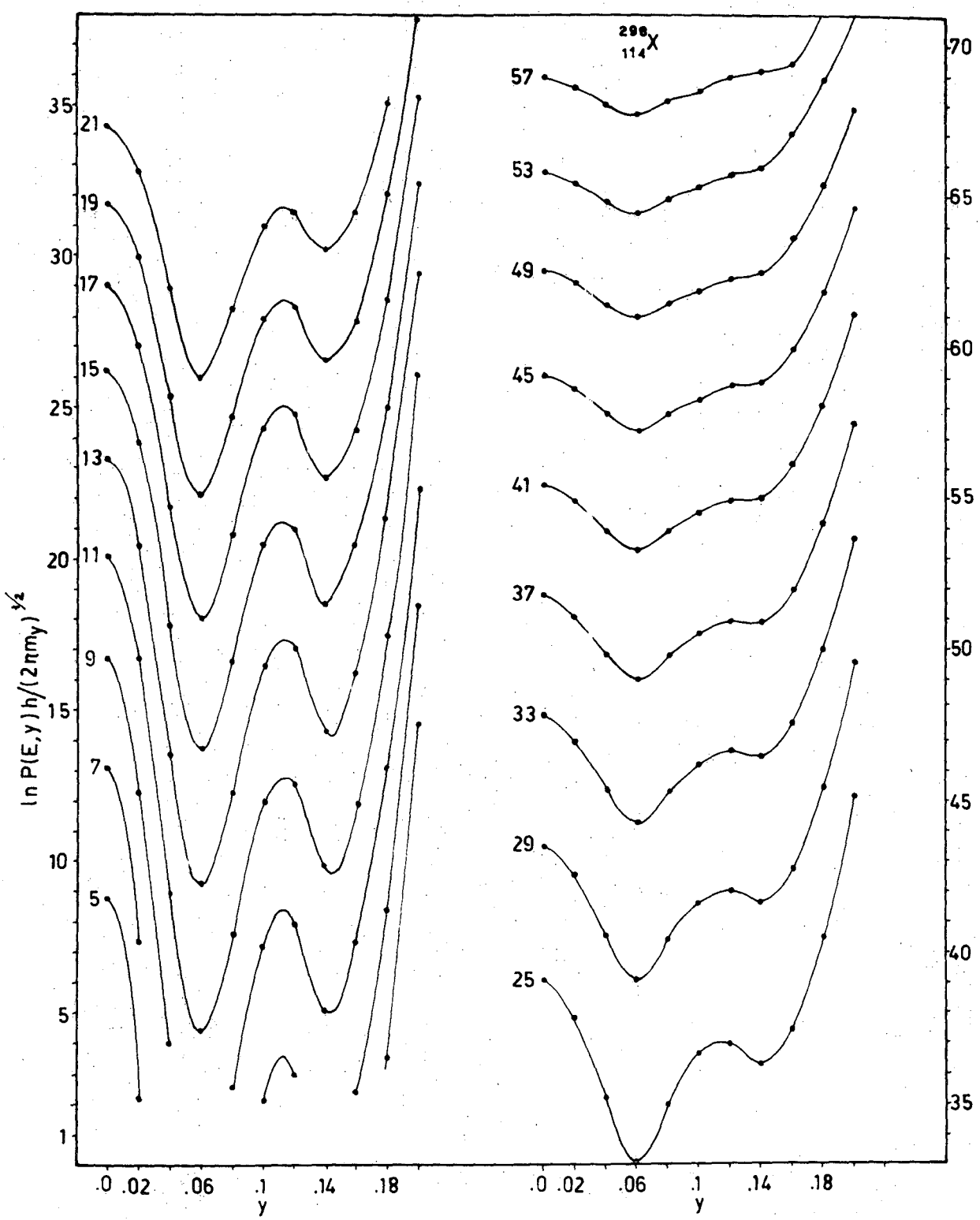
Fig. 14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35 40 45 50 55 60 65 70
5 7 9 11 13 15 17 19 21
25 29 33 37 41 45 49 53 57

