

# Many- Body Methods at Finite Temperature

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# **I NUCLEAR PARTITION FUNCTIONS**

### 1 Introduction

Tools to deal with many- body systems at finite temperature were developped long ago. As early as 1932 R. E. Peierls [1] established the general framework of thermodynamic perturbation theory for quantum systems. In 1955 T. Matsubara [2] worked out the details of thermal perturbation theory for many body systems (see also [3]). Several textbooks in the field have by now been available for some time. Among these we wish to mention those of Baym and Kadanoff [4], Abrikosov, Gorkov and Dzyaloshinsky [5], Thouless [6], Fetter and Walecka [7]. More recent reviews including a presentation of functional methods [8] can be found in the monographs by Negele and Orland [9] and Blaizot and Ripka [10]. It is also worthwhile mentionning some of the classic articles in the field such as the elegant construction given by M. Gaudin in 1960 [11] of Wick's theorem at finite temperatures, which exploits the algebra of exponentials of quadratic forms in the field operators. As a second example we mention the exhaustive discussion of the mean field approximation (including small amplitude collective motion in hot Fermi systems) given by des Cloizeaux in his 1967 les Houches lectures [12] using the framework of the variational principle.

The motivation for the present lectures arises from the renewed interest in finite temperature many body methods which has appeared recently in several different domains of nuclear and particle physics. These include in particular the physics of hot nuclei, which is the main purpose of these lectures, but also the restauration of broken symmetries in the standard model [13, 14, 15] or the physics of the quark gluon plasma [16, 17, 18, 19, 20]. These methods are also important for the description of type- II supernovae or the discussion of meson properties in hot dense matter.

The possibility of producing thermalized hot nuclei with temperatures of the order of several MeV's (1MeV  $\simeq 10^{10}$  K) has been demonstrated in the early eighties by performing collisions of two nuclei at intermediate energies. The first experiments where carried with a 720 MeV carbon beam at CERN [21] and a 44 MeV per nucleon Argon beam at GANIL [22]. For a review of recent developments in this field the reader is referred to the lectures presented at the 1992 Predeal School by B. Tamain[23]. It is worthwhile emphasizing that temperatures of about 5 MeV are precisely those which are reached during the collapse of massive stars which are believed to lead to type II supernovae explosions. The measurement of thermal properties of nuclei in this temperature range is thus of significance for an accurate description of the collapse of massive stars. Among such properties is the specific heat and level density parameter of hot nuclei. Their values indeed determine how much energy and entropy can be stored in nuclear

excited states. It is also important to have good estimates of the limiting temperature beyond which nucleons will no longer be bound into nuclei. Beyond this temperature one indeed expects a sharp increase in the interior pressure of the star due to the sudden appearance of the contribution of nucleons.

Another reason for the renewed interest in hot many body methods was the observation by the Berkeley group in the early eighties of the persistance of giant collective oscillations in hot nuclei up to temperatures of the order of several MeV's [24]. The possibility of giant collective oscillations built on nuclear excited states was anticipated in 1955 by D. M. Brink in his thesis work [25]. Shortly after the discovery of giant resonances in hot nuclei several theoretical studies using linear response theory at finite temperature were performed [26, 27, 28, 29]. Several applications of this approach were investigated at the same time. For instance the long standing question of the contribution of collective modes to nuclear partition functions [30, 31] was reexamined.

The purpose of the present lectures is to review the approximation methods relevant to describe many -fermion systems at finite temperature. In the next section we review the grand canonical formalism for independent fermions and discuss its applicability to the case of finite nuclei for which fluctuations arising from the small number of particles involved are expected to be sizeable. In section 3 we present a derivation of the mean field equations based on the variational method. In the second part we discuss perturbation expansions of partition functions. We consider a particularly important subseries containing the so called ring diagrams whose summation leads to the random phase approximation (RPA). In the third part an application to the physics of giant resonances in hot nuclei is described.

### **2** Partition functions in astrophysics

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hot clear The basic tool for calculating thermodynamic properties of atomic nuclei is the familiar grand canonical partition function

$$Z(\alpha,\beta) = \text{Trace } \exp(\alpha \hat{N} - \beta \hat{H}), \qquad (2.1)$$

where the Trace is taken over the entire Fock space i.e. runs over all possible quantum states of all possible nuclei. Denoting by  $E_n(A)$  the energy of the *n*-th excited state of the nucleus of mass number A this definition implies

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$$Z(\alpha,\beta) = \sum_{A} \sum_{n} \exp(\alpha A - \beta E_n(A)). \qquad (2.2)$$

The canonical partition function  $Z_A(\beta)$  is defined by a similar formula

$$Z_A(\beta) = \sum_n \exp(-\beta E_n(A)). \qquad (2.3)$$

Partition functions are involved in a large number of applications. As a first example they appear in the determination of chemical (or thermonuclear) equilibrium. For a reaction

$$A + B \rightarrow AB$$

the densities  $n_A = N_A/\Omega$ ,  $n_B = N_B/\Omega$ ,  $n_{AB} = N_{AB}/\Omega$  indeed satisfy Saha's equation

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$$\frac{n_{AB}}{n_A n_B} = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{-3/2} \frac{\tilde{Z}_{AB}(\beta)}{\tilde{Z}_A(\beta)\tilde{Z}_B(\beta)} e^{\beta(E_A + E_B - E_{AB})} , \qquad (2.4)$$

where  $\beta = 1/kT$  is the inverse temperature and where  $\tilde{Z}$  is the internal partition function

$$\tilde{Z}(\beta) = 1 + e^{-\beta E_1^*} + e^{-\beta E_2^*} + \dots$$
(2.5)

where  $E_n^* = E_n - E_0$  is the excitation energy of the *n*-th state of the system and *m* the reduced mass  $m_A m_B / (m_A + m_B)$ .

Nuclear partition functions are also important to determine which nuclei are present in the hot dense matter encountered e.g. in collapsing stars. Let us use a single label i to specify the neutron number N and the proton number Z of a nucleus. With this notation the density  $n_i$  of the nucleus i is given by

$$n_i = g_i \left(\frac{m_i}{2\pi\hbar^2\beta}\right)^{3/2} e^{\alpha_i - \beta E_i} \tilde{Z}_i(\beta).$$
(2.6)

In this formula  $m_i$  is the mass of the nucleus *i*,  $E_i$  its energy and  $g_i = 2J_i + 1$  its ground state degeneracy. The quantity  $\alpha_i$  is often referred to as the degeneracy parameter and is given by

$$k_T \alpha_i \simeq N \mu_n + Z \mu_p, \tag{2.7}$$

where  $\mu_n$  and  $\mu_p$  are the neutron and proton chemical potentials. These should be adjusted in order to have the desired total nucleon density and proton fractions of the medium. Actually equation 2.7 is approximate only. It neglects the interactions inside the nucleon vapor in which nuclei are immersed. This is a reasonable approximation provided the density of the vapor is not too high.

To conclude this subsection we mention that partition functions are a useful tool to construct approximate expressions for nuclear level densities. Indeed the partition function can be expressed as

$$Z(\alpha,\beta) = \int \int \rho(E,A) \exp(\alpha A - \beta E) dA dE, \qquad (2.8)$$

where  $\rho(E, A)$  is the level density. By taking the inverse Laplace transform of this expression we find

$$\rho(E,A) = \left(\frac{1}{2\pi i}\right)^2 \int \int_{-i\infty}^{+i\infty} Z(\alpha,\beta) \exp(-\alpha A + \beta E) d\alpha d\beta.$$
(2.9)

As will be shown below the use of the saddle point method for this integral leads to useful approximations to the nuclear level density.

# **3** grand canonical formalism for independent nucleons

The most convenient formalism to deal with independent fermions is the grand canonical formalism. In contrast in the microcanonical or canonical formalisms the Pauli principle is difficult to implement. A non trivial question however arises since nuclei are finite systems containing a rather small number of particles. Fluctuations are thus expected to be sizeable. For this reason we present in this section a critical review of the basic formulae in the grand canonical formalism and discuss their applicability to the case of atomic nuclei.

Let us consider independent nucleons moving in a potential V(r), described by the one body hamiltonian:

$$h = \frac{p^2}{2m} + V(r).$$
 (3.1)

In this case the grand partition function

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$$Z_0 = \operatorname{Trace} \exp(\alpha \hat{N} - \beta H_0), \qquad (3.2)$$

is easily calculable. Using  $H_0 = h(1) + h(2) + ..$  we find

$$\log Z_0 = \sum_i \log(1 + e^{\alpha - \beta \epsilon_i}). \tag{3.3}$$

In this equation the index *i* labels the single particle levels of *h* and  $\epsilon_i$  is the single particle energy defined by

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$$(\frac{p^2}{2m}+V)\varphi_i(\mathbf{r})=\epsilon_i\varphi_i(\mathbf{r}). \tag{3.4}$$

The number of particles is obtained by means of the standard formula

$$N = \frac{\partial}{\partial \alpha} \log Z_0 = \sum_i f_i, \qquad (3.5)$$

where  $f_i$  is the occupation number

$$f_i = \frac{1}{1 + \exp\{\beta(\epsilon_i - \mu)\}}.$$
(3.6)

Similarly the energy is given by

$$E = -\frac{\partial}{\partial\beta} \log Z_0 = \sum_i \epsilon_i f_i.$$
(3.7)

To evaluate the entropy we use the definition

and the construction

 $S = -\operatorname{Trace}(D_0 \log D_0). \tag{3.8}$ 

where  $D_0$  is the density matrix

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$$D_0 = Z_0^{-1} \exp(\alpha \hat{N} - \beta \hat{H}_0), \qquad (3.9)$$

This formula leads to:

$$S = (1 - \alpha \frac{\partial}{\partial \alpha} - \beta \frac{\partial}{\partial \beta}) \log Z_0(\alpha, \beta).$$
(3.10)

Using equation (3.3) this gives the familiar expression

$$S = -\sum_{i} \{f_i \log f_i + (1 - f_i) \log(1 - f_i)\}.$$
(3.11)

As an application of the above formulae let us now construct an approximate expression for the level density of a nucleus. We start from eq.(2.9) which we rewrite as

$$\rho(E,A) = \left(\frac{1}{2\pi i}\right)^2 \int \int_{-i\infty}^{+i\infty} e^{\beta E - \alpha A + \log Z(\alpha,\beta)} d\alpha d\beta.$$
(3.12)

Dominant contributions to this integral will occur from the neighborhood of the point  $(\alpha_0, \beta_0)$  where the integrand is stationary i.e.

$$A = \frac{\partial}{\partial \alpha} \log Z(\alpha_0, \beta_0), \quad E = -\frac{\partial}{\partial \beta} \log Z(\alpha_0, \beta_0). \tag{3.13}$$

Expanding the argument of the exponential to second order in  $\alpha - \alpha_0$  and  $\beta - \beta_0$  we find

$$\rho(E,A) = \frac{1}{2\pi\sqrt{D}} \exp S(\alpha_0,\beta_0), \qquad (3.14)$$

where  $S(\alpha_0, \beta_0)$  is the entropy calculated at the saddle point  $(\alpha_0, \beta_0)$  and D the determinant of the matrix of the second derivatives of log Z

$$D = \begin{vmatrix} \partial^2 \log Z / \partial \alpha^2 & \partial^2 \log Z / \partial \alpha \partial \beta \\ \partial^2 \log Z / \partial \alpha \partial \beta & \partial^2 \log Z / \partial \beta^2 \end{vmatrix} .$$
(3.15)

Actually this formula corresponds to a nucleus with an equal number of neutron and protons. For asymmetric nuclei one needs different chemical potentials for neutrons and protons [32].

Equation (3.14) is the well known formula expressing the fact the entropy is the log of the number of accessible levels. Here however we have an additional correction appearing as a preexponential factor. While in macroscopic systems this prefactor is negligible it is important to include it in the case of atomic nuclei. A comparison between the grand canonical formula (3.14) and a microcanonical enumeration of states performed by Jacquemin [33] in the case of

calcium-40 is shown in Fig.3.1. It can be seen that a good agreement is obtained for excitation energies above  $E^* = 10$  MeV.



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Figure 3.1 Level density in calcium-40 calculated in the grand canonical formalism and with an exact enumeration of states [33]. Single particle energies are taken from [32].

