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1970 J. Phys. A: Gen. Phys. 3 342

(http://iopscience.iop.org/0022-3689/3/4/004)

J. Phys. A: Gen. Phys., 1970, Vol. 3. Printed in Great Britain

A note on ring integrals and the Fermi function

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MS. received 24*th February* 1970

Abstract. A method which proceeds in a natural fashion via the symmetry properties of the wave functions of a many-body fermion (boson) system of independent identical particles, is employed for the derivation of the Fermi (Bose) function. The analysis makes use of the grand partition function expressed in terms of ring integrals. Spin considerations are included in the case of electrons in a constant uniform magnetic field.

1. Introduction and derivation of the Fermi function

It is well known that in dealing with a many-body system of identical particles, whose dynamical development is determined by the Schrödinger equation, the admissible wave functions are antisymmetric if the system is composed of fermions and symmetric for boson systems.

For the study of the equilibrium thermodynamic properties of an N-body system, one requires the partition function of the system:

$$\begin{aligned} Z_N^{(\mp)} &= \mathrm{Tr}^{(\mp)} \exp(-\beta H_N) \\ &= \int \sum_{\{n\}} \overset{*}{\psi}_n{}^{\mp}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) \exp(-\beta H_N) \psi_n{}^{\mp}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) \prod_{j=1}^{N} \mathrm{d}\boldsymbol{x}_j \end{aligned} \tag{1}$$

where the trace operation is taken against a complete set of antisymmetric$^{(-)}$ (symmetric$^{(+)}$) wave functions of the N-particle Hamiltonian H_N, in the case of fermions (bosons).

In dealing with independent particles (weakly interacting) the N-particle partition function for fermions can be written in terms of the single-particle Green function of the Bloch equation

$$\left(\frac{\partial}{\partial\beta} + H_1\right)\psi(\boldsymbol{x}, \beta) = 0, \qquad \beta = \frac{1}{kT} \tag{2}$$

as

$$Z_N^{(-)} = \frac{1}{N!} \int \prod_{j=1}^{N} \mathrm{d}\boldsymbol{x}_j \begin{vmatrix} \mathrm{G}(\boldsymbol{x}_1\beta|\boldsymbol{x}_1 0) \ldots \mathrm{G}(\boldsymbol{x}_1\beta|\boldsymbol{x}_N 0) \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ \mathrm{G}(\boldsymbol{x}_N\beta|\boldsymbol{x}_1 0) \ldots \mathrm{G}(\boldsymbol{x}_N\beta|\boldsymbol{x}_N 0) \end{vmatrix} \tag{3}$$

(see Montroll and Ward 1958). The case of bosons is obtained by replacing the determinant by a permanent. Ter Haar (1966) gives an interesting derivation of (3).

The direct evaluation of the partition function is in general extremely difficult, and one proceeds via the grand partition function:

$$\Xi^{(\mp)} = \sum_{N=0}^{\infty} z^N Z_N^{(\mp)} \tag{4}$$

for which an asymptotic evaluation of the partition function for large N is feasible. The $(+)$ sign is associated with the permanent form of (3). Now, Fredholm's theory of integral equations, in relation to iterated kernels, provides the following expression for the grand partition function (4):

$$\Xi^{(\mp)} = \exp\left\{ \mp \sum_{l=1}^{\infty} (\mp z)^l \frac{A_l}{l} \right\} \tag{5}$$

where A_l stands for the lth ring integral

$$A_l = \int_V \ldots \int \mathrm{G}(\boldsymbol{x}_1\beta|\boldsymbol{x}_2 0)\mathrm{G}(\boldsymbol{x}_2\beta|\boldsymbol{x}_3 0)\ldots\mathrm{G}(\boldsymbol{x}_l\beta|\boldsymbol{x}_1 0) \prod_{j=1}^{l} \mathrm{d}\boldsymbol{x}_j. \tag{6}$$

Expression (5) is the cumulant version of (4). Outline of its derivation may be found in Kubo's book (1965).