Fig. 12

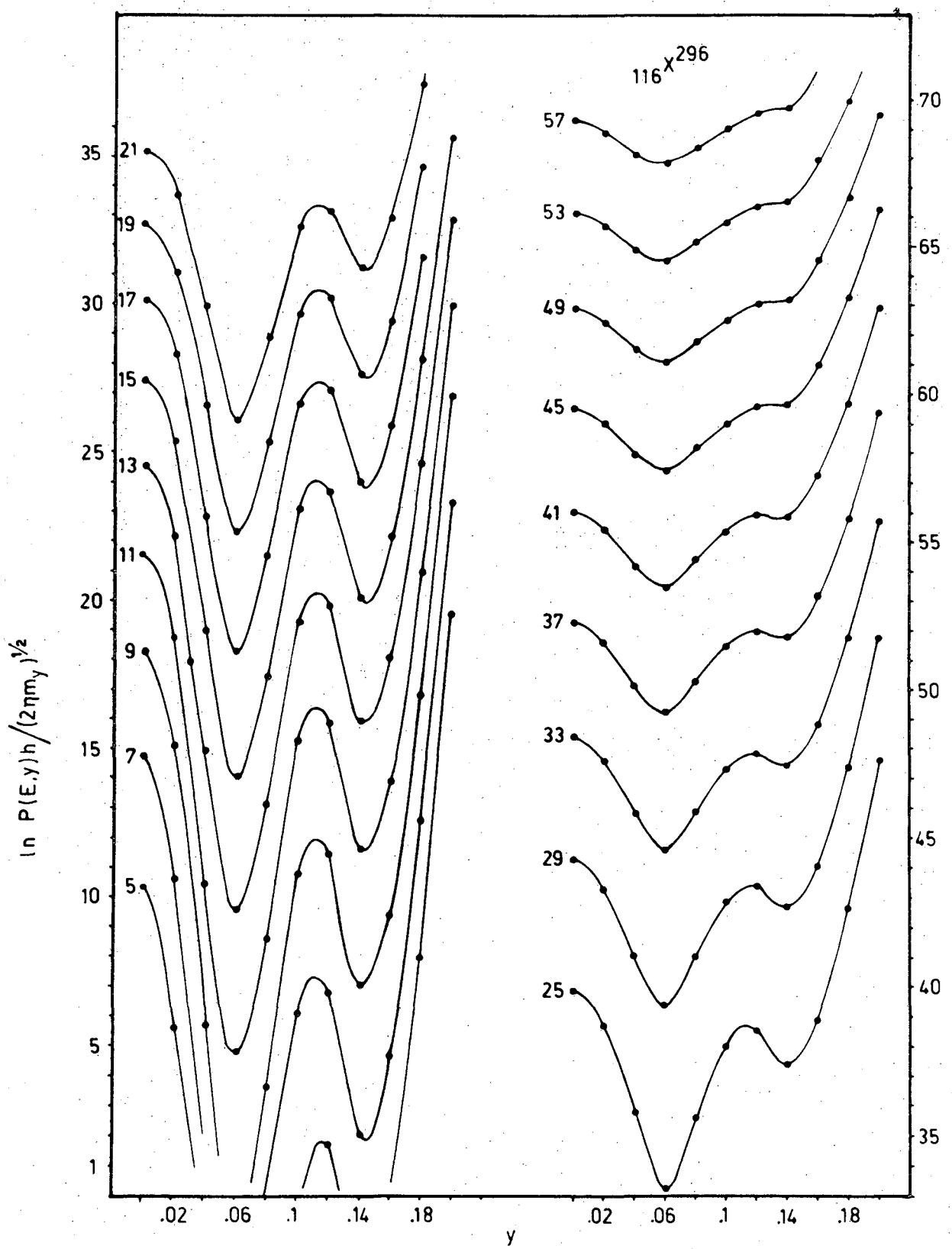
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Fig. 13

$$+ \beta \sum_{\alpha\gamma} W_{\alpha\gamma} \frac{f_\gamma}{e^{\beta E_\alpha} + 1} \quad . \tag{2.22}$$

The term

$$- \frac{\beta}{2} \sum W_{\alpha\gamma} \delta_{\alpha\gamma} \frac{e^{\beta E_\alpha}}{(e^{\beta E_\alpha} + 1)^2}$$

was dropped from the above equation, since it is of order A^{-1}.

$\ell n\ Z_1$ contains 2 sets of adjustable parameters. U, W_α, $W_{\alpha\gamma}$ depend on the choice of representation. They are functions of a set of independent parameters, say ϕ_α. The f_α form of a second set. Applying the variational principle means maximizing $\ell n\ Z_1$. Therefore we have

$$\frac{\partial \ell n\ Z_1}{\partial f_\delta} = \frac{\partial \ell n\ Z_1}{\partial \phi_\delta} = 0 \quad . \tag{2.23}$$