# 4 Variational method and mean field approximation

The variational method is based on the principle of maximum entropy. This principle states that for a given family of density matrices, the best density matrix D is that for which the entropy functional

$$S(D) = -k \operatorname{Trace}(D \log D) \tag{4.1}$$

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is maximum. This maximization has to be performed for a fixed particle number and a fixed energy. If we introduce two Lagrange multipliers to account for these constraints we find that the functional

$$-k\operatorname{Trace}(D\log D) - \beta\operatorname{Trace}(D\hat{H}) + \alpha\operatorname{Trace}(D\hat{N}), \qquad (4.2)$$

should be maximum for the optimal density matrix. It is customary in the litterature to consider the functional

$$A(D) = \operatorname{Trace}(D\hat{H}) - kTS(D) - \mu\operatorname{Trace}(D\hat{N}), \qquad (4.3)$$

where we have introduced the chemical potential  $\mu = \alpha/\beta$  and the temperature  $T = 1/k\beta$ . The previous functional is referred to as the grand potential. Minimizing the grand potential is thus equivalent to maximizing the entropy while including the adequate constraints due to

energy and particle number conservation. If this minimization is performed for the most general density matrix one obtains the usual Gibbs distribution [34]

$$D = Z^{-1} \exp(\alpha \tilde{N} - \beta \tilde{H}). \tag{4.4}$$

Unfortunately for interacting systems, expectation values with this distribution cannot in general be calculated exactly. One thus has to rely in this case on approximation methods. A convenient and powerful method is to minimize the grand potential within a restricted set of density matrices for which calculations are feasible. An important example is the mean field or Hartree-Fock approximation. This approximation corresponds to the case where the trial set of density matrices is taken to be of the form

$$D = Z^{-1} \exp(\sum_{ij} M_{ij} a_i^+ a_j), \qquad (4.5)$$

This choice corresponds to a density matrix of independent Fermions. In this case the entropy is found to be

$$S(D) = -k \operatorname{trace} \{ \rho \log \rho + (1 - \rho) \log(1 - \rho) \}, \qquad (4.6)$$

where the trace is over single particle indices and where  $\rho$  is the single particle density matrix

$$\rho_{ji} = \operatorname{Trace}(Da_i^+a_j) = \langle j|\rho|i \rangle.$$
(4.7)

Performing the Trace in this equation leads to

$$\rho = \frac{1}{1 + \exp(-M)}.$$
(4.8)

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exercise 4.1

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Prove the relation

$$Da_k^+ = \sum_i (e^M)_{ik} a_i^+ D.$$

Use this relation to derive equation 4.8.

answer The desired relation is obtained by expanding, in powers of the matrix M, the quantity

$$Da_k^+ D_{-1} = a_k^+ + [\sum_{ij} M_{ij}a_i^+ a_j, a_k^+] + \dots$$

and by using the commutation relation

$$\sum_{ij} M_{ij}a_i^+a_j, a_k^+] = \sum_i a_i^+ M_{ik}.$$

Equation 4.8 is then established by writing

$$\operatorname{Trace}(Da_k^+a_l) = \sum_m (e^M)_{mk} \operatorname{Trace}(a_m^+Da_l).$$

By exploiting the anticommutation relations of a and  $a^+$  one obtains

$$\rho = e^M - \rho e^M.$$

exercise 4.2

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Using the results of the previous exercise prove that

$$\operatorname{Trace}(Da_i^+a_j^+a_la_k) = < k|\rho|i> < l|\rho|j> - < l|\rho|i> < k|\rho|j>$$

(Wick's theorem).

answer

Using the commutation relation of D and  $a^+$  gives

$$\operatorname{Trace}(Da_i^+a_j^+a_la_k) = \sum_m \operatorname{Trace}(a_m^+Da_j^+a_la_k)(e^M)_{mi}.$$

The next step is to reorder the fermion operators by means of the anticommutation relations. This leads to

$$\sum_{\substack{m \\ (e^{M})_{ki} < l | \rho | j > -(e^{M})_{li} < k | \rho | j > .}} (4.9)$$

Multiplying both sides by  $(1 + e^M)_{in}^{-1}$  and summing over *i* gives the answer.

Let us now evaluate the grand potential corresponding to our trial density matrix. We assume that the hamiltonian of the system is of the form H = T + V with

$$T = \sum_{i} \epsilon_{i} a_{i}^{+} a_{i}, \qquad (4.10)$$

and

$$V = \frac{1}{2} \sum_{ijkl} \langle ij|V|kl \rangle a_i^+ a_j^+ a_l a_k.$$
 (4.11)

The expectation value of the number operator is

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$$\langle \hat{N} \rangle = \operatorname{trace}(\rho).$$
 (4.12)

Let us now calculate the expectation value of the energy. The kinetic energy is

$$< T > = \sum_{ij} < i|t|j > < i|\rho|j > .$$
 (4.13)

Using the result of exercise 4.2 the potential energy is found to be

$$\langle \hat{V} \rangle = \sum_{ijkl} \langle ij|\tilde{V}|kl\rangle \langle i|\rho|j\rangle \langle k|\rho|l\rangle, \qquad (4.14)$$

where  $\langle ij|\bar{V}|kl\rangle = \langle ij|V|kl\rangle - \langle ij|V|lk\rangle$ .

In order to determine the optimal density matrix  $D_{HF}$  we now have to perform a variation of the grand potential with respect to the variational parameters  $M_{ij}$  or equivalently  $\rho_{ij}$ . Two different types of variations can be envisaged. The first type corresponds to transformations of the form

$$\rho = e^{i\chi} \rho_{HF} e^{-i\chi}. \tag{4.15}$$

Such transformations do not change the entropy and do not change the number of particles. The change in the grand potential therefore reduces to the change in the energy. This change is conveniently expressed by introducing the mean field operator W defined by

$$\delta E = \operatorname{Trace}(W\delta\rho). \tag{4.16}$$

Its explicit expression is given by

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$$\langle i|W|k\rangle = \sum_{jl} \langle ij|\tilde{V}|kl\rangle \langle l|\rho|j\rangle.$$
(4.17)

Since  $\delta \rho = i[\chi, \rho_{HF}]$  we learn that  $\operatorname{Trace}([W, \rho_{HF}]\chi)$  vanishes for any operator  $\chi$  i.e.

$$[W, \rho_{IIF}] = 0. (4.18)$$

Thus W and  $\rho_{HF}$  can be simultaneously diagonalized. We denote their common eigenvectors by  $\varphi_i$ 

$$W|\varphi_i\rangle = \epsilon_i |\varphi_i\rangle, \qquad (4.19)$$
  
$$\rho_{HF}|\varphi_i\rangle = f_i |\varphi_i\rangle.$$

We can also perform a second type of variation for which only the eigenvalues of the one body density matrix are modified e.g.

$$\delta \rho = \delta f_i |\varphi_i\rangle < |\varphi_i|. \tag{4.20}$$

Requiring the change in the grand potential to be zero we find that the eigenvalues of the one body density matrix should be given by Fermi occupation numbers

$$f_{i} = \frac{1}{1 + \exp\{\beta(\epsilon_{i} - \mu)\}}.$$
 (4.21)

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Equations 4.17, 4.18 and 4.21 are referred to as mean field or Hartree-Fock equations at finite temperature. In these equations the chemical potential is to be adjusted in such a way that the total number of nucleons equals A i.e.

$$\sum_{i} f_i = A. \tag{4.22}$$

exercise 4.3 For a spin saturated symmetric nucleus (i.e. N=Z) work out the expression of the mean field W in the case of a simplified Skyrme force which is a sum of two and three body forces

$$V = v_{12} + v_{123}, \tag{4.23}$$

where the two and three- body terms  $v_{12}$  and  $v_{123}$  are respectively given by

$$v_{12}=t_0\delta(\mathbf{r}_1-\mathbf{r}_2),$$

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$$v_{123} = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3).$$

answer

In second quantized form the hamiltonian density of the nucleus reads

$$\mathcal{H} = \frac{\hbar^2}{2m} \nabla \psi^+(\mathbf{r}) \cdot \nabla \psi(\mathbf{r}) + \frac{t_0}{2} : (\psi^+(\mathbf{r})\psi(\mathbf{r}))^2 : + \frac{t_3}{6} : (\psi^+(\mathbf{r})\psi(\mathbf{r}))^3 :, \qquad (4.24)$$

where the notation :: indicates that the operators should be normal ordered i.e. all creation operators placed to the left of annihilation operators as prescribed by equation (4.11). Note that in the previous equation  $\psi$  is a two component spinor whose components are:

$$\psi^{+}(\mathbf{r},\sigma) = \sum_{i} \varphi_{i}^{*}(\mathbf{r},\sigma) a_{i}^{+}. \qquad (4.25)$$

The expectation value of the energy density is obtained by applying Wick's theorem with the result:

$$<\mathcal{H}>=rac{\hbar^2}{2m} au(\mathbf{r})+rac{3}{8}t_0
ho^2(\mathbf{r})+rac{1}{16}t_3
ho^3(\mathbf{r}),$$
 (4.26)

where  $\rho$  and  $\tau$  are respectively the density and kinetic energy density

$$\rho(\mathbf{r}) = \langle \psi^{+}(\mathbf{r})\psi(\mathbf{r}) \rangle = \sum_{i} f_{i} |\varphi_{i}(\mathbf{r})|^{2}, \qquad (4.27)$$

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$$\tau(\mathbf{r}) = \langle \nabla \psi^{+}(\mathbf{r}) \nabla \psi(\mathbf{r}) \rangle = \sum_{i} f_{i} |\nabla \varphi_{i}(\mathbf{r})|^{2}.$$
(4.28)

Requiring the grand potential to be stationary leads to the mean field equation

$$(-\frac{\hbar^2}{2m}\Delta + U)\varphi_i(\mathbf{r}) = \epsilon_i \varphi_i(\mathbf{r}), \qquad (4.29)$$

where the average potential U is given in terms of the density distribution by

$$U(\mathbf{r}) = \frac{3}{4}t_0\rho(\mathbf{r}) + \frac{3}{16}t_3\rho^2(\mathbf{r}).$$
(4.30)

#### exercise 4.4

Let us define the grand partition function in the Hartree- Fock approximation as

$$\log Z_{HF}(\alpha,\beta) = -\beta A(D). \tag{4.31}$$

Show that this definition preserves the thermodynamic identities

$$E = -\frac{\partial}{\partial\beta}\log Z, \quad N = \frac{\partial}{\partial\alpha}\log Z,$$
 (4.32)

and

$$S = \left(1 - \frac{\partial}{\partial \alpha} - \frac{\partial}{\partial \beta}\right) \log Z.$$
 (4.33)

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#### answer

Let us evaluate the change in log Z when  $\alpha$  and  $\beta$  are increased by  $\delta \alpha$  and  $\delta \beta$  respectively:

$$\delta \log Z = -\delta\beta \operatorname{Trace}(D\hat{H}) + \delta\alpha \operatorname{Trace}(D\hat{N}). \tag{4.34}$$

Note that there is no term arising from the variation of the density matrix because the grand potential is stationary. Identification of the variations in  $\alpha$  and  $\beta$  provides the desired result. Note also that the Hartree-Fock partition function is not the free particle one  $Z_0$ .

### References

 See e.g. L.D. Landau and I.E. Lifschitz, Statistical Mechanics, Mir, Moscow, 1976, section 32; see also R.E. Peierls, Surprises in Theoretical Physics, Princeton series in Physics, Princeton University Press, Princeton, New Jersey, 1979

[2] T. Matsubara, Prog. Theor. Phys. (Kyoto) 14(1955) 351 [3] P. Martin and J. Schwinger, Phys. Rev. 115 (1959) 1342 [4] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics, Benjamin, Reading Mass., 1962 [5] A.A. Abrikosov, L.P. Gorkov and I.E. Dzyaloshinsky, Methods of Quantum Field Theory in Statistical Physics, Dover, New York, 1963 [6] D.J. Thouless, Quantum Mechanics of Many Body Systems, Academic, New York, 1964 [7] A.L. Fetter and J.D. Walecka, Quantum Theory of Many Particle Systems, Mc Graw Hill, New York, 1971 [8] A.K. Kerman and S. Levit, Phys. Rev. C24 (1981) 1029 [9] J.W. Negele and H. Orland, Quantum many- particle systems, Addison Wesley, Reading, Mass. 1988 [10] J.P. Blaizot and G. Ripka, Quantum Theory of Finite Systems, MIT Press, Cambridge Mass., 1988 [11] M. Gaudin, Nucl. Phys. 15 (1960) 89 [12] M. des Cloizeaux, in Many Body Physics, Les Houches Lectures, 1967, C. de Witt and R. Balian eds., Gordon and Breach, New York, 1968. [13] D.A. Kirznits and A.D. Linde, Phys. Lett. 42B (1972) 471 [14] S. Weinberg, Phys. Rev. D9 (1974) 3357 [15] L. Dolan and R. Jackiw, Phys. Rev. D9 (1974) 3320 [16] A.M. Polyakov, Phys. Lett. 72B (1978) 477 [17] C. Bernard, Phys. Rev. D9 (1974) 3312 [18] D. Gross, R. Pisarsky and L. Yaffe, Rev. Mod. Phys. 53 (1981) 43 [19] B. Peterson, Nucl. Phys. A525 (1991) 237c [20] J. Kapusta, Finite Temperature Field Theory, Cambridge University Press, 1989 [21] S. Song et. al., Phys. Lett. 130B (1984) 14 [22] J. Galin, Nucl. Phys. A488 (1988) 297c

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- [23] B. Tamain, Lectures presented at the 1992 Predeal summer school in Physics
- [24] M. Draper et. al., Phys. Rev. Lett. 49 (1982)
- [25] D.M. Brink, D. Phil. Thesis, University of Oxford 1955, as quoted by J.E. Lynn, The Theory of Neutron Resonance Reactions, Clarendon, Oxford, 1968
- [26] D. Vautherin and N. Vinh Mau, Nucl. Phys. A422 (1984) 140
- [27] J. Bar Touv, Phys. Rev. C32 (1985) 1369

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- [28] H. Sagawa and G.F. Bertsch, Phys. Lett. 146B (1984) 138
- [29] M. Gallardo, M. Dievel, T. Dossing and R.A. Broglia, Nucl. Phys. A443 (1985) 415
- [30] G.F. Bertsch and T.T.S. Kuo, Nucl. Phys. A112 (1968) 204
- [31] N. Vinh Mau and D. Vautherin, in Windsurfing the Fermi sea, vol.2, T.T.S Kuo and J. Speth Eds., Elsevier 1987; N. Vinh Mau, Nucl. Phys. A491 (1989) 246
- [32] A. Bohr and B. Mottelson, Nuclear Structure, Vol.1, Benjamin, New York, 1969.
- [33] C. Jacquemin and S.K. Kataria, Z. Phys. A324 (1986) 261; C. Jacquemin, private communication
- [34] R. Balian, From microphysics to macrophysics, vol.1, Texts and monographs in physics, Springer, Berlin, 1992