For statistical evaluations it is more convenient to deal with the free energy of the system, rather than with the partition function. This is obtained, as is well known, from the grand partition function as

$$F^{(\mp)} = \kappa T N \ln z - \kappa T \ln \Xi^{(\mp)} \tag{7}$$

where z, the fugacity of the system, determined by the number of particles N in the system, can be expressed in terms of the chemical potential μ, as: $z = \exp(\beta\mu)$. We then write (7) as

$$F^{(\mp)} = N\mu - \kappa T \sum_{l=1}^{\infty} (\mp)^{l+1} \exp(l\beta\mu) \frac{A_l}{l}. \tag{7a}$$

Before we proceed any further, we shall show that the lth ring integral can be expressed in terms of the single-particle partition function,

$$Z_1(\beta) = \int_V \mathrm{G}(\boldsymbol{x}\beta|\boldsymbol{x}0)\, \mathrm{d}\boldsymbol{x} \tag{8}$$

as

$$A_l = Z_1(l\beta). \tag{9}$$

Relation (9) can be derived very simply by utilizing the eigenfunction expansion of the single-particle Green function

$$\mathrm{G}(\boldsymbol{x}\beta|\boldsymbol{x}'0) = \sum_{\{n\}} \Phi_n(\boldsymbol{x})\Phi_n^*(\boldsymbol{x}') \exp(-\beta E_n). \tag{10}$$

Repeatedly substituting (10) into (6), for the ring integral A_l, and recalling the orthogonality of the eigenfunctions Φ_n, we obtain

$$A_l = \sum_{\{n\}} \exp(-l\beta E_n) = Z_1(l\beta).$$

Having established (9), let us express the ring integrals as a Laplace transform of a function of energy, $g(\epsilon)$, as

$$A_l = Z_1(l\beta) = \int_0^{\infty} \mathrm{d}\epsilon\, g(\epsilon) \exp(-l\beta\epsilon). \tag{11}$$

Since (11) is valid for arbitrary $\beta > 0$, we can also write

$$Z_1(\beta) = \int_0^{\infty} \mathrm{d}\epsilon\, g(\epsilon) \exp(-\beta\epsilon). \tag{11a}$$

Therefore (11*a*) tells us that the function $g(\epsilon)$, which generates A_l in (11) as a Laplace transform, is just the single-particle density of states (see Sondheimer and Wilson 1951). Introducing (11) into (7*a*) for the free energy, and summing over the resulting series we obtain

$$F^{(\mp)} = N\mu \mp \kappa T \int_0^\infty d\epsilon\, g(\epsilon) \ln[1 \pm \exp\{-\beta(\epsilon-\mu)\}]. \tag{12}$$

This is the form of the free energy in Fermi–Dirac (Bose–Einstein) statistics.

The Fermi (Bose) function can now be obtained from

$$\frac{\partial F^{(\mp)}}{\partial \mu} = N - \int_0^\infty d\epsilon \frac{g(\epsilon)}{\exp\{\beta(\epsilon-\mu)\} \pm 1} = 0. \tag{12a}$$

Derivation of (12), based on the symmetry properties of the wave functions of a many-body system, has been done in the particular case of free particles (no external interaction), by direct evaluation of the ring integral (6). This may be found in Montroll and Ward (1958). However, such an evaluation of A_l involves multiple integration and is by no means an easy task even in the case without external interaction. Our approach evades all these difficulties and is quite general. The central role in our derivation is played by the Laplace transform representation of the ring integrals A_l, given in (11).

So far we have silently restricted the discussion to the case of spinless particles. We think that we can best show how to take account of the spin in the grand partition scheme by treating a particular case: that of electrons in a constant uniform magnetic field B. We shall ignore the spin interaction with possible electric fields.