The first condition yields

$$0 = \sum_{\alpha\gamma} W_{\alpha\gamma} W_{\alpha\delta} \frac{e^{\beta E_\alpha}}{(e^{\beta E_\alpha} + 1)^2} \left(\frac{1}{e^{\beta E_\gamma} + 1} - f_\gamma \right) \quad ,$$

which requires that

$$f_\gamma = \frac{1}{e^{\beta E_\gamma} + 1} \quad . \tag{2.24}$$

With the help of (2.24) the second condition gives

$$0 = \frac{\partial U}{\partial \phi_\delta} + \sum_\alpha \frac{\partial W_\alpha}{\partial \phi_\delta} f_\alpha + \frac{1}{2} \sum_{\alpha\gamma} \frac{\partial W_{\alpha\gamma}}{\partial \phi_\delta} f_\alpha f_\gamma \quad . \tag{2.25}$$

(2.25) is equivalent to

$$0 = \frac{\partial \overline{H}}{\partial \phi_\delta} \quad , \tag{2.26}$$

in which

$$\overline{H} = U + \sum_\alpha W_\alpha f_\alpha + \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} f_\alpha f_\gamma \quad . \tag{2.27}$$

$\overline{H}$ is a "thermal average" of the Hamiltonian. It is the same as H_d (see Eq. (2.12)) with the number operators n_α replaced by their "thermal averages" f_α.

Substituting (2.24) into (2.22), $\ln Z_1$ can be rewritten as

$$\ln Z_1 = -\beta U + \sum_\alpha \ln (1 + e^{-\beta E_\alpha}) + \frac{\beta}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} \frac{1}{(e^{\beta E_\alpha} + 1)(e^{\beta E_\alpha} + 1)} , \tag{2.28}$$

or

$$\ln Z_1 = -\beta U - \sum_\alpha \ln (1 - f_\alpha) + \frac{\beta}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} f_\alpha f_\gamma \quad . \tag{2.29}$$

To summarize the variational principle:

a) express the diagonal part of the Hamiltonian in the chosen representation as

$$H_d = U + \sum_{\alpha} W_{\alpha} n_{\alpha} + \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} n_{\alpha} n_{\gamma} \quad ,$$

b) vary the parameters in the choice of representation by minimizing

$$\overline{H} = U + \sum_{\alpha} W_{\alpha} f_{\alpha} + \frac{1}{2} \sum_{\alpha\gamma} W_{\alpha\gamma} f_{\alpha} f_{\gamma} \quad ,$$

keeping the f's constant;

c) the approximate value of the grand partition function is given by Eq. (2.28) or (2.29), where

$$f_{\alpha} = \frac{1}{e^{\beta E_{\alpha}} + 1}$$

$$E_{\alpha} = W_{\alpha} + \sum_{\gamma} W_{\alpha\gamma} f_{\gamma} \quad .$$

The following section gives an application of this variational principle.

III. SPECIAL BOGOLIUBOV TRANSFORMATION

Most recent work on level densities[3-6] has used a simple pairing model in which all pairing matrix elements are equal and all others are zero. The quasiparticle operators a_α^+, a_α are connected to the single-particle operators c_α^+, c_α by the special Bogoliubov transformation

$$a_\alpha^+ = u_\alpha c_\alpha^+ - v_\alpha c_{\bar{\alpha}}$$

$$a_\alpha = u_\alpha c_\alpha - v_\alpha c_{\bar{\alpha}}^+ \quad . \tag{3.1}$$

u_α and v_α are real numbers. The notation $\bar{\alpha}$ refers to the time-reversed state of α.

In this section the variational principle previously derived will be applied to the case of the special Bogoliubov transformation.

It can be assumed that the interaction is time-reversal invariant and therefore, with a proper choice of phases, the matrix elements are real. Bearing in mind Eq. (2.6) this means that

$$V_{\gamma\delta\alpha\beta} = V_{\alpha\beta\gamma\delta}$$

$$V_{\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}} = V_{\alpha\beta\gamma\delta} \quad . \tag{3.2}$$

The a_α^+, a_α satisfy the usual anticommutation rules

$$[a_\alpha^+, a_\beta^+]_+ = [a_\alpha, a_\beta]_+ = 0$$

$$[a_\alpha^+, a_\beta]_+ = \delta_{\alpha\beta} \quad , \tag{3.3}$$

if

$$u_{\bar{\alpha}} = u_\alpha$$

$$v_{\bar{\alpha}} = -v_\alpha \tag{3.4}$$

The inverse transformation is

$$c_\alpha^+ = u_\alpha\, a_\alpha^+ + v_\alpha\, a_{\bar{\alpha}}$$

$$c_\alpha = u_\alpha\, a_\alpha + v_\alpha\, a_{\bar{\alpha}}^+ \quad . \tag{3.5}$$