# **II THERMODYNAMIC PERTURBATION THEORY**

# 5 Dyson's expansion

Suppose that we have to deal with a many fermion system whose hamiltonian H is the sum H = T + V of a one body operator T (e.g. the kinetic energy for an electron gas or the average field for a nucleus)

$$T = \sum_{ij} \langle i|T|j \rangle a_i^+ a_j = \sum_i \epsilon_i a_i^+ a_i, \qquad (5.1)$$

and a residual two-body interaction V

$$V = \frac{1}{2} \sum_{ijkl} \langle ij|V|kl \rangle a_i^+ a_j^+ a_l a_k.$$
 (5.2)

As was mentionned in section 2 the partition function

$$Z(\alpha,\beta) = \operatorname{Trace} \exp(\alpha \hat{N} - \beta \hat{H}), \qquad (5.3)$$

cannot in general be calculated explicitly in this case. In this section we present a method to construct Z as a perturbation series in the residual interaction V. Let us first write the partition function as

$$Z(\alpha,\beta) = \operatorname{Trace} e^{-\beta(H_0+V)},\tag{5.4}$$

where the operator  $H_0$  collects the one body terms

$$H_0 = \sum_i (\epsilon_i - \mu) a_i^+ a_i, \qquad (5.5)$$

and where  $\mu$  is the chemical potential

$$\mu = \alpha/\beta. \tag{5.6}$$

In order to construct a perturbation expansion for Z it is convenient to make explicit the contribution of the unperturbed hamiltonian

$$Z_0 = \text{Trace } e^{-\beta H_0}, \tag{5.7}$$

(which is calculable by the methods of section 4), and to write

$$Z(\alpha,\beta) = Z_0 \operatorname{Trace} \{ \frac{e^{-\beta H_0}}{Z_0} [e^{\beta H_0} e^{-\beta (H_0+V)}] \}.$$
 (5.8)

The attractive feature of this expression is that it is well adapted to the case of a weak residual interaction. Indeed it expresses Z as the product of bare partition function  $Z_0$  by a correction

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factor. This factor is the thermal expectation value in the unperturbed state of an operator close to unity when V is small. Explicitly

$$Z(\alpha,\beta) = Z_0 < U_I(\beta) >$$
(5.9)

with

$$U_{I}(\beta) = e^{\beta H_{0}} e^{-\beta (H_{0}+V)}.$$
 (5.10)

This operator is reminiscent of evolution operator in the interaction representation. Indeed it satisfies the following evolution equation (sometimes referred to as the Bloch equation [1])

$$\frac{\partial}{\partial \beta} U_I(\beta) = -V_I(\beta) U_I(\beta), \qquad (5.11)$$

where  $V_i$  is the residual interaction in the interaction representation

$$V_{I}(\beta) = e^{+\beta H_{0}} V e^{-\beta H_{0}}.$$
 (5.12)

The only difference with ordinary perturbation theory is that we now have an imaginary value of the time variable. For this reason the formalism described below is called imaginary time formalism.

Integration of the above evolution equation yields

$$U_I(\beta) = 1 - \int_0^\beta V_I(\tau) U_I(\tau) d\tau, \qquad (5.13)$$

which can be expanded as (Dyson's expansion)

$$U_{I}(\beta) = \sum_{n} \frac{(-1)^{n}}{n!} \int_{0}^{\beta} \dots \int_{0}^{\beta} d\tau_{1} \dots d\tau_{n} T\{V_{I}(\tau_{1}) \dots V_{I}(\tau_{n})\}.$$
(5.14)

In this equation the notation T denotes the time ordering operator defined by

$$\begin{split} T\{A(\tau_1)B(\tau_2)\} &= A(\tau_1)B(\tau_2) & \text{if } \tau_1 > \tau_2, \\ &= (-1)^P B(\tau_2)A(\tau_1) & \text{if } \tau_1 < \tau_2, \end{split}$$
 (5.15)

where A (resp. B) is a product of an arbitrary number of creation and annihilation operators with the same time argument  $\tau_1$  (resp.  $\tau_2$ ) and P is the parity of the permutation bringing the fermion field operators in the desired order.

exercise 5.1 Establish equation (5.14).

answer

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Iterating equation (5.13) twice gives

$$U_{I}(\beta) = 1 - \int_{0}^{\beta} V_{I}(\tau) d\tau + \int_{0}^{\beta} d\tau_{1} \int_{0}^{\tau_{1}} d\tau_{2} V_{I}(\tau_{1}) V_{I}(\tau_{2}) + \dots \qquad (5.16)$$

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which can be rewritten in the form (5.14) for the first two terms. Higher order terms are obtained by induction.

To evaluate the partition function  $Z = Z_0 < U_I >$  we are thus left with the calculation of the thermal expectation value of time ordered products of interaction terms in the unperturbed density matrix. The implementation of this step is achieved by means of the following two lemma.

lemma 5.1

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In the interaction representation the two body interaction reads

$$V_l(\tau) = \frac{1}{2} \sum_{ijkl} \langle ij|V|kl \rangle \tilde{a}_i(\tau) \tilde{a}_j(\tau) a_l(\tau) a_k(\tau), \qquad (5.17)$$

where the notation  $a(\tau)$  denotes creation and anihilation operators in the interaction representation

$$a_{i}(\tau) = e^{+\tau H_{0}} a_{i} e^{-\tau H_{0}} = a_{i} \exp\{-(\epsilon_{i} - \mu)\tau\},$$
  

$$\tilde{a}_{i}(\tau) = e^{+\tau H_{0}} a_{i}^{+} e^{-\tau H_{0}} = a_{i}^{+} \exp\{+(\epsilon_{i} - \mu)\tau\}.$$
(5.18)

Note that  $\tilde{a}(\tau)$  is no longer the hermitian conjugate of the annihilation operator  $a(\tau)$  in thermal perturbation theory, unless  $\tau = 0$ .

#### proof

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The derivation of (5.17) is straightforward. In order to establish (5.18) we expand  $\tilde{a}(\tau)$  as:

$$\tilde{a}_i(\tau) = a_i^+ + \tau [H_0, a_i^+] + \frac{\tau^2}{2!} [H_0, [H_0, a_i^+]] + \dots$$
(5.19)

The commutator appearing in this equation is given by

$$[H_0, a_i^+] = (\epsilon_i - \mu)a_i^+, \tag{5.20}$$

which leads to the result. A similar calculation can be made to establish the expression for  $a(\tau)$ .

### lemma 5.2

The thermal expectation value of a time ordered product of creation and annihilation operators in the unperturbed state is obtained by grouping the operators by pairs, multiplying the expectation values of each time ordered pair, adding the contributions of all possible pairings with a sign determined by the parity of the permutation which sets the operators in the required sequence (Wick's theorem).

#### example

$$< T\{\tilde{a}_{i}(\tau_{1})\tilde{a}_{j}(\tau_{2})a_{k}(\tau_{3})a_{l}(\tau_{4})\} > = < T\{\tilde{a}_{i}(\tau_{1})a_{l}(\tau_{4})\} > < T\{\tilde{a}_{j}(\tau_{2})a_{k}(\tau_{3})\} > - < T\{\tilde{a}_{i}(\tau_{1})a_{k}(\tau_{3})\} > < T\{\tilde{a}_{j}(\tau_{2})a_{l}(\tau_{4})\} > + < T\{\tilde{a}_{i}(\tau_{1})\tilde{a}_{j}(\tau_{2})\} > < T\{a_{k}(\tau_{3})a_{l}(\tau_{4})\} > .$$

$$(5.21)$$

The last term in fact vanishes since it involves the expectation value of two creation operators.

#### proof

Let us first restrict ourselves to the case of four operators mentionned in the previous example. A possible -though tedious- way to prove Wick's theorem is to exploit the time independent version of this theorem discussed in exercise 4.2. A more elegant proof however [1] is obtained by applying to both sides of equation (5.21) the operator  $\partial/\partial \tau_1 - \epsilon_i + \mu$ . Note that, although the action of this operator on  $\tilde{a}_i(\tau_1)$  vanishes, such is not the case for a time ordered product involving this operator because of the step functions implied by the time ordering. As a result

$$\begin{array}{l} (\partial/\partial\tau_1 - \epsilon_i + \mu) < T\{\tilde{a}_i(\tau_1)\tilde{a}_j(\tau_2)a_k(\tau_3)a_l(\tau_4)\} > \\ = \delta(\tau_1 - \tau_4)\delta_{il} < T\{\tilde{a}_j(\tau_2)a_k(\tau_3)\} > -\delta(\tau_1 - \tau_3)\delta_{ik} < T\{\tilde{a}_j(\tau_2)a_l(\tau_4)\} > . \end{array}$$

$$(5.22)$$

It can thus be seen that both sides satisfy the same differential equation with the same antiperiodic boundary conditions on the interval  $[0,\beta]$ . The extension to an arbitrary number of operators is straightforward.

#### **Definition 5.1**

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According to Wick's theorem all expectation values of products of creation and annihilation operators can be expressed in terms of the quantities

$$G_{ij}^{(0)}(\tau - \tau') = \text{Trace } \left\{ \frac{e^{-\beta H_0}}{Z_0} T[\tilde{a}_i(\tau) a_j(\tau')] \right\}$$
(5.23)

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These quantities, which depend only on  $\tau - \tau'$  are called unperturbed propagators or unperturbed single particle Green's functions in analogy with the zero temperature case. Exact Green's functions G are defined in the same way provided the full hamiltonian H is substituted to the unperturbed one ir the above formula.

#### exercise 5.2

Unperturbed propagators are needed only in the interval  $0 < \tau < \beta$  i.e.  $-\beta < \tau - \tau' < +\beta$ . Show that in this interval  $G^{(0)}(\tau)$  is antiperiodic with a period  $\beta$ .

#### answer

Assume  $\tau$  to belong to the interval  $[0,\beta]$ . We have in this case

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$$Z_{0}G_{ij}^{(0)}(\tau - \beta) = \operatorname{Trace} \left\{ e^{-\beta H_{0}}T[\tilde{a}_{i}(\tau - \beta)a_{j}(0)] \right\}$$
  
= -Trace  $\left\{ e^{-\beta H_{0}}a_{j}e^{(\tau - \beta)H_{0}}a_{i}^{+}e^{-(\tau - \beta)H_{0}} \right\}$   
= -Trace  $\left\{ e^{-\beta H_{0}}e^{\tau H_{0}}a_{i}^{+}e^{-\tau H_{0}}a_{j} \right\}$   
=  $-Z_{0}G_{ij}^{(0)}(\tau)$  (5.24)

which establishes the result. Note that the antiperiodicity of Green's functions holds only in the restricted interval  $[-\beta, +\beta]$ .

### exercise 5.3

Show that in the basis in which the single particle hamiltonian  $H_0$  is diagonal the unperturbed Green's function  $G^{(0)}$  are given by

$$G_{ij}^{(0)}(\tau) = \delta_{ij} f_i e^{(\epsilon_i - \mu)\tau} \quad \text{if} \quad \tau > 0$$
  
=  $-(1 - f_i) \delta_{ij} e^{-(\epsilon_i - \mu)\tau} \quad \text{if} \quad \tau < 0$  (5.25)

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where  $f_i$  is the Fermi occupation number defined by equation (3.6).

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### hint

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۰. چ Use the definition (5.15) and equation (5.18). Note that equation (5.25) satisfies the antiperiodicity condition studied in the previous exercise.

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.23) percact The unperturbed propagators can thus be represented by a Fourier series as

$$G_{ij}^{(0)}(\tau) = \frac{1}{\beta} \sum_{\nu=-\infty}^{+\infty} e^{-i\omega_{\nu}\tau} G_{ij}^{(0)}(\omega_{\nu}), \qquad (5.26)$$

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where

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$$\omega_{\nu}=(2\nu+1)\pi/\beta,$$

with  $\nu$  being an arbitrary positive or negative integer. The frequencies  $\omega_{\nu}$  are called Matsubara frequencies. From the previous equation we find

$$G_{ij}^{(0)}(\omega_{\nu}) = \int_0^\beta e^{i\omega_{\nu}\tau} G_{ij}^{(0)}(\tau) d\tau = \frac{\delta_{ij}}{\epsilon_i - \mu + i\omega_{\nu}}.$$
 (5.27)

It is interesting to see how equation (5.26) is able to reproduce the discontinuity at  $\tau = 0$ . Suppose that  $\tau$  is greater than zero. By using the two previous formulae, we can write the propagator as

$$G_{ij}^{(0)}(\tau) = \delta_{ij} \frac{1}{\beta} \int_C f(z) dz$$
(5.28)

where the function f is defined by

$$f(z) = \frac{1}{(\epsilon_i - \mu) - z} \frac{e^{z\tau}}{e^{\beta z} + 1},$$
 (5.29)

and where the contour C encloses the poles of f located at i times the Matsubara frequencies i.e. at  $z = i\omega_{\nu}$ . Now when |z| is large the function f(z) behaves as

$$f(z) \simeq e^{-(\beta-\tau)\text{Re}z} \quad if \quad \text{Re}z > 0, \qquad (5.30)$$

and

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$$f(z) \simeq e^{\tau \operatorname{Re} z} \quad if \quad \operatorname{Re} z < 0. \tag{5.31}$$

In both cases the fuction f(z) vanishes exponentially at large |z| and the contour C can thus be deformed into a single loop around the remaining pole at  $z = (\epsilon_i - \mu)$ . This gives

$$G_{ij}^{(0)}(\tau) = \frac{e^{(\epsilon_i - \mu)\tau}}{e^{\beta(\epsilon_i - \mu)} + 1} \qquad (\tau > 0).$$
 (5.32)

In the case where  $\tau$  is negative the above procedure fails because f(z) no longer vanishes at large |z|. However it is possible to use another function namely

$$g(z) = \frac{1}{(\epsilon_i - \mu) - z} \frac{e^{z\tau}}{e^{-\beta z} + 1}.$$
 (5.33)

Indeed this function g(z) behaves for large z as

$$g(z) \simeq e^{(\beta+\tau)\text{Re}z} \quad if \quad \text{Re}z < 0, \tag{5.34}$$