The accommodation of spin in the above formalism is effected via the following modifications: The Green functions $G(\boldsymbol{x}\beta|\boldsymbol{x}'0)$ employed in (3) and given in eigenfunction expansion form in (10) will take the form:

$$G(\boldsymbol{x}\sigma\beta|\boldsymbol{x}'\sigma'0) = \sum_{\{n\}} \Phi_n^*(\boldsymbol{x}', \sigma') \exp\{-\beta(H_1+W)\}\Phi_n(\boldsymbol{x}, \sigma) \tag{10$'$}$$

where W is the spin part of the Hamiltonian and the variable σ (values -1, $+1$) stands for the spin variable. We have

$$\int \Phi_{n'}^*(\boldsymbol{x}, \sigma')\Phi_n(\boldsymbol{x}, \sigma)\, d\boldsymbol{x} = \delta_{nn'}\delta_{\sigma\sigma'} \tag{10$'a$}$$

and

$$(H_1+W)\Phi_n(\boldsymbol{x}, \sigma) = (E_n + \sigma\mu_B B)\Phi_n(\boldsymbol{x}, \sigma) \tag{10$'b$}$$

where μ_B is the Bohr magneton and E_n is the eigenvalue of the Hamiltonian operator H_1 associated with the eigenfunction $\Phi_n(\boldsymbol{x})$, to which the wave functions $\Phi_n(\boldsymbol{x}, \sigma)$ coalesce if the spin magnetic field interaction is removed.

With this modification the form (5) of the grand partition function is preserved and the ring integrals (6) now take the form:

$$A_l = \sum_{\sigma_1,\sigma_2,\ldots,\sigma_l} \int_V \ldots \int G(\boldsymbol{x}_1\sigma_1\beta|\boldsymbol{x}_2\sigma_2 0) \,.\, G(\boldsymbol{x}_2\sigma_2\beta|\boldsymbol{x}_3\sigma_3 0) \ldots G(\boldsymbol{x}_l\sigma_l\beta|\boldsymbol{x}_1\sigma_1 0) \prod_{j=1}^{l} d\boldsymbol{x}_j. \tag{6$'$}$$

Taking into account (10$'$, 10$'a$, 10$'b$), we find that (6$'$) yields

$$A_l = \{\exp(-l\beta\mu_B B) + \exp(l\beta\mu_B B)\} Z_1(l\beta) \tag{9$'$}$$

where $Z_1(\beta)$ is the single-particle partition function for 'spinless electrons'.

The single-particle partition function for an electron in a magnetic field B is given by:

$$\{\exp(-\beta\mu_B B)+\exp(\beta\mu_B B)\}Z_1(\beta) \tag{10'}$$

where

$$Z_1(\beta) = V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \frac{\beta\mu_B B}{\sinh(\beta\mu_B B)} \tag{10'a}$$

may be cited, which shows that the ring integral A_l in the case where the spin is included is again obtained via the rule established earlier on, namely that of replacing β by $l\beta$ in the appropriate single-particle partition function. Therefore, formulae (11) and (11*a*) are still applicable in (12) and (12*a*) for the derivation of the Fermi function, spin inclusive. We may remark that by taking the magnetic field B in (9′) equal to zero the factor in front of $Z_1(l\beta)$ becomes 2, which is the usual factor for electrons to account for the two possible spin orientations.

The above considerations can be easily generalized to include bosons or fermions of any spin.

In the case of interacting particles (two-body interactions), the expression (5) for the grand partition function still holds, but the symbols A_l no longer represent ring integrals. Their role is taken up by the quantities $(\mp)^l l b_l^{(\mp)}$, b_l being the lth cluster integral discussed in Montroll and Ward (1958). However, we do not yet know the analytic properties of the quantities $lb_l(\beta)$. We can only say that if the above formalism is to apply equally well to the interacting case it should be possible to write $lb_l(\beta)$ as a function of the form $J(l\beta)$.

Acknowledgments

One of us (G.J.P.) would like to thank Professor S. F. Edwards for a useful discussion, and one of us (A.V.J.) would like to express his thanks to the British Council for financial support.

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