To apply the variational principle we must first obtain the diagonal terms of the Hamiltonian in the quasi-particle representation. This requires the evaluation of contractions of pairs of c^+, c operators and of diagonal terms of normal products of c^+, c operators. The contractions of c^+, c operators are

$$\langle c_\alpha^+ c_\beta^+ \rangle = -\langle c_\alpha c_\beta \rangle = \delta_{\alpha\bar{\beta}}\, u_\alpha v_\alpha$$

$$\langle c_\alpha^+ c_\beta \rangle = \delta_{\alpha\beta}\, v_\alpha^2 \quad . \tag{3.6}$$

The fully-contracted term of the transformed Hamiltonian follows from Eq. (2.9) and (3.6):

$$U = \sum_\alpha T_{\alpha\alpha}\, v_\alpha^2 + \frac{1}{2} \sum_{\alpha\gamma} V_{\alpha\gamma\alpha\gamma}\, v_\alpha^2\, v_\alpha^2 + \frac{1}{4} \sum_{\alpha\gamma} V_{\alpha\bar{\alpha}\gamma\bar{\gamma}}\, u_\alpha v_\alpha\, u_\gamma v_\gamma \quad . \tag{3.7}$$

The other terms of the transformed Hamiltonian, Eq. (2.10) and (2.11), require the evaluation of the diagonal terms of some normal products of c^+, c operators. After some algebra these emerge as

$$: c_\alpha^+ c_\beta^+ :_d = - : c_\alpha c_\beta :_d = - \delta_{\alpha\bar\beta} u_\alpha v_\alpha [a_\alpha^+ a_\alpha + a_{\bar\alpha}^+ a_{\bar\alpha}]$$

$$: c_\alpha^+ c_\beta :_d = \delta_{\alpha\beta} [u_\alpha^2 a_\alpha^+ a_\alpha - v_\alpha^2 a_{\bar\alpha}^+ a_{\bar\alpha}] \quad , \tag{3.8}$$

and

$$: c_\alpha^+ c_\beta^+ c_\delta c_\gamma :_d$$

$$= (\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})(u_\alpha^2 u_\beta^2 a_\alpha^+ a_\beta^+ a_\beta a_\alpha + v_\alpha^2 v_\beta^2 a_{\bar\alpha}^+ a_{\bar\beta}^+ a_{\bar\beta} a_{\bar\alpha}$$

$$- v_\alpha^2 u_\beta^2 a_{\bar\alpha}^+ a_\beta^+ a_\beta a_{\bar\alpha} - u_\alpha^2 v_\beta^2 a_\alpha^+ a_{\bar\beta}^+ a_{\bar\beta} a_\alpha) + \delta_{\alpha\bar\beta}\delta_{\gamma\bar\delta} u_\alpha v_\alpha u_\gamma v_\gamma (a_\alpha^+ a_\gamma^+ a_\gamma a_\alpha + a_\alpha^+ a_{\bar\gamma}^+ a_{\bar\gamma} a_\alpha$$

$$+ a_{\bar\alpha}^+ a_\gamma^+ a_\gamma a_{\bar\alpha} + a_{\bar\alpha}^+ a_\gamma^+ a_{\bar\gamma} a_\alpha) \quad . \tag{3.9}$$

Substituting (3.6), (3.8), and (3.9) into (2.10) and (2.11) gives the diagonal terms of H_2 and H_4, namely H_{2d} and H_{4d}:

$$H_{2d} = \sum_\alpha n_\alpha \left\{ u_\alpha^2 (T_{\alpha\alpha} + \sum_\gamma V_{\alpha\gamma\alpha\gamma} v_\gamma^2) - v_\alpha^2 (T_{\bar\alpha\bar\alpha} + \sum_\alpha V_{\bar\alpha\gamma\bar\alpha\gamma} v_\gamma^2) \right\}$$

$$- \sum_\alpha n_\alpha u_\alpha v_\alpha \sum_\gamma u_\gamma v_\gamma V_{\alpha\bar\alpha\gamma\bar\gamma} \quad , \tag{3.10}$$

$$H_{4d} = \frac{1}{2} \sum_{\alpha\gamma} n_\alpha n_\gamma \left\{ (u_\alpha^2 u_\gamma^2 + v_\alpha^2 v_\gamma^2) V_{\alpha\gamma\alpha\gamma} - (u_\alpha^2 v_\gamma^2 + v_\alpha^2 u_\gamma^2) V_{\alpha\bar\gamma\alpha\bar\gamma} \right\}$$

$$+ \sum_{\alpha\gamma} n_\alpha n_\gamma u_\alpha v_\alpha u_\gamma v_\gamma V_{\alpha\bar\alpha\gamma\bar\gamma} \quad . \tag{3.11}$$