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$$g(z) \simeq e^{\tau \operatorname{Re} z}$$
 if  $\operatorname{Re} z > J$ . (5.35)

A deformation of the contour C thus leads in this case to

$$G_{ij}^{(0)}(\tau) = \frac{e^{(\epsilon_i - \mu)\tau}}{e^{-\beta(\epsilon_i - \mu)} + 1} \qquad (\tau < 0).$$
 (5.36)

From the calculation we have just made we also learn that the expression we have written for the propagator in terms of its Fourier components is not a convergent one for  $\tau = 0$ . In order to have a formula valid for all values of  $\tau$  it should be modified into

$$G_{ij}^{(0)}(\tau) = \lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\nu = -\infty}^{+\infty} e^{i\eta\tau} e^{-i\omega_{\nu}\tau} G_{ij}^{(0)}(\omega_{\nu})$$
(5.37)

exercise 5.4

Establish the correction to the partition function in first order perturbation theory.

answer

From equations (5.9) and (5.13) we have

$$Z(\beta) = Z_0 < (1 - \int_0^\beta V_I(\tau) U_I(\tau) d\tau) > .$$
 (5.38)

Up to first order  $Z = Z_0 + Z_1$  with:

$$Z_{1}/Z_{0} = -\int_{0}^{\beta} < V_{l}(\tau) > d\tau$$
  
=  $-\frac{\beta}{2} < ij|V|kl > \{G_{ik}^{0}(+0)G_{jl}^{0}(+0) - G_{il}^{0}(+0)G_{jk}^{0}(+0)\}$   
=  $-\frac{\beta}{2} < ij|\tilde{V}|ij > f_{i}f_{j},$  (5.39)

where  $\tilde{V}$  denotes an antisymmetrized matrix element:

$$\langle ij|\tilde{V}|kl\rangle = \langle ij|V|kl\rangle - \langle ij|V|lk\rangle.$$
(5.40)

## 6 Diagrams

As for zero temperature perturbation theory it is convenient to visualize the various terms in the perturbation expansion by means of graphs or diagrams. These terms involve the two body interaction V and the single particle propagators G. To each of them one can associate a graph in the following way. An interaction matrix element  $\langle ij|\tilde{V}|kl \rangle$  is represented by a dotted horizontal line:

$$\langle ij|\tilde{V}|kl\rangle = i_j \geq --- <^k_l$$
 (6.1)

whose altitude characterizes the imaginary time  $\tau$  when it is taking place. Propagators  $G_{ij}^{(0)}(\tau - \tau')$  are represented by a solid line beginning at imaginary time  $\tau$  and ending at time  $\tau'$  and oriented from  $\tau$  to  $\tau'$ . With these conventions the first order contribution  $Z_1$  to the partition function is represented by the following graph

$$Z_1 = 0 - - - 0 \tag{6.2}$$

It is also possible to define graphs with interaction matrix elements which are not antisymmetrized. One has in this case a larger number of graphs in a given order.

disconnected graphs. Some terms in the perturbation expansion can be factorized as a product of two or more thermal expectation values in the unperturbed state. Such terms lead to disconnected graphs. As an example in second order one encounters for the partition function the following diagrams

$$\begin{array}{c} 0 - - - - 0 \\ 0 - - - 0 \end{array} \tag{6.3}$$

which correspond to the contribution

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$$Z_2/Z_0 = \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 < V_I(\tau_1) > < V_I(\tau_2) > = \frac{1}{2} (\frac{\beta}{2} \sum_{ij} < ij |\tilde{V}| ij > f_i f_j)^2.$$
(6.4)

In contrast contributions which cannot be factorized are called connected graphs.

linked cluster expansion As for zero temperature the sum of all graphs, connected and disconnected, is equal to the exponential of the sum including connected graphs only. Let us illustrate this property on the following example

exercise 6.1 Calculate the sum of the corrections to the partition function  $Z_0$  defined by the following graphs:

$$\tilde{Z}/Z_0 = 1 + 0 - - - 0 + 0 - - - 0 + 0 - - - 0 + ..$$
 $0 - - - 0 + 0 - - - 0 + ..$ 
 $0 - - - 0 + ..$ 
 $0 - - - 0 + ..$ 
(6.5)

answer. The n-th order contribution is

$$Z_N/Z_0 = \int_0^\beta d\tau_1 \dots \int_0^{\tau_{N-1}} d\tau_N < V_I(\tau_1) > \dots < V_I(\tau_N) >, \qquad (6.6)$$

which is equal to

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$$Z_N/Z_0 = \frac{1}{N!} (\beta \sum_{ij} < ij | \tilde{V} | ij >)^N.$$
(6.7)

s;

The sum of all such graphs is thus

$$\tilde{Z}/Z_0 = \exp\{-\frac{\beta}{2}\sum_{ij} < ij|\tilde{V}|ij > f_if_j\}.$$
 (6.8)

This sum enjoys the following property.

exercise 6.2 Show that when the unperturbed hamiltonian is chosen to be the kinetic energy operator T and the perturbation to be the two body interaction V, then the sum of all disconnected graphs generated from the first order one has an expression similar to the Hartree-Fock partition function but with the Hartree-Fock occupation numbers replaced by the unperturbed ones.

answer. Using the expression of the unperturbed partition function and equation (6.6) we obtain:

$$-\beta \log \bar{Z} = -\beta \sum_{i} \log\{1 + e^{\beta(u-t_i)}\} + \frac{1}{2} \sum_{ij} < ij |\bar{V}| ij > f_i f_j.$$
(6.9)

The first term can be transformed into

$$Trace(TD_0) - S(D_0)/\beta - \mu N(D_0),$$
 (6.10)

where  $S(D_0)$  and  $N(D_0)$  are the unperturbed entropy and particle number respectively. The last term is equal to Trace $(D_0V)$ . Combining these results we have

$$-\beta \log \tilde{Z} = \operatorname{Trace}(D_0 H) - S(D_0)/\beta - \mu \operatorname{Trace}(D_0 N).$$
(6.11)

This expression looks similar to the Hartree-Fock partition function  $Z_{HF}$  but in fact differs from it because the occupation numbers  $f_i$  are not the Hatree-Fock ones.

To conclude this section we now perform two additional exercises which will be usefull in the next section.

exercise 6.3 List the second order connected graphs for the partition function and evaluate their contributions.

answer. In second order one has two possible connected graphs which are displayed in the following figure

$$Z_{2a}/Z_0 = \left( \int_{-}^{-} \int_{-}^{-} \int_{-}^{-} Z_{2b}/Z_0 = \left( \int_{-}^{-} -O \right)$$
 (6.12)

The contribution of the first graph is given by

$$\frac{Z_{2a}}{Z_0} = -\frac{\beta}{8} \sum_{php'h'} \frac{(1-f_p)f_h(1-f_{p'})f_{h'}}{\epsilon_p - \epsilon_h + \epsilon_{h'} - \epsilon_{p'}} | < ph|V|p'h' > |^2 \{1 - e^{-\beta(\epsilon_p - \epsilon_h + \epsilon_{h'} - \epsilon_{p'})}\}.$$
 (6.13)

The labels of single particle states have been classified as p or h depending on whether they become particle or hole states at zero temperature. The contribution of the second graph is

$$Z_{2b}/Z_0 = \frac{1}{2}\beta^2 \sum_{ijk} f_i f_j (1 - f_j) f_k < ij |\tilde{V}| ij > < jk |\tilde{V}| jk > .$$
(6.14)

Note that this graph would not occur in zero temperature perturbation theory because the factor f(1-f) would vanish in this case. It would also not occur in the Hartree-Fock basis as shown in the next exercise.

exercise 6.4 Examine the case where the unperturbed Hamiltonian is chosen to be the Hartree- Fock Hamiltonian. Prove that in this case all graphs containing insertions of the form

$$i_i > - - - 0 \tag{6.15}$$

vanish identically.

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answer The Hamiltonian  $H_0$  is  $\hat{T} + \hat{U} - \mu \hat{N}$ , where  $\hat{U}$  is the Hartree-Fock potential, and the perturbation is  $\hat{V} - \hat{U}$  where  $\hat{V}$  is the two-body interaction. An insertion of the form (6.15) contributes a factor

$$\Sigma_{ij} = \sum_{k} f_k < ik |\tilde{V}| jk > - < i |U| j > . \qquad (6.16)$$

Using the definition of the Hartree- Fock potential one finds  $\Sigma = 0$ .

# 7 Thermal Green's functions

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In the previous sections we already encountered one body Green functions. For the discussion of the random phase approximation it is also convenient to introduce the so called particle hole Green functions which involve expectation values of time ordered products of two pairs of creation and annihilation operators. More precisely we define the unperturbed particle hole Green function as

$$< ph\tau | G_2^{(0)} | p'h'\tau' > = < T\{\tilde{a}_h(\tau)a_p(\tau)\tilde{a}_{p'}(\tau')a_{h'}(\tau')\} > .$$
(7.1)

The definition of exact Green functions is obtained by substituting the exact Hamiltonian to the unperturbed one in this equation. Using Wick's theorem one obtains:

$$< ph\tau |G_2^{(0)}| p'h'\tau' >= G_{hp}^{(0)}(+0)G_{p'h'}^{(0)}(+0) - G_{pp'}^{(0)}(\tau-\tau')G_{hh'}^{(0)}(\tau'-\tau).$$
(7.2)

The applications considered below involve only the second term in equation (7.2). From now on we thus focus on this particular function which we denote by  $\hat{G}_2^{(0)}$ :

$$\hat{G}_{2}^{(0)} = -G_{pp'}^{(0)}(\tau - \tau')G_{hh'}^{(0)}(\tau' - \tau)$$
(7.3)

The function  $\hat{G}_2$  is periodic with a period  $\beta$  in the interval  $[-\beta, +\beta]$ . It can thus be represented by a Fourier series

$$\hat{G}_{2}^{(0)}(\tau) = \frac{1}{\beta} \sum_{\nu=-\infty}^{+\infty} e^{-i\omega_{\nu}\tau} \hat{G}_{2}^{(0)}(\omega_{\nu}), \qquad (7.4)$$

with  $\omega_{\nu} = 2\pi\nu/\beta$ ,  $\nu$  being an arbitrary positive or negative integer. The Fourier coefficients are found to be

$$\hat{G}_{2}^{(0)}(\omega_{\nu}) = \int_{0}^{\beta} e^{i\omega_{\nu}\tau} \hat{G}_{2}^{(0)}(\tau) d\tau, \qquad (7.5)$$

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$$\langle ij|\hat{G}_{2}^{(0)}(\omega_{\nu})|kl\rangle = -\delta_{ij}\delta_{kl}f_{i}(1-f_{k})\int_{0}^{\beta}e^{(i\omega_{\nu}+\epsilon_{i}-\epsilon_{k})r}d\tau.$$
(7.6)

Using the expression of the occupation numbers this formula leads to

$$\hat{G}_2^{(0)}(\omega_{\nu}) = \frac{1}{\Delta \epsilon + i\omega_{\nu}}F,\tag{7.7}$$

where the matrices  $\Delta \epsilon$  and F are given by

$$< ph|\Delta\epsilon|p'h'> = \delta_{pp'}\delta_{hh'}(\epsilon_p - \epsilon_h),$$
 (7.8)

$$< ph|F|p'h' > = -\delta_{pp'}\delta_{hh'}(f_p - f_h).$$

$$(7.9)$$

If we work in a model space containing N single particle levels, then the matrices  $\Delta \epsilon$  and F are both  $N^2$  by  $N^2$  matrices (in fact N(N-1) by N(N-1) matrices since the matrix elements with p = h vanish). It is worthwhile noting that with this notation the second order graph  $Z_{2a}$ considered in the previous section can be written as

$$Z_{2a}/Z_0 = \frac{1}{4} \operatorname{Trace} \{ \mathcal{V}\hat{G}_2^{(0)} \mathcal{V}\hat{G}_2^{(0)} \},$$
 (7.10)

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where the indices in the above matrices are of the form  $(\tau, p, h)$ ,  $\tau$  being the imaginary time variable belonging to the interval  $[0, \beta]$ , while p and h are single particle indices. The interaction matrix  $\mathcal{V}$  is defined by

$$< ph\tau |\mathcal{V}| p'h'\tau' > = < ph' |\tilde{\mathcal{V}}| hp' > \delta(\tau - \tau').$$

$$(7.11)$$

Note on this specific example that the function of interest is  $\hat{G}_2$  and not  $G_2$ . The function  $G_2$  would not be useful since it would include undesirable disconnected graphs.

Note also that the Fourier decomposition of the product of two operators

$$< au|A| au'>=rac{1}{eta}\sum_
u e^{i\omega_
u( au- au')}A(\omega_
u),$$

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$$< au|B| au'>=rac{1}{eta}\sum_
u e^{i\omega_
u( au- au')}B(\omega_
u),$$

is, according to the standard properties of Fourier transforms, equal to

$$\int_0^\beta <\tau |A|\tau''><\tau''|B|\tau'>=\frac{1}{\beta}\sum_\nu e^{i\omega_\nu(\tau-\tau')}A(\omega_\nu)B(\omega_\nu).$$

In this formula the product of the matrices A and B now involves a summation over the indices (p, h) only.

# 8 The random phase approximation (RPA)

#### ring diagrams

The notation introduced in equation (7.10) suggests that the subset of the perturbation series leading to contributions of the form :

$$C(N) = A_N \operatorname{Trace} \left( \mathcal{V} G_2^{(0)} \right)^N \tag{8.1}$$

should be worthwhile investigating. Due to the structure of the two particle Green's function  $G_2^{(0)}$  we see that the corresponding graphs contain two one-particle propagators originating both a time  $\tau$  and ending at time  $\tau'$ . They have the structure shown in the figure below

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Such graphs are called ring diagrams.

summation of ring diagrams Enumerating the various possible ways of constructing term of the form (8.2) we find that

$$A_N = \frac{1}{2N} \quad \text{for} \quad N > 2 \tag{8.3}$$

while  $A_2 = 1/4$ .

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**proof** Let us diplay the interactions  $\overline{V}$  at the various times  $\tau_1, \tau_2...\tau_N$  as shown on the figure below

1	>< 2	$ au_1$	
	><	$ au_2$	(8.4)
	•••		(011)
3	>< 4	$ au_N$	

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There are 2(N-1) possibilities to link the first particle hole pair (labeled 1 on the figure) to another one. Suppose we pick the pair labeled 3 on the figure. We now have to link the pair labeled 4 to another one. Except for N=2 the pair number 2 is excluded since this would give rise to a disconnected diagram. We thus have 2(N-2) possibilities for this second step. By induction we find that the total number of possibilities is  $2^{N-1}(N-1)!$  except for N=2 where there is a single possibility. To obtain the expression for  $A_N$  we must incorporate an extra factor  $(1/2)^N$  due to the N interactions V and another factor  $(-1)^N/N!$  arising from the Dyson expansion.

The sum of all ring diagrams which we denote by  $Z_{RPA}$  can thus be expressed as

$$2\log(Z_{RPA}/Z_{HF}) = -\mathrm{Trace}\log(1+\mathcal{V}\hat{G}_2^{(0)}) + \mathrm{Trace}(\mathcal{V}\hat{G}_2^{(0)}) - \frac{1}{4}\mathrm{Trace}(\mathcal{V}\hat{G}_2^{(0)})^2.$$
(8.5)

The value  $Z_{RPA}$  is generally referred to as the partition function in the random phase approximation. By using the Fourier representation of the unperturbed Green's function the first term in this formula can be rewritten as

$$\operatorname{Trace}\log(1+\mathcal{V}\hat{G}_{2}^{(0)}) = \sum_{\nu}\operatorname{trace}\log\{1+\hat{G}_{2}^{(0)}(\omega_{\nu})\mathcal{V}\},\tag{8.6}$$

Note that in this formula we have two different types of traces denoted respectively Trace and trace. The notation Trace involves a summation over the indices  $(p, h, \tau)$  while the notation trace implies a sum over the indices p, h only. Similarly, matrix multiplications on the right hand side involve summations over the particle hole indices (p, h) only, while the left hand side also includes an integration over the imaginary time variable. In particular, although we have kept the same notation, the interaction matrix  $\mathcal{V}$  in the left hand side is an operator in the space  $(p, h, \tau)$  while in the right hand side it is an operator in the space (p, h). Using the

relation trace log  $M = \log \det M$  (valid for any matrix M) and the explicit form of the Fourier coefficient we obtain

Trace log(1 + 
$$\mathcal{V}\hat{G}_{2}^{(0)}$$
) =  $\sum_{\nu} \log \det\{\frac{1}{\Delta\epsilon + i\omega_{\nu}}(\Delta\epsilon + F\mathcal{V} + i\omega_{\nu})\}.$  (8.7)

This formula unvails the important role played by the eigenvalue equation

$$(\Delta \epsilon + F \mathcal{V})|Y_n\rangle = E_n|Y_n\rangle, \tag{8.8}$$

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which is known in the litterature as RPA equation at finite temperature. This equation has the following properties.

property 1 If  $|Y_n >$  is an eigenstate of the RPA matrix, then the vector

$$|X_n>=F^{-1}|Y_n>, (8.9)$$

is an eigenvector of the matrix  $(\Delta \epsilon + \mathcal{V}F)$  with the eigenvalue  $E_N$ .

property 2 The eigenvalues of the RPA equations (8.8) are real when the unperturbed Hartree-Fock ground state corresponds to a true minimum of the Hartree-Fock grand potential.

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Let us perform a small variation of the Hartree- Fock density matrix  $D_{HF}$  defined by

$$D = e^{i\chi} D_{HF} e^{-i\chi}, \tag{8.10}$$

where  $\chi$  is a small hermitian operator. The change in the one- body density matrix  $\rho$  to second order is

 $\rho = \rho_0 + \rho_1 + \rho_2 + \dots \tag{8.11}$ 

with

$$\rho_1 = i[\chi, \rho_0], \tag{8.12}$$

and

$$\rho_2 = -\frac{1}{2}[\chi, [\chi, \rho_0]]. \tag{8.13}$$

In this transformation the entropy and particle number are unchanged. The variation of the grand potential is thus the change in the energy i.e.

$$\delta A = \langle \chi | (F \Delta \epsilon + F \mathcal{V} F) | \chi \rangle, \tag{8.14}$$

where  $|\chi\rangle$  is a vector whose components are related to the matrix elements of the operator  $\chi$  by

 $\chi_{ph} = \langle h | \chi | p \rangle . \tag{8.15}$ 

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Since  $\delta A > 0$  for any  $\chi$  we find, by considering the particular choice  $|\chi\rangle = |X_n\rangle$  that

$$E_n < X_n |F| X_n > 0.$$
 (8.16)

Since F is a hermitian matrix  $E_n$  should be real.

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The eigenstates of the RPA matrix corresponding to two different eigenvalues  $E_n$  and  $E_m$  satisfy the generalized orthogonality relation

$$\langle X_n|F|X_m \rangle = 0$$
 if  $E_n \neq E_m$ . (8.17)

### proof

This property is obtained by using the fact that the matrices F and  $\Delta \epsilon$  commute and by calculating in two different ways the matrix element  $\langle X_n | (F\Delta \epsilon + FVF) | X_m \rangle$ .

#### property 4

If  $X_n(p,h)$  is a solution of the RPA equation corresponding to the eigenvalue  $E_n$  then  $X_n^*(h,p)$  is a solution corresponding to the eigenvalue  $-E_n$ .

#### proof

This property is a consequence of the symmetries of the matrices involved in the RPA equation

In the following we shall denote negative energy states as  $|X_n^+>$ .

### property 5

The RPA eigenvectors can be normalized by means of the following relation

$$\langle X_n|F|X_m \rangle = \delta_{mn} \operatorname{sign}(E_n)$$
 (8.19)

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This is a direct consequence of the previous property.

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Provided the RPA eigenvectors form a closed set one has the following closure relations

$$\sum_{n>0} \{ |X_n| - |X_n^+| < X_n^+| \} F = 1,$$
(8.20)

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and

$$\sum_{n>0} \frac{1}{F} \{ |Y_n \rangle < Y_n| - |Y_n^+ \rangle < Y_n^+| \} = 1,$$
(8.21)

where the summation over the index n runs over positive energy states only. We will now show that the properties of the RPA equation allow one to obtain an explicit formula for the RPA partition function.

### Explicit expression of the RPA partition function

Using the RPA eigenvalues it is possible to derive a more explicit expression of the partition function in the RPA approximation. Indeed from properties 2, 3 and 4 we obtain

Trace 
$$\log(1 + \mathcal{V}G_2^{(0)}) = \frac{\prod_{p>h} \omega_{\nu}^2 + (\epsilon_p - \epsilon_h)^2}{\prod_{n>0} \omega_{\nu}^2 + E_n^2},$$
 (8.22)

where the notation n > 0 implies a summation over positive RPA roots only. The next step is to use the representation of the hyperbolic sine as

$$\frac{1}{z}\sinh z = \prod_{\nu>0} (1 + \frac{z^2}{\nu^2 \pi^2}), \qquad (8.23)$$

where the product runs over all positive integer values of  $\nu$ . This formula allows one to perform the infinite product over the Matsubara frequencies with the result

$$\log(Z_{RPA}/Z_{HF}) = \sum_{p>h} \log \sinh\{\beta(\epsilon_p - \epsilon_h)/2\} - \sum_{n>0} \log \sinh\{\beta(E_n/2)\} + \frac{\beta}{2} \sum_{p\neq h} (1 - f_p) f_h < ph|V|ph >$$

$$-\frac{\beta}{8} \sum \frac{(1 - f_p) f_h (1 - f_{p'}) f_{h'}}{\epsilon_p - \epsilon_h + \epsilon_{h'} - \epsilon_{p'}} | < ph|V|p'h' > |^2 \times \left\{1 - e^{-\beta(\epsilon_p - \epsilon_h + \epsilon_{h'} - \epsilon_{p'})}\right\}.$$
(8.24)

Since the partition function of a quantum harmonic oscillator is  $Z(\beta) = 1/2 \sinh(\beta \omega/2)$  we see that the partition function in the random phase approximation can be interpreted as being that of an assembly of independent harmonic oscillators whose frequencies are just the RPA frequencies. There are however two important correction terms which must be introduced to obtain the correct coefficients of the first and second order terms in the perturbation expansion.

# 9 The time dependent mean field approximation and RPA

The time dependent mean field approximation is obtained by assuming [2] that at each time the density matrix D is the exponential of a one body operator. By considering the one body reduction of the Liouville von Neuman equation for D,  $i\dot{D} = [H, D]$ , we obtain the evolution equation for the one body density matrix  $\rho$  defined by

$$\langle i|\rho|j\rangle = \operatorname{Trace}\{D(t)a_i^+a_j\}.$$
(9.1)

The result is

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$$i\dot{\rho} = [W,\rho],\tag{9.2}$$

where W is the mean field hamiltonian, defined as the functional derivative of the energy functional with respect to one body density i.e.

$$\delta E = \operatorname{Trace}(W\delta\rho). \tag{9.3}$$

Using

$$E = \operatorname{Trace}(T\rho) + \frac{1}{2} \sum_{ijkl} \langle ij|\tilde{V}|kl\rangle \langle k|\rho|i\rangle \langle l|\rho|j\rangle, \qquad (9.4)$$

where T is the kinetic energy operator we find, as in section 4,

$$\langle i|W|k\rangle = \sum_{jl} \langle ij|\tilde{V}|kl\rangle \langle l|\rho|j\rangle.$$
(9.5)

As for zero temperature the thermal RPA equations are related to the linearized mean field equations. Let us consider small amplitude oscillations around a solution of the static Hartree-Fock equations at finite temperature characterized by a one body density matrix  $\rho_0$  such that

$$[W_0, \rho_0] = 0. \tag{9.6}$$

Substituting  $\rho(t) = \rho_0 + \delta \rho(t)$  into the evolution equation, and retaining only linear terms in  $\delta \rho$ , we obtain

$$i\frac{\partial}{\partial t}\delta\rho = [W_0, \delta\rho] + [\delta W, \rho_0]. \tag{9.7}$$

Considering the matrix element m, n of this equation we find

$$i\frac{\partial}{\partial t} < m|\delta\rho|n > = (\epsilon_m - \epsilon_n) < m|\delta\rho|n > + < m|\delta W|n > (f_n - f_m), \qquad (9.8)$$

where  $f_n = \langle n | \rho_0 | n \rangle$  is the usual Fermi occupation number. Note that the structure of this equation implies that only the matrix elements with  $m \neq n$  need to be considered. In contrast matrix elements of  $\delta \rho$  with m = n are constants of the motion.

Calculating the change  $\delta W$  in the mean field from equation (9.5) we find that the linearized evolution equation can be written as

$$i\dot{X} = (\Delta \epsilon + F \mathcal{V})X, \tag{9.9}$$

where the vector X is defined by its components

$$X_{mn} = \langle m | \delta \rho | n \rangle, \tag{9.10}$$

and where the matrices  $\Delta \epsilon, F, V$  are the matrices which were introduced in section 7 to define the particle hole Green functions (equations 7.8,7.9,7.11).

The matrix  $(\Delta \epsilon + F \mathcal{V})$  is also related to the response of the system to a small external field. Suppose that at time minus infinity the system is in thermal equilibrium, described by a static Hartree Fock density matrix  $\rho_0$ , and submitted at later times to the external field

$$V_{ext} = \lambda \{ e^{-i(\omega+i\eta)t}O + e^{i(\omega-i\eta)t}O^+ \}.$$
(9.11)

In this equation O is a one body operator (e.g. the dipole operator in the case of an external electric field). The quantity  $\eta$  is a vanishingly small number corresponding to an adiabatic switching of the external perturbation. We consider the limit where the strength  $\lambda$  goes to zero for which linearized evolution equations can be used. In this case we find:

$$i\frac{\partial}{\partial t} < m|\delta\rho|n > = (\epsilon_m - \epsilon_n) < m|\delta\rho|n > + < m|\delta W + V_{ext}|n > (f_n - f_m), \qquad (9.12)$$

If we define a vector |O> whose components are

$$O_{mn} = \langle m | O | n \rangle, \tag{9.13}$$

we find that  $\langle m | \delta \rho | n \rangle = X_{mn}(t) + X_{nm}^{*}(t)$  where the vector X satisfies the evolution equation

$$\{i\partial_t - (\Delta \epsilon + F\mathcal{V})\}|X\rangle = -\lambda e^{-i(\omega + i\eta)t}F|O\rangle.$$
(9.14)

The solution of this equation satisfying the boundary condition X = 0 at large negative times is

$$|X\rangle = -\lambda e^{-i(\omega+i\eta)t} R(\omega)|O\rangle, \qquad (9.15)$$

where  $R(\omega)$  is the response function

$$R(\omega) = \frac{1}{\omega + i\eta - (\Delta \epsilon + F \mathcal{V})} F.$$
 (9.16)