The n_α are number operators for quasiparticles:

$$n_\alpha = a_\alpha^+ a_\alpha \quad .$$

$\overline{H}$ is obtained by replacing the n_α operators in $H_d = U + H_{2d} + H_{4d}$ by the parameters f_α. After some manipulation

$$\overline{H} = \sum_\alpha f_\alpha T_{\alpha\alpha} + \frac{1}{2} \sum_{\alpha\gamma} f_\alpha f_\gamma V_{\alpha\gamma\alpha\gamma} + \sum_\alpha T_{\alpha\alpha} v_\alpha^2 (1 - f_\alpha - f_{\bar{\alpha}})$$

$$+ \frac{1}{2} \sum_{\alpha\gamma} V_{\alpha\gamma\alpha\gamma} v_\alpha^2 v_\gamma^2 (1 - f_\alpha - f_{\bar{\alpha}})(1 - f_\gamma - f_{\bar{\gamma}})$$

$$+ \sum_{\alpha\gamma} f_\alpha V_{\alpha\gamma\alpha\gamma} v_\alpha^2 (1 - f_\gamma - f_{\bar{\gamma}})$$

$$+ \frac{1}{4} \sum_{\alpha\gamma} V_{\alpha\bar{\alpha}\gamma\bar{\gamma}} u_\alpha v_\alpha u_\gamma v_\gamma (1 - f_\alpha - f_{\bar{\alpha}})(1 - f_\gamma - f_{\bar{\gamma}}) \quad . \tag{3.12}$$

Putting

$$\overline{u}_\alpha \equiv u_\alpha (1 - f_\alpha - f_{\bar{\alpha}})^{1/2}$$

$$\overline{v}_\alpha \equiv v_\alpha (1 - f_\alpha - f_{\bar{\alpha}})^{1/2} \quad ,$$

gives a relatively simple form for $\overline{H}$:

$$\overline{H} = \sum_\alpha f_\alpha T_{\alpha\alpha} + \frac{1}{2} \sum_{\alpha\gamma} f_\alpha f_\gamma V_{\alpha\gamma\alpha\gamma} + \sum_{\alpha\gamma} f_\alpha V_{\alpha\gamma\alpha\gamma} \overline{v}_\gamma^2 + \sum_\alpha T_{\alpha\alpha} \overline{v}_\alpha^2$$

$$+ \frac{1}{2} \sum_{\alpha\gamma} V_{\alpha\gamma\alpha\gamma} \bar{v}_\alpha^2 \bar{v}_\alpha^2 + \frac{1}{4} \sum_{\alpha\gamma} V_{\alpha\bar{\alpha}\gamma\bar{\gamma}} \bar{u}_\alpha \bar{v}_\alpha \bar{u}_\gamma \bar{v}_\gamma \quad . \tag{3.13}$$

Application of the variational principle consists in minimizing $\bar{H}$ with respect to a set of independent transformation parameters, keeping the f_α constant. The $\bar{v}_\alpha$ can be taken as the independent parameters. Since

$$\bar{u}_\alpha^2 + \bar{v}_\alpha^2 = 1 - f_\alpha - f_{\bar{\alpha}} \quad ,$$

we have

$$\frac{\partial \bar{u}_\alpha}{\partial \bar{v}_\alpha} = - \frac{\bar{v}_\alpha}{\bar{u}_\alpha} \quad .$$

Bearing in mind Eq. (3.4), the requirement

$$\frac{\partial \bar{H}}{\partial \bar{v}_\alpha} = 0 \quad ,$$

leads to

$$0 = 2\bar{u}_\alpha \bar{v}_\alpha [T_{\alpha\alpha} + \sum_\gamma V_{\alpha\gamma\alpha\gamma}(\bar{v}_\gamma^2 + f_\gamma) + T_{\bar{\alpha}\bar{\alpha}} + \sum_\gamma V_{\bar{\alpha}\gamma\bar{\alpha}\gamma}(\bar{v}_\gamma^2 + f_\gamma)]$$

$$+ (\bar{u}_\alpha^2 - \bar{v}_\alpha^2) \sum_\gamma V_{\alpha\bar{\alpha}\gamma\bar{\gamma}} \bar{u}_\gamma \bar{u}_\gamma \quad . \tag{3.14}$$