This equation can also be written as

$$R(\omega) = F \frac{1}{\omega + i\eta - (\Delta \epsilon + \mathcal{V}F)}.$$
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$$(\Delta \epsilon + F \mathcal{V}) = \sum_{n>0} E_n \{ |Y_n| > \langle Y_n| + |Y_n^+| > \langle Y_n^+| \} \frac{1}{F}$$
(9.18)

where

$$|Y_n\rangle = F|X_n\rangle. \tag{9.19}$$

Indeed the action of this operator on the basis vectors  $|Y_n >$  provides the expected result. We can therefore write

$$R(\omega) = \sum_{n>0} \{ \frac{|Y_n| > < Y_n|}{\omega + i\eta - E_n} - \frac{|Y_n^+| > < Y_n^+|}{\omega + i\eta + E_n} \}.$$
 (9.20)

Displaying the indices explicitely we find the following formula

$$< ph|R(\omega)|p'h'> = \sum_{n>0} \{ \frac{Y_{ph}^{(n)}Y_{p'h'}^{\star(n)}}{\omega + i\eta - E_n} - \frac{Y_{hp}^{(n)}Y_{h'p'}^{\star(n)}}{\omega + i\eta + E_n} \}.$$
(9.21)

### 10 Linear response theory in hot nuclear matter

The formalism presented in the previous section becomes particularly simple in the case of nuclear matter, for which the single particle states are plane waves. Single particle states are thus labeled by the three quantum numbers  $(\mathbf{k}, \sigma, \tau)$  where  $\mathbf{k}$  is the wave number,  $\sigma$  the spin and  $\tau$  the isospin. Matrix elements of the response function  $R(\omega)$  are thus of the form

$$<\mathbf{k}_{1},\sigma_{1},\tau_{1};\mathbf{k}_{2},\sigma_{2},\tau_{2}|R(\omega)|\mathbf{k}_{3},\sigma_{3},\tau_{3};\mathbf{k}_{4},\sigma_{4},\tau_{4}>.$$
(10.1)

Let us suppose that the two- body interaction V is invariant under spin and isospin rotations. In this case, if we couple in the above matrix element particles 1 and 2 to a total spin  $(S, M_S)$ , total isospin  $(T, M_T)$  and particles 3 and 4 to  $(S', M'_S), (T', M'_T)$ , then the matrix R will be diagonal in the quantum numbers  $S, M_S, T, M_T$  and will not depend on  $M_S$  or  $M_T$ . The matrix R thus falls into four blocks characterized by the four possible values of the quantum numbers (S, T)

$$<\mathbf{k}_1,\mathbf{k}_2|R_{ST}(\omega)|\mathbf{k}_3,\mathbf{k}_4>. \tag{10.2}$$

Let us now specialize to the case of a local interaction  $V_{ST}(\mathbf{r}_1 - \mathbf{r}_2)$  in the channel (S, T) and let us furthermore ignore exchange terms in a first step. From the definition of the interaction matrix  $\mathcal{V}$  we have

$$\langle \mathbf{k}_1, \mathbf{k}_2 | \mathcal{V}_{ST} | \mathbf{k}_3, \mathbf{k}_4 \rangle = \langle \mathbf{k}_1, \mathbf{k}_4 | \mathcal{V}_{ST} | \mathbf{k}_2, \mathbf{k}_3 \rangle \\ = \delta(\mathbf{q} - \mathbf{q}') \tilde{\mathcal{V}}_{ST}(\mathbf{q}) / (2\pi)^3.$$

$$(10.3)$$

In this formula we have introduced the momentum transfer variables

$$q = k_1 - k_2$$
  $q' = k_3 - k_4$ , (10.4)

and  $\overline{V}$  is the Fourier transform of V

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$$\tilde{V}(\mathbf{q}) = \int V(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r}.$$
 (10.5)

We thus see that the response function  $R(\omega)$  is diagonal in the momentum transfer q. In contrast the matrix elements of  $\mathcal{V}$  are independent of the total momentum variables

$$K = k_1 + k_2$$
  $K' = k_3 + k_4$ . (10.6)

Therefore  $\mathcal{V}$  is not diagonal in K. However it is possible to construct an explicit expression for the matrix elements of  $R(\omega)$  in the basis  $|\mathbf{K}, \mathbf{q} \rangle$ . The first step is to expand the RPA response function as

$$R(\omega) = R_0(\omega) + R_0(\omega) \mathcal{V} R_0(\omega) + \dots$$
(10.7)

where  $R_0(\omega)$  is the bare response corresponding to  $\mathcal{V} = 0$ . The second step is to examine the structure of the matrix elements of the successive terms in the basis  $|\mathbf{K}, \mathbf{q}\rangle$ . We first find

$$< \mathbf{K}, \mathbf{q} | R_0 \mathcal{V} R_0 | \mathbf{K}', \mathbf{q}' > = \delta(\mathbf{q} - \mathbf{q}') R_0(\mathbf{K}, \mathbf{q}) R_0(\mathbf{K}', \mathbf{q}) \overline{\mathcal{V}}(\mathbf{q}) / (2\pi)^3,$$
 (10.8)

where  $R_0(\mathbf{K}, \mathbf{q})$  is defined as

$$R_0(\mathbf{K},\mathbf{q}) = -\frac{f(\mathbf{K}+\mathbf{q}/2) - f(\mathbf{K}-\mathbf{q}/2)}{\omega - \epsilon(\mathbf{K}+\mathbf{q}/2) + \epsilon(\mathbf{K}-\mathbf{q}/2) + i\eta}.$$
 (10.9)

Similarly, by using the closure relation

$$\mathbf{1} = \int d\mathbf{K} d\mathbf{q} | \mathbf{K}, \mathbf{q} \rangle \langle \mathbf{K}, \mathbf{q} |, \qquad (10.10)$$

and the previous relation, we obtain

$$<\mathbf{K},\mathbf{q}|R_{0}\mathcal{V}R_{0}\mathcal{V}R_{0}|\mathbf{K}',\mathbf{q}'>=\delta(\mathbf{q}-\mathbf{q}')R_{0}(\mathbf{K},\mathbf{q})R_{0}(\mathbf{K}',\mathbf{q})\tilde{V}(\mathbf{q})\Pi_{0}(\omega,\mathbf{q})\tilde{V}(\mathbf{q}),\qquad(10.11)$$

where  $\Pi_0(\omega, \mathbf{q})$  is the so called Lindhard function, defined as [3]

$$\Pi_0(\omega, \mathbf{q}) = \frac{1}{(2\pi)^3} \int d\mathbf{K} R_0(\mathbf{K}, \mathbf{q}).$$
(10.12)

By induction the expression of the response function is found to be

$$(2\pi)^{3} < \mathbf{K}, \mathbf{q} | R(\omega) | \mathbf{K}', \mathbf{q}' > = (2\pi)^{3} \delta(\mathbf{q} - \mathbf{q}') \delta(\mathbf{K} - \mathbf{K}') R_{0}(\mathbf{K}, \mathbf{q}) + \delta(\mathbf{q} - \mathbf{q}') R_{0}(\mathbf{K}, \mathbf{q}) R_{0}(\mathbf{K}', \mathbf{q}) \frac{\tilde{V}(\mathbf{q})}{1 - \Pi_{0}(\omega, \mathbf{q}) \tilde{V}(\mathbf{q})}.$$
(10.13)

The response function is thus seen to have poles when  $1 = \prod_0 \tilde{V}$ . The location of these poles determines the energy  $\omega$  and the lifetime of the collective modes. For a more detailed discussion see [3].

When exchange terms are included an additional contribution to the interaction matrix  $\delta(\mathbf{q} - \mathbf{q}')\tilde{V}(\mathbf{K} - \mathbf{K}')$  arises and the construction of the response function is more complicated. An important exception is the case of zero range forces for which the direct and exchange terms have the same structure. The case of a zero range force including a quadratic velocity dependence can also be rather easily handled provided generalized Lindhard functions are introduced [4].

The Lindhard function  $II_0$  occurs in a wide variety of problems. As an illustrative example we now consider the problem of the determination of the mean free path of neutrinos in neutron matter. In this case the optical potential  $\Gamma$  governing the propagation of a neutrino with a momentum k is given by [5, 6, 7]

$$\Gamma(\mathbf{k}) = \frac{G_F^2}{(2\pi)^3} \int f(E_{\mathbf{p}}) \{1 - f(E_{\mathbf{p}+\mathbf{q}})\} \delta(\omega + E_{\mathbf{p}} - E_{\mathbf{p}+\mathbf{q}}) d\mathbf{p} d\mathbf{k}', \qquad (10.14)$$

where  $G_F$  is the Fermi constant,  $\mathbf{q} = \mathbf{k} - \mathbf{k}', \, \omega = |\mathbf{k}| - |\mathbf{k}'|, \, E_{\mathbf{p}} = p^2/2m$ . Using the relation

$$f(E_{\mathbf{p}})\{1 - f(E_{\mathbf{p}+\mathbf{q}})\} = \frac{1}{1 - \exp(-\beta\omega)}\{f(E_{\mathbf{p}}) - f(E_{\mathbf{p}+\mathbf{q}})\},$$
 (10.15)

we see that the integrand is related, up to a factor  $1 - \exp(-\beta\omega)$ , to the imaginary part of the Lindhard function. Explicitly

$$\Gamma(\mathbf{k}) = -\frac{G_F^2}{(2\pi)^2} \int \frac{1}{1 - \exp(-\beta\omega)} \mathrm{Im}\Pi_0(\mathbf{q},\omega) d\mathbf{k}', \qquad (10.16)$$

where  $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ ,  $\omega = |\mathbf{k}| - |\mathbf{k}'|$ . The imaginary part of the Lindhard function can be evaluated analytically due to the presence of the  $\delta$  function. The result is

$$\mathrm{Im}\Pi_{0}(\mathbf{q},\omega) = -\frac{m^{2}}{2\pi g}\log\frac{1+e^{\beta(A+\omega/2)}}{1+e^{\beta(A-\omega/2)}},$$
(10.17)

with

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$$A = \mu - \frac{m\omega^2}{2q^2} - \frac{q^2}{8m^2},$$
 (10.18)

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 $\mu$  being the chemical potential of the neutrons. In the range  $T \ll \mu$ , which is relevant for supernovae explosions ( $\mu \simeq 50 \text{MeV}, T < 10 \text{MeV}$ ), the following approximate formula can be derived

$$\Gamma(\mathbf{k}) = \frac{G_F^2}{3(2\pi)^3} \left(\frac{km}{m+p_F}\right)^3 \left(\frac{3T}{k} + \frac{m+p_F}{p_F} + 1 + \ldots\right)$$
(10.19)

where  $p_F = \sqrt{2m\mu/\hbar^2}$ . It is worthwhile noting that for neutron matter just above nuclear density (e.g.  $p_F = 300 \text{MeV}$ , k = 5 MeV, T = 10 MeV, m = 940 MeV) the previous equation gives a mean free path of the order of 1.5 km. In contrast just below nuclear density, the presence of nuclei allows coherent neutrino scattering which leads to a mean free path of the order of 1 cm only [7].

## References

- [1] D.J. Thouless, Quantum Mechanics of Many Body Systems, Academic, New York, 1964.
- [2] J. des Cloizeaux, in Many Body Physics, Les Houches Lectures, 1967, C. de Witt and R. Balian Eds., Gordon and Breach, New York, 1968.
- [3] A.L. Fetter and J.D. Walecka, cited in chapter 1. The definition given by these authors in their formula 15.9 is a factor two larger than ours because it already includes the trace over spin variables.
- [4] C. Garcia- Recio, J. Navarro, Nguyen van Giai and L.L Salcedo Ann. Phys. 214 (1992) 293
- [5] N. Iwamoto and C.J. Pethick, Phys. Rev. D25 (1982) 313
- [6] P. Haensel and A.J. Jerzak, Astron. Astrophys. 179 (1987) 127
- [7] J.L. Basdevant, Ph. Chomaz and D. Vautherin, Neutrino propagation in hot dense neutron matter, Orsay preprint IPNO/TH 90-48

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# **III GIANT RESONANCES IN HOT NUCLEI**

### 11 Photoabsorption by hot nuclei

Let us consider a nucleus in thermal equilibrium at temperature T. We describe it in the mean field approximation by its one body density matrix  $\rho_0$ . We suppose that at time t=0, it begins to interact with an electromagnetic plane wave, described by the vector potential

$$\mathbf{A}(\mathbf{r},t) = \mathbf{e}_{z} \frac{\mathcal{E}}{\omega} \sin(ky - \omega t). \tag{11.1}$$

In the long wavelength limit  $kR \ll 1$ , where R is the nuclear radius, the interaction hamiltonian can be approximated by

$$V_{ext} = -\mathbf{d}.\mathbf{E}(t) = -q\mathcal{E}z\cos\omega t \tag{11.2}$$

where d = qz is the dipole operator, E the electric field  $-\partial A/\partial t$  and q the proton charge. To calculate the response of the nucleus we use the results of the previous section. The one body density matrix at time t can be expressed as

$$< m|\rho|n> = < m|\rho_0|n> + x_{mn}(t) + x_{nm}^*(t)$$
 (11.3)

where the vector x is given by

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n

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n

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$$2|x > = \sum_{n>0} \mathcal{E}\left\{\frac{1}{\omega + i\eta + E_n} |Y_n| < Y_n |d > (e^{i(\omega + i\eta)t} - e^{-iE_nt}) - \frac{1}{\omega + i\eta - E_n} |Y_n^+| < Y_n^+ |d > (e^{i(\omega + i\eta)t} - e^{iE_nt})\right\},$$
(11.4)

and where  $d_{mn} = \langle m|qz|n \rangle$ . To obtain this relation we have first constructed a particular solution of the evolution equation. In a second step we have subtracted, in order to satisfy the boundary condition  $\rho(t=0) = \rho_0$ , a superposition of the solutions  $|Y_n \rangle \exp(-iE_n t)$  and  $|Y_n^+ \rangle \exp(iE_n t)$  of the homogeneous equation. This formula can also be written as

$$\begin{aligned} |x\rangle &= i\mathcal{E}\sum_{n>0} \left\{ |Y_n\rangle < Y_n | d\rangle e^{i(\omega - E_n)t/2} \frac{\sin(\omega + E_n)t/2}{\omega + E_n} \\ &- |Y_n^+\rangle < Y_n^+ | d\rangle e^{-i(\omega + E_n)t/2} \frac{\sin(\omega - E_n)t/2}{\omega - E_n} \right\}, \end{aligned}$$
(11.5)

where the limit  $\eta \to 0$  has been performed. At sufficiently large times (but not too large for first order perturbation theory to be valid) it is legitimate to make the substitution :

$$\frac{\sin(\omega-E_n)t/2}{(\omega-E_n)/2}\sim 2\pi t\delta(\omega-E_n). \tag{11.6}$$

The excitation of the system at time t is given by the expectation value of the matrix  $(\Delta \epsilon + F \mathcal{V})$ :

$$E(t) - E(t=0) = \langle x(t) | (\Delta \epsilon + F \mathcal{V}) F | x(t) \rangle. \qquad (11.7)$$

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#### exercise 9.1

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Why is it possible to obtain an expression up to second order in the external field  $\mathcal{E}$  for the energy while the change in the density matrix was calculated only up to first order in  $\mathcal{E}$ ?

#### answer

The mean field evolution equation preserves the eigenvalues of one body density matrix  $\rho$ . It can thus be written at all times as

$$\rho(t) = e^{i\chi} \rho_{HF} e^{-i\chi}, \qquad (11.8)$$

where  $\chi$  is a one body operator

$$\chi = \sum_{mn} \langle n | \chi | m \rangle a_m^+ a_n. \tag{11.9}$$

If we expand the one body density matrix up to second order in  $\chi$  as

$$\rho(t) = \rho_{HF} + \rho_1 + \rho_2 + \dots \tag{11.10}$$

we thus find that the matrix elements of the first order term  $i[\chi, \rho_{HF}]$  automatically determine those of the second order term. The contribution of  $\rho_2$  can thus be hidden in the above expression for the excitation energy. This generates the term  $\Delta \epsilon$  in this formula.

Using the properties of the RPA solutions we thus find

$$\frac{E(t) - E(0)}{t} = 2\pi \sum_{n > 0} |\langle d|F|X_n \rangle|^2 E_n \{\delta(\omega - E_n) + \delta(\omega + E_n)\}$$
(11.11)

The photoabsorption cross section is the energy absorbed per unit time by the nucleus divided by the modulus of the Poynting vector of the incident plane wave :

$$G = \epsilon_0 c^2 |\mathbf{E} \times \mathbf{B}| = \epsilon_0 c \mathcal{E}^2 / 2. \tag{11.12}$$

This procedure provides the following result :

$$\sigma(\omega) = 4\pi^2 \alpha \sum_{n>0} |\langle d|F|X_n \rangle|^2 E_n \delta(E_n - \omega), \qquad (11.13)$$

where  $\alpha$  is the fine structure constant  $q^2/4\pi\epsilon_0\hbar c$ .

The strength function is  $\sigma(\omega)/4\pi^2 \alpha \omega$  i.e.

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$$S(\omega) = \langle d|\Im mR(\omega)|d\rangle$$
(11.14)

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where R is the response function defined in the previous section. The present result misses a factor  $1 - \exp(-\beta\omega)$  discussed in section 10 and reference [1]. This is because our calculation allows both absorption and emission of photons from the hot nucleus and is not restricted to absorption only.

### 12 sum rules at finite temperature

For nuclei at zero temperature the photoabsorption cross section calculated in the random phase approximation satisfies the well known sum rule

$$\int_0^\infty \sigma(\omega) d\omega = \frac{1}{2} < HF | [\mathbf{d}, [H, \mathbf{d}] ] | HF >, \qquad (12.1)$$

where d is the dipole operator and  $|HF\rangle$  the Hartree-Fock ground state. For a local interaction without exchange terms only the kinetic energy operator contributes to the double commutator and the result is

$$\int_0^\infty \sigma(\omega)d\omega = \frac{3}{4\pi} \frac{\hbar^2}{2M} \frac{NZ}{A} \times 4\pi^2 \alpha.$$
(12.2)

In this formula M is the nucleon mass while N, Z and A are the neutron, proton and mass numbers respectively.

The above equations can be generalized to the case of photoabsorption at finite temperature. Indeed from the RPA expression of the cross section we find

$$\int_0^\infty \sigma(\omega)d\omega = 4\pi^2 \alpha \sum_{n>0} |\langle d|F|X_n \rangle|^2 E_n.$$
(12.3)

The right hand side of this expression is a special case of the moment of order k of the RPA distribution of eigenvalues at temperature T, which for a given one body operator  $\chi$  is defined by

$$m_k(\chi,T) = \sum_{n>0} |\langle \chi|F|X_n \rangle|^2 E_n^k.$$
(12.4)

Note that in this equation the temperature dependance of the right hand side is contained not only in the RPA eigenvalues and eigenvectors E and X but also in the occupation number matrix F.

Let us now show that, in the random phase approximation at finite temperature, one has the following sum rule

$$m_1(\chi, T) = \frac{1}{2} \operatorname{Trace} \{ D_{HF}(T)[\chi, [H, \chi]] \}$$
(12.5)

where  $D_{HF}$  is the Hartree-Fock density matrix at temperature T. To establish this relation we consider a small change of the density matrix defined by

$$D = \exp(i\epsilon\chi)D_{HF}\exp(-i\epsilon\chi)$$
(12.6)

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where  $\epsilon$  is a small number. In this transformation the first order change in the one body density matrix is

$$< m |\delta^{(1)}\rho|n> = i\epsilon < m |[\chi,\rho]|n>, \qquad (12.7)$$

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$$< m |\delta^{(1)}\rho|n> = i\epsilon(f_n - f_m) < m |\chi|n>,$$
 (12.8)

while the second order change is given by

$$< m |\delta^{(2)}\rho|n> = -\frac{\epsilon^2}{2} < m |[\chi, [\chi, \rho]]|n>.$$
 (12.9)

The change in the grand potential A is thus, in the notations of section 8

$$\Delta A = \frac{1}{2}\epsilon^2 < \chi |F(\Delta \epsilon + \mathcal{V}F)|\chi > . \qquad (12.10)$$

By using the completeness of the RPA solutions we can transform this formula into

$$\Delta A = \epsilon^2 \sum_{n>0} E_n |<\chi|F|X_n > |^2.$$
(12.11)

However the change  $\Delta A$  can also be evaluated directly from the expression of the density matrix with the result

$$\Delta A = -\frac{1}{2}\epsilon^2 \operatorname{Trace} \{ D_{HF}[[H,\chi],\chi] \}, \qquad (12.12)$$

which establishes the sum rule (12.5).

For the dipole operator

$$d = \sum_{i=1}^{Z} \{ r_i Y_{10}(\theta_i, \varphi_i) - R Y_{10}(\hat{R}) \}, \qquad (12.13)$$

one has (for a local interaction without charge exchange terms)

$$m_1(d,T) = \frac{3}{4\pi} \frac{\hbar^2}{2M} \frac{NZ}{A},$$
 (12.14)

which is exactly the zero temperature result.

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For the isoscalar quadrupole operator

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$$Q = \sum_{i=1}^{Z} r_i^2 Y_{20}(\theta_i, \varphi_i), \qquad (12.15)$$

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there is in contrast a temperature dependence since

$$m_1(Q,T) = \frac{5}{4\pi} \frac{\hbar^2}{M} A \operatorname{Trace}\{r^2 D_{HF}(T)\}.$$
 (12.16)

## 13 Observation of giant resonances in hot nuclei

As was already mentioned in the introduction of this course giant collective oscillations were first observed in the early eighties by the Berkeley group [2]. This group used an 1150 MeV <sup>136</sup>Xe beam to produce deep inelastic collisions with a <sup>181</sup>Ta target. Excitation energies of the target nucleus of 40, 80, 120, 160, 200 MeV were selected and the photons emitted from these highly excited nuclei were observed. These experiments revealed that the photon spectrum contains in addition to the thermal spectrum  $N(E) = \exp(-E/kT)$  a broad and well developed peak. As an example we show in the figure below more recent data obtained at the GANIL facility for very hot nuclei ( $T \simeq 5$ MeV) formed in the Argon-36 + Zirconium-90 reaction at 27 MeV per nucleon bombarding energy. This figure gives the number of photons emitted by a hot Tin-115 nucleus as a function of the photon energy [3]. The dotted lines are exponential fits to the statistical and bremsstrahlung part of the spectrum while the upper right corner gives the difference between the sum of these two curves and the observed spectrum.





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As for zero temperature the peak occurring around 15 MeV is interpreted as a collective dipole oscillation in which neutrons oscillate against protons. As was mentioned in the introduction the possibility of having giant resonances built on nuclear excited states was suggested in 1955 by David Brink in his thesis [4].

A large amount of information on giant resonances is by now available. It has first been verified that there is a good evidence of thermalization of the nucleus in these reactions. This has been checked by observing photons emitted from compound nuclei obtained by the fusion of various systems e.g.  ${}^{63}Cu$  obtained in  ${}^{4}He + {}^{59}Co, {}^{6}Li + {}^{57}Fe, {}^{12}C + {}^{51}V$  and  ${}^{18}O + {}^{45}Sc$  reactions [5]. Spectra obtained from these four reactions were found to be indistinguishable. The data obtained by now indicate that, to a good precision, the energy of the giant dipole resonance is independent of temperature while its width increases strongly at moderate excitation (about 130 MeV in Sn isotope) with a saturation for higher excitation energies [6, 7, 3, 8, 9].

## 14 The schematic model at finite temperature

The simplest description of giant resonances is through the schematic model of Brown and Bolsterli [10]. We consider a simple version of this model in which N active particles occupy 2N levels, N with a single particle energy  $\epsilon_1$  and N with an energy  $\epsilon_2 > \epsilon_1$  as described in the

figure below.

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N particles  $\mu = (\epsilon_1 + \epsilon_2)/2$  (14.1)

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 N levels  $\epsilon_1$ 

The chemical potential is thus independent of temperature

$$\mu = (\epsilon_1 + \epsilon_2)/2, \tag{14.2}$$

and the occupation numbers of the levels 1 and 2 are respectively

$$f_1 = \frac{1}{1 + exp(\frac{\epsilon_1 - \epsilon_2}{T})},$$
 (14.3)

and

$$f_2 = \frac{1}{1 + exp(\frac{c_2 - c_1}{T})}.$$
 (14.4)

A further assumption of the model is that the two body interaction is separable i.e.

$$< ph|\mathcal{V}|p'h'> = \lambda v_{ph} v_{p'h'}^*, \tag{14.5}$$

with  $v_{ph} = v_{hp}^*$ . This equation can be written as

$$\mathcal{V} = \lambda |v\rangle \langle v| . \tag{14.6}$$

For such a model the RPA matrix

$$M_{ij,kl} = \langle i, j | (\Delta \epsilon + F \mathcal{V}) | k, l \rangle, \qquad (14.7)$$

is a 2 by 2 matrix since the indices (i, j) can take only the values (1, 2) and (2, 1). The single particle energy matrix reads

$$\Delta \epsilon = \begin{pmatrix} -\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}, \tag{14.8}$$

with  $\epsilon = \epsilon_2 - \epsilon_1$ . The occupation number matrix is given by

$$F = \begin{pmatrix} -f & 0 \\ 0 & f \end{pmatrix}, \tag{14.9}$$

with

$$f = f_1 - f_2 = \tanh(\frac{\epsilon_2 - \epsilon_1}{2T}). \tag{14.10}$$

From these formulae we construct the explicit expression of the RPA matrix

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$$(\Delta \epsilon + F \mathcal{V}) = \begin{pmatrix} -\epsilon - f |v|^2 & -f v^2 \\ f v^{*2} & \epsilon + f |v|^2 \end{pmatrix}.$$
 (14.11)

The positive eigenvalue of this matrix gives the excitation energy E of the giant resonance at temperature T

$$E = \pm (\epsilon_2 - \epsilon_1) \sqrt{1 + \frac{2\lambda |v|^2}{(\epsilon_2 - \epsilon_1)} \tanh(\frac{\epsilon_2 - \epsilon_1}{2T})}$$
(14.12)

As an illustration let us consider the case of lead-208 for which we take the distance between shells to be  $\epsilon_2 - \epsilon_1 = 7$  MeV. If we adjust the strength of the interaction to reproduce the energy of the giant dipole state at zero temperature E = 14MeV we find

$$\frac{2\lambda|v|^2}{\epsilon_2-\epsilon_1}=3. \tag{14.13}$$

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With this value of the strength parameter the energy of the giant dipole is found to be

$$E = 12 \text{ MeV for } T = 2.5 \text{ MeV}$$
  

$$E = 10 \text{ MeV for } T = 5 \text{ MeV}$$
  

$$E = 8 \text{ MeV for } T = 10 \text{ MeV}.$$
(14.14)

The energy of the giant dipole thus decreases slowly when temperature increases. This is in contradiction with experimental observations which suggest a value independent of temperature. The reason for this discrepancy is that we assumed all the particle states to have the same energy  $\epsilon_2$  and all the hole states to have the same energy  $\epsilon_1$ . As a result when temperature increases the matrix  $\Delta \epsilon + \mathcal{V}F$  tends to  $\Delta \epsilon$  i.e. collective effects decrease. In more realistic calculations many configurations of the form pp' or hh' appear at non zero temperature since  $f_p - f_{p'}$  or  $f_h - f_{h'}$  is no longer zero. These new configurations induce additional collective effects which compensate the decrease of the matrix  $\mathcal{V}F$ . As a result the location of the giant dipole state remains unchanged as we will show in the next section.