With the definitions

$$H_\alpha = T_{\alpha\alpha} + \sum_\gamma V_{\alpha\gamma\alpha\gamma}(\bar{v}_\gamma^2 + f_\gamma) = T_{\alpha\alpha} + \sum_\gamma V_{\alpha\gamma\alpha\gamma}[f_\gamma + v_\gamma^2(1 - f_\gamma - f_{\bar{\gamma}})] \tag{3.15}$$

$$\Delta_\alpha = \frac{1}{2} \sum_\gamma V_{\alpha\bar{\alpha}\gamma\bar{\gamma}}\, \bar{u}_\gamma \bar{v}_\gamma = \frac{1}{2} \sum_\gamma V_{\alpha\bar{\alpha}\gamma\bar{\gamma}}\, u_\gamma v_\gamma (1 - f_\gamma - f_{\bar{\gamma}}) \quad , \tag{3.16}$$

(3.14) gives

$$0 = \bar{u}_\alpha \bar{v}_\alpha (H_\alpha + H_{\bar{\alpha}}) + (\bar{u}_\alpha^2 - \bar{v}_\alpha^2)\, \Delta_\alpha \quad . \tag{3.17}$$

This equation is formally the same as the usual BCS equation for u and v. In fact, multiplying (3.17) by $(1 - f_\alpha - f_{\bar{\alpha}})$ gives

$$0 = u_\alpha v_\alpha (H_\alpha + H_{\bar{\alpha}}) + (u_\alpha^2 - v_\alpha^2)\, \Delta_\alpha \quad ,$$

and thus

$$v_\alpha^2 = \frac{1}{2} \left(1 - \frac{\varepsilon_\alpha}{\sqrt{\varepsilon_\alpha^2 + \Delta_\alpha^2}} \right)$$

$$u_\alpha^2 = \frac{1}{2} \left(1 + \frac{\varepsilon_\alpha}{\sqrt{\varepsilon_\alpha^2 + \Delta_\alpha^2}} \right) \quad , \tag{3.18}$$

where

$$\varepsilon_\alpha = \frac{1}{2} (H_\alpha + H_{\bar{\alpha}}) \quad . \tag{3.19}$$

Substituting (3.18) back into (3.16) gives the "generalized gap equation"

$$\Delta_\alpha = \frac{1}{4} \sum_\gamma V_{\alpha\bar{\alpha}\gamma\bar{\gamma}}\, (1 - f_\gamma - f_{\bar{\gamma}}) \frac{|\Delta_\gamma|}{\sqrt{\varepsilon_\gamma^2 + \Delta_\gamma^2}} \quad . \tag{3.20}$$

In the simple pairing theory, all the nonpairing matrix elements are zero and all the pairing matrix elements are equal, within a phase factor. In other words

$$|V_{\alpha\beta\gamma\delta}| = G\ \delta_{\bar{\alpha}\beta}\ \delta_{\bar{\gamma}\delta} \quad . \tag{3.21}$$

In this simple theory H_α is usually set equal to $T_{\alpha\alpha}$. The other terms in Eq. (3.15) are taken to represent a self-energy term which is effectively included in $T_{\alpha\alpha}$. Equation (3.16) gives

$$|\Delta_\alpha| = \frac{1}{2} \sum_\gamma G|u_\gamma v_\gamma|\ (1 - f_\gamma - f_{\bar{\gamma}}) \quad , \tag{3.22}$$

and thus $|\Delta_\alpha|$ is independent of the state α in the simple pairing theory. So there is just one "gap equation"

$$\frac{4}{G} = \sum_\gamma (1 - f_\gamma - f_{\bar{\gamma}})\ \frac{1}{\sqrt{\varepsilon_\gamma^2 + \Delta^2}} \quad . \tag{3.23}$$

The general equations differ in the details from the equations of the simple pairing theory. The "single particle energy" ε_α includes self-consistent energy terms. In the simple pairing theory, the ε_α are taken to be constant; the general theory allows for temperature dependence of the self-consistent field.

In general, the pairing matrix elements of the form $V_{\alpha\bar{\alpha}\alpha\bar{\alpha}}$ are larger than those of form $V_{\alpha\bar{\alpha}\gamma\bar{\gamma}}$, $\gamma \neq \alpha$. This will make the temperature dependence of Δ_α qualitatively different from that of Δ in the simple pairing theory.

The theory presented here is not the most general one. With the special Bogoliubov transformation, Eq. (3.1), we have put constraints on what we allow to happen as the temperature is varied. In effect we are saying that the only thing that changes is the pairing (i.e. the admixture of a state with the corresponding time-reversed state in a given quasiparticle state).