### 15 Numerical solution of the thermal RPA equations

For more simplicity we consider a density dependent effective interaction of the form

$$V = \{t_0 + \frac{t_3}{6}\rho^{\sigma}(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2})\}\delta(\mathbf{r}_1 - \mathbf{r}_2).$$

For such an interaction the single particle Hartree- Fock wave functions can be written as

$$\varphi_i(\mathbf{r},\sigma) = R_{n_i\ell_i}(\tau)Y_{\ell_im_i}(\theta,\varphi)\chi_{\sigma_i}(\sigma).$$
(15.1)

In order to show how the angular reduction of the RPA equations is performed in this simple case we introduce the following notation. We use a single index  $\alpha$  to denote the set of quantum numbers

$$\alpha \equiv \{n_p; \ell_p; n_h, \ell_h\}.$$
 (15.2)

Similarly we define

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$$\boldsymbol{\beta} \equiv \{\boldsymbol{n}_{p'}, \boldsymbol{\ell}_{p'}; \boldsymbol{n}_{h'}, \boldsymbol{\ell}_{h'}\}. \tag{15.3}$$

The notation  $\alpha > 0$  means that the single particle energy of the particle state is higher than that of the hole state i.e.

$$\epsilon(n_p, \ell_p) > \epsilon(n_h, \ell_h). \tag{15.4}$$

We also denote by  $\bar{\alpha}$  the set of quantum numbers in which particles and holes are interchanged

$$\bar{\alpha} \equiv \{n_h, \ell_h; n_p \ell_p\}. \tag{15.5}$$

For a spherical nucleus we decompose the RPA eigenvectors  $X_{ph} = X(n_p, \ell_p, m_p; n_h, \ell_h, m_h)$ into their angular components as

$$X_{ph} = (-1)^{m_p} \sum_{LM} (2L+1) \begin{pmatrix} \ell_p & \ell_h & L \\ -m_p & m_h & M \end{pmatrix} X_{\alpha}^{LM}.$$
 (15.6)

By using the orthogonality of the Wigner coefficients this relation can be inverted to give

$$X_{\alpha}^{LM} = \sum_{m_{p}m_{h}} (-1)^{m_{p}} \begin{pmatrix} \ell_{p} & \ell_{h} & L \\ -m_{p} & m_{h} & M \end{pmatrix} X_{ph}.$$
 (15.7)

With this decomposition we find that the RPA matrix is diagonal by block, each block being characterized by the quantum numbers L and M, and being independent of M. For instance the linearized evolution equation for the amplitude  $X_{\alpha}$  reads for  $\alpha > 0$ :

$$i\hbar \dot{X}_{\alpha}^{LM} = \Delta \epsilon_{\alpha} X_{\alpha}^{LM} + F_{\alpha} \sum_{\beta > 0} A_{\alpha\beta}^{(L)} X_{\beta}^{LM} + B_{\alpha\beta}^{(L)} X_{\bar{\beta}}^{LM}$$
(15.8)

where

$$\Delta \epsilon_{\alpha} = \epsilon(n_p, \ell_p) - \epsilon(n_h, \ell_h),$$
  

$$F_{\alpha} = -f(n_p, \ell_p) + f(n_h, \ell_h).$$
(15.9)

The matrices A and B depend on the quantum number L only :

$$A_{\alpha\beta}^{L} = \frac{1}{4\pi} I_{\alpha\beta} \hat{\ell}_{p} \hat{\ell}_{l} \hat{\ell}_{p'} \hat{\ell}_{l'} \begin{pmatrix} \ell_{p} & \ell_{h} & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_{p'} & \ell_{l'} & L \\ 0 & 0 & 0 \end{pmatrix}$$

$$B_{\alpha\beta}^{L} = A_{\alpha\beta}^{L}$$
(15.10)

where the notation  $\hat{\ell}$  stands for  $(2\ell+1)^{1/2}$  and where I is the radial integral

$$I_{\alpha\beta} = \int_{0}^{\infty} Rn_{p}\ell_{p}(r)Rn_{p'}\ell_{p'}(r)Rn_{h}\ell_{h}(r)Rn_{h'}\ell_{h'}(r) \\ \{\frac{3}{4}t_{0} + \frac{t_{3}}{16}(1+\sigma)(2+\sigma)\rho^{\sigma}(r)\}r^{2}dr.$$
(15.11)

Results of an RPA calculation for the dipole mode in calcium -40 are shown in figure 15.1. This calculation uses a model space including 1s, 1p, 2s, 1d, 2p, 1f and 1g levels. It requires the diagonalisation of a 30  $\times$ 30 matrix (equation 15.8). The single particle wave functions are chosen to be oscillator wave functions with a parameter b = 1.8 fm and the single particle energies were taken from reference [11]. The interaction is a simple delta force  $t_0 = -700$  MeV  $\times$  fm<sup>3</sup>,  $t_3 = 0$ .



#### Figure 15.1

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In figure 15.1, each RPA state is represented by a line, the length of which is proportional to the dipole strength  $S_n = |\langle d|F|X_n \rangle|^2$ . While at zero temperature all the strength is concentrated near E = 20 MeV it can be seen that at temperatures of T = 2 MeV and T = 4MeV the presence of new particle-particle and hole-hole configurations produces the appearance of a wider spreading of the dipole strength. This effect provides a mechanism suitable to explain a broadening of the giant dipole when temperature increases. The present calculation is however too crude to reproduce the observed saturation in the increase of the dipole width at high temperature. We wish to point out that the calculation we have described should be taken as a pedagogical exercise only. More realistic calculations including spin orbit terms, pairing, nuclear rotations and nuclear deformations can be found in the literature [12, 13, 14, 15, 16, 17]

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# 16 The level density parameter in excited nuclei

In section 3 we showed that the number of levels per unit energy interval in a nucleus of mass A,  $\rho(E, A)$ , can be evaluated from the approximate formula [18]:

$$\rho(E,A) = \frac{1}{2\pi\sqrt{D(\alpha_0\beta_0)}} \exp S(\alpha_0,\beta_0). \tag{16.1}$$

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In this formula the quantities appearing on the right side are calculated at the saddle point  $\alpha_0, \beta_0$  such that

$$A = \frac{\partial}{\partial \alpha} \log Z(\alpha_0, \beta_0), \qquad E = -\frac{\partial}{\partial \beta} \log Z(\alpha_0, \beta_0). \tag{16.2}$$

The quantity  $S(\alpha_0, \beta_0)$  is the entropy

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$$S = (1 - \alpha \frac{\partial}{\partial \alpha} - \beta \frac{\partial}{\partial \beta}) \log Z(\alpha, \beta), \qquad (16.3)$$

and D the determinant of the second derivatives of  $\log Z(\alpha,\beta)$  at the saddle point

$$D = \begin{vmatrix} \partial^2 \log Z / \partial \alpha^2 & \partial^2 \log Z / \partial \alpha \partial \beta \\ \partial^2 \log Z / \partial \alpha \partial \beta & \partial^2 \log Z / \partial \beta^2 \end{vmatrix}.$$
 (16.4)

Applying these formulae to a Fermi gas at a temperature T much smaller than the Fermi energy  $\epsilon_F$  one obtains the well known Bethe formula [18]

$$\rho(E^*, A) = \frac{1}{E^* \sqrt{48}} \exp \sqrt{2aE^*}, \qquad (16.5)$$

where  $E^* = E - E_0$  is the excitation energy with respect to the ground state and *a* the so called level density parameter

$$a = \frac{\pi}{6} \mathcal{D}(\epsilon_F). \tag{16.6}$$

In this formula  $\mathcal{D}(\epsilon_F)$  is the density of single particle levels at the Fermi surface. For a Fermi gas

$$\mathcal{D}(\epsilon_F) = \frac{3A}{2\epsilon_F}.$$
 (16.7)

To a given excitation energy  $E^*$  one can associate a temperature T by the formula

$$E^* = aT^2. \tag{16.8}$$

In terms of the temperature the entropy is

 $S = 2aT. \tag{16.9}$ 

The argument of the exponential in Bethe's formula is thus the entropy of the nucleus as prescribed by equation (16.1).

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Empirically the level density parameter a is found to be A/8 levels per MeV whereas the Fermi gas value is a factor two smaller. Recently renewed interest in this parameter has been reported. Indeed measurements of both temperature and excitation energy in hot nuclei have been performed [19], which allow via the relation  $E^* = aT^2$  a determination of temperature dependence of the level density parameter a(T). Whereas the Fermi gas model predicts a(T) to be independent of T, a sharp decrease in nuclei of mass A = 160 was found near T = 4 MeV from a value a = A/8 levels per MeV to a = A/13 levels per MeV. Why is there such a large deviation from the Fermi gas predictions? It is the purpose of the present section to show that the contribution of giant collective excitations to the partition function can provide part of the explanation.

In order to be able to obtain analytic formulae we consider the schematic model of Brown and Bolsterli. We specialize to the case of lead-208 for which we assume the difference  $\epsilon_2 - \epsilon_1$ between shells to be 7 MeV. We include five collective states : the giant dipole 1<sup>-</sup> observed at 14 MeV, the quadrupole state observed at 4.1 MeV, and the 3<sup>-</sup> (2.6 MeV), 4<sup>+</sup> (4.3 MeV) and 5<sup>-</sup> (3.3 MeV). We adjust the strength  $\lambda_n$  of the separable interaction in each channel in order to reproduce these data at zero temperature.

In this model the change in the partition function due to collective modes can be worked out explicitly through the formulae given above. The result is

$$\log \frac{Z_{RPA}}{Z_{HF}} = -\frac{\beta}{2} \sum_{n} \{E_n - \Delta \epsilon - \frac{1}{2} C_n \Delta \epsilon \coth \beta \frac{\Delta \epsilon}{2}\} - \sum_{n} \log(\frac{1 - e^{-\beta E_n}}{1 - e^{-\beta \Delta \epsilon}}),$$
(16.10)

where  $\Delta \epsilon = \epsilon_2 - \epsilon_1$  and where the sum over *n* runs over the five collective modes listed above. The coefficient  $C_n$  is related to the interaction strength by

$$C_n = 2\frac{\lambda_n}{\Delta\epsilon} < v|v>. \tag{16.11}$$

To obtain the correction to the Hartree-Fock level density parameter we divide the excitation energy  $E^*$  by the square of the temperature. This procedure gives

$$\Delta a = \frac{1}{T^2} \sum_{n} \left\{ \frac{1}{4} C_n \Delta \epsilon \left( \frac{\Delta \epsilon}{2T} \frac{1}{\sinh^2(\beta \Delta \epsilon/2)} + 1 - \coth\left(\frac{\beta \Delta \epsilon}{2}\right) \right) + \frac{E_n}{\exp(\beta E_n) - 1} - \frac{\Delta \epsilon}{\exp(\beta \Delta \epsilon) - 1} \right\}.$$
(16.12)

As a function of temperature this formula leads to the following corrections to the Hartree-Fock level density parameter (expressed in levels per MeV)

$$\Delta a = 3.23(T = 1 \text{ MeV}), 2.97(T = 2 \text{ MeV}), 1.77(3 \text{ MeV})$$
  
$$\Delta a = 1.10(4 \text{ MeV}), 0.73(T = 5 \text{ MeV})$$
 (16.13)

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Compared to the Hartree-Fock value  $a_{HF} \simeq 10 - 15$  levels per MeV [20], we see that collective states increase the level density parameter at zero temperature by about 20 to 30 percent. The increase however is not so pronounced at higher temperatures which explains part of the observed experimental variation. Other effects have been invoked in the literature to explain the remaining part of the variation with temperature of a(T) [21].

#### acknowledgements

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### References

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- [1] Ph. Chomaz, D. Vautherin and N. Vinh Mau, Phys. Lett. B242 (1990) 313
- [2] J.E. Draper et al. Phys. Rev. Lett. 49 (1982) 434
- [3] J.H. Le Faou et al. Proceedings of the XXXI Winter Meeting on Nuclear Physics, Bormio, January 25- 30, 1993
- [4] D.M. Brink, D. Phil. Thesis, University of Oxford 1955, as quoted by J.E. Lynn, The Theory of Neutron Resonance Reactions, Clarendon, Oxford, 1968
- [5] M. Kicinska et al. Phys. Rev. C36 (1987) 612
- [6] J.J. Gaardhoje et al. Phys. Rev. Lett. 56 (1986) 1783
- [7] D.R. Chakrabarty et al. Phys. Rev. C36 (1987) 1886
- [8] A. Bracco et al. Nucl. Phys. A519 (1990) 47c

[9] B. Fornal et al. Zeit. f. Phys. A340 (1991) 59

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[10] G.E. Brown and M. Bolsterli, Phys. Rev. Lett. 3 (1959) 472

[11] D. Vautherin and N. Vinh Mau, Nucl. Phys. A422 (1984) 140

[12] H. Sagawa and G.F. Bertsch, Phys. Lett. B146 (1984) 138

[13] P. Ring et al. Nucl. Phys. A419 (1984) 261

[14] M. Gallardo, M. Dievel, T. Dossing and R.A. Broglia, Nucl. Phys. A443 (1985) 415

• •

. .

[15] J. Bar Touv Phys. Rev. C32 (1985) 1364

[16] M. Sommermann, Ann. Phys. 151 (1983) 163

[17] N. Vinh Mau, Nucl. Phys. A548 (1992) 381

[18] A. Bohr and B. Mottelson, Nuclear Structure, Vol.1, Benjamin, New York, 1969.

 [19] G. Nebbia et al. Phys. Lett. B176 (1986) 20; B. Natowitz et al. Nucl. Phys. A482 (1988) 171c

[20] P. Bonche, S. Levit and D. Vautherin, Nucl. Phys. A427 (1984) 278

[21] R. W. Hasse and P. Schuck Phys. Lett. 179B (1986) 313