In order to allow for mixing of single-particle states with each other, the transformation to use is the general Bogoliubov transformation:

$$a_\alpha^+ = \sum_\mu (A_{\alpha\mu}\, c_\mu^+ + B_{\alpha\mu}\, c_\mu) \quad .$$

The application of the variational principle for the grand partition function to the case of the general Bogoliubov transformation is currently being worked on, and will be the object of a future paper.

APPENDIX A

The Convexity Theorem

A function is convex in a given interval if its second derivative is always of the same sign in that interval. The sign of the second derivative can be chosen as positive (by multiplying by -1 if necessary).

We can easily prove the convexity theorem:

If $\frac{d^2f}{dx^2} > 0$ in a given interval, x_α are a set of points in that interval, w_α are a set of weights such that

$$w_\alpha \geqslant 0$$

and

$$\sum_\alpha w_\alpha = 1 \quad , \tag{A1}$$

then

$$\sum_\alpha w_\alpha \, f(x_\alpha) \quad \geqslant \quad f\left(\sum_\alpha w_\alpha \, x_\alpha \right) \quad . \tag{A2}$$

Proof: Define $\bar{x} \equiv \sum_\alpha w_\alpha \, x_\alpha$. (A3)

Taylor's expansion gives

$$f(x_\alpha) = f(\bar{x}) + (x_\alpha - \bar{x}) \, f'(\bar{x}) + \frac{1}{2}(x_\alpha - \bar{x})^2 \, f''(\xi_\alpha)$$

where

$$|\xi_\alpha| < |x_\alpha - \bar{x}| \quad .$$

Multiply the above equation by w_α and sum over α:

$$\sum_\alpha w_\alpha f(x_\alpha) = f(\bar{x})\sum_\alpha w_\alpha + f'(\bar{x})\sum_\alpha w_\alpha(x_\alpha - \bar{x})$$

$$+ \frac{1}{2}\sum_\alpha w_\alpha(x_\alpha - \bar{x})^2 f''(\xi_\alpha) \quad .$$

The second term on the right-hand side vanishes because of (A1) and (A3). So

$$\sum_\alpha w_\alpha f(x_\alpha) = f(\bar{x}) + \frac{1}{2}\sum_\alpha w_\alpha (x_\alpha - \bar{x})^2 f''(\xi_\alpha) \quad .$$

Since $f''(\xi_\alpha)$ is positive

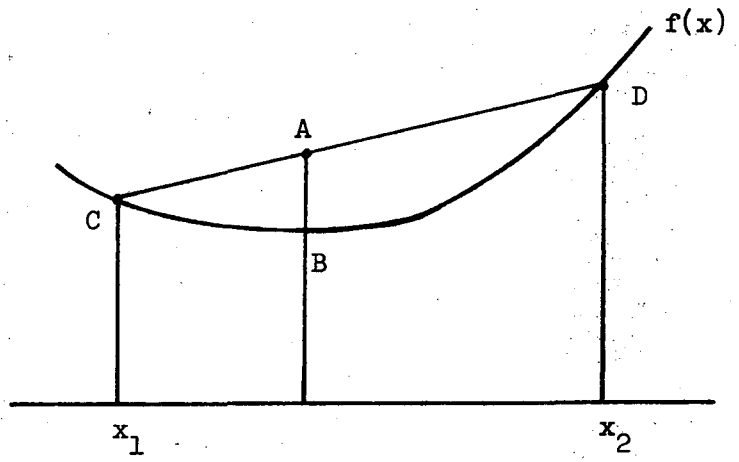
$$\sum_\alpha w_\alpha f(x_\alpha) \geqslant f(\bar{x}) = f\left(\sum_\alpha w_\alpha x_\alpha\right) \qquad \text{QED} \quad .$$

We get equality only if $x_\alpha = \bar{x}$.

The convexity theorem has a simple geometric interpretation in the case of 2 points, x_1 and x_2 let $w_1 = 1 - w_2 = w$. From (A2)

$$w\, f(x_1) + (1 - w)\, f(x_2) \geqslant f[wx_1 + (1 - w)x_2] \quad .$$

This means that for a function with a positive second derivative any point A on the chord CD is above the point B on the curve with the same abscissa.



APPENDIX B

Peierls' Theorem

The convexity theorem can be used to prove some theorems about diagonal matrix elements, including Peierls' theorem.

We begin with the following theorem:

Given an operator X and an arbitrary set of orthonormal states $|k\rangle$, then for any function f(x) with a positive second derivative, then

$$\langle k|f(X)|k\rangle \geqslant f(\langle k|X|k\rangle) \quad . \tag{B1}$$

Proof: Let x_α be the eigenvalues of X, and $|\alpha\rangle$ its eigenstates. There is a unitary transformation connecting the states $|\alpha\rangle$ with the states $|k\rangle$, with coefficients $\langle k|\alpha\rangle$ such that

$$\sum_\alpha |\langle k|\alpha\rangle|^2 = 1 \quad .$$

We can apply the convexity theorem (A2) with $w_\alpha = |\langle k|\alpha\rangle|^2$:

$$\sum_\alpha |\langle k|\alpha\rangle|^2 f(x_\alpha) \geqslant f\left(\sum_\alpha |\langle k|\alpha\rangle|^2 x_\alpha\right) \quad . \tag{B2}$$

The left-hand side of (B2) equals

$$\sum_\alpha \langle k|\alpha\rangle\langle\alpha|f(X)|\alpha\rangle\langle\alpha|k\rangle = \langle k|f(X)|k\rangle \quad .$$

Similarly the right hand side of (B2) is $f(\langle k|X|k\rangle)$. This immediately yields (B1).

If we sum (B1) over all states $|k\rangle$ we get an inequality involving the trace of $f(X)$:

$$\mathrm{Tr}\, f(X) \geqslant \sum_k f(\langle k|X|k\rangle) \quad . \tag{B3}$$

In the particular case where $f(x) = e^{-\beta x}$ and the operator X is the Hamiltonian we get Peierls' theorem:[7]

$$\mathrm{Tr}\, e^{-\beta H} \geqslant \sum_k e^{-\beta \langle k|H|k\rangle} \quad . \tag{B4}$$

APPENDIX C

The Bogoliubov Inequality

The Bogoliubov inequality follows from the convexity theorem and Peierls' theorem.

If we decompose the Hamiltonian H into the sum $H_0 + H_1$ the Bogoliubov inequality gives a lower bound for the partition function:

$$\ln \mathrm{Tr}\, e^{-\beta(H_0 + H_1)} \geqslant \ln \mathrm{Tr}\, e^{-\beta H_0} - \beta \frac{\mathrm{Tr}(H_1 e^{-\beta H_0})}{\mathrm{Tr}\, e^{-\beta H_0}} \quad . \tag{C1}$$

Proof: Let ε_α be the eigenvalues of H_0 and $|\alpha\rangle$ its eigenstates. From Peierls' theorem:

$$\mathrm{Tr}\, e^{-\beta(H_0 + H_1)} \geqslant \sum_\alpha \exp - \beta \langle \alpha | H_0 + H_1 | \alpha \rangle \quad ,$$

or

$$\mathrm{Tr}\, e^{-\beta(H_0 + H_1)} \geqslant \sum_\alpha \exp - \beta [\varepsilon_\alpha + \langle \alpha | H_1 | \alpha \rangle] \quad , \tag{C2}$$

let us apply the convexity theorem with

$$f(x) = e^{-\beta x}$$

$$x_\alpha = \langle \alpha | H_1 | \alpha \rangle$$

$$w_\alpha = e^{-\beta\varepsilon_\alpha} / \sum_\alpha e^{-\beta\varepsilon_\alpha}$$

$$= e^{-\beta\varepsilon_\alpha} / \operatorname{Tr} e^{-\beta H_0} \quad .$$

(A2) gives

$$\sum_\alpha \frac{e^{-\beta\varepsilon_\alpha}}{\operatorname{Tr} e^{-\beta H_0}} e^{-\beta \langle \alpha | H_1 | \alpha \rangle} \geqslant \exp\left[-\beta \sum_\alpha \frac{e^{-\beta\varepsilon_\alpha}}{\operatorname{Tr} e^{-\beta H_0}} \langle \alpha | H_1 | \alpha \rangle\right] \quad . \qquad \text{(C3)}$$

But

$$\sum_\alpha e^{-\beta\varepsilon_\alpha} \langle \alpha | H_1 | \alpha \rangle = \operatorname{Tr}(H_1 e^{-\beta H_0}) \quad . \qquad \text{(C4)}$$

(C2), (C3), and (C4) combine to give

$$\operatorname{Tr} e^{-\beta(H_0 + H_1)} \geqslant \operatorname{Tr} e^{-\beta H_0} \exp\left[-\beta \frac{\operatorname{Tr}(H_1 e^{-\beta H_0})}{\operatorname{Tr} e^{-\beta H_0}}\right] \text{ QED} .$$

FOOTNOTES AND REFERENCES

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