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Author

Baym, Gordon

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ABSTRACT

Highly convenient rules are given for the general term in the time-independent perturbation-theory expansion for the self-energy operator of quantum statistical mechanics. The rules are derived by starting from the usual formalism involving time-dependent Green's functions. The well-known formulas for thermodynamic quantities in terms of the self-energy operator are included for completeness.

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I. INTRODUCTION

In 1933 Peierls¹ developed a perturbation theory for quantum statistical mechanics that suffered because (1) the general term was not easy to characterize, and (2) spurious terms in the total number of particles seemed to appear (although we now know that these terms all cancel). In 1958, Montroll and Ward² gave a perturbation theory in which the spurious terms were absent and the general term could be described, but their formalism, involving an unnecessary expansion in powers of the fugacity, is exceedingly complicated.

In recent years any number of formalisms have been proposed.³ These are all essentially equivalent, varying only in details. Thus the procedure of Glassgold, Heckrotte, and Watson involves a contour integration, that of Bloch and de Dominicis multiple temperature integrations, that of Luttinger and Ward infinite sums. Thouless,⁴ however, has given a very convenient expression for the logarithm of the partition function.

To propose still another formalism would appear to be both inconsiderate and imprudent. Our motivation is that we are convinced that the rules we

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[†] Department of Physics, University of California, Berkeley, California

describe here are considerably simpler than any other prescription previously proposed. The rules are closely related to those by Thouless,⁴ but we shall work with the self-energy operator in terms of which one can find not only the partition function but also the single-particle excitations. Furthermore it should be observed that the derivation of the rules is not restricted to the single-particle self-energy operator but, rather, is quite general. Thus, for example, one can easily use the method described here to obtain convenient and explicit time-independent rules for the space-time correlation function of any two physical observables.

The rules for calculating are given in Section II. These rules were first obtained intuitively more than a year ago⁵ by means of the following reasoning: In quantum statistical mechanics one computes the equilibrium properties of a given system by constructing an ensemble of similar systems, then (employing quantum mechanics in the calculation) computing the properties of each system in the ensemble and finally averaging over the ensemble. We know from the work of Darwin and Fowler that the average over the ensemble is strongly peaked in the neighborhood of the most probable system in the ensemble. This suggests interchanging the order of (i) the averaging procedure and (ii) the quantum-mechanical calculation of the properties of one system. Thus one is led to consider the quantum mechanics of a system in a state that is the most probable in the ensemble, and consequently one expects that the usual rules for ground-state perturbation theory⁶ will be modified only by replacing the step functions associated with particle and hole lines with single-particle statistical-distribution factors of the most probable state. In Sec. III we derive this result, starting from the time-dependent formalism for perturbation theory.⁷

After this work had been completed the rules of Sec. II appeared in the literature, but without an explicit derivation of the general term.⁸

II. RULES

1. Formalism

The thermodynamic properties of a system can all be deduced from the grand potential Ω defined by

$$\Omega = - \frac{1}{\beta} \log \text{Tr} \left[e^{-\beta \mathcal{H}} \right] , \quad (\text{II-1})$$

where $\mathcal{H} = H - \mu N$ with H and N the Hamiltonian and number operators, respectively. The pressure is given by $P = - \Omega/V$, while the number of particles N and the entropy S are given by

$$N = - \left(\frac{\partial \Omega}{\partial \mu} \right)_{\beta, V}$$

and

(II-2)

$$S = k\beta^2 \left(\frac{\partial \Omega}{\partial \beta} \right)_{\mu, V} .$$

There are several useful ways of calculating Ω , in addition to calculating it directly from its definition (II-1). One can compute it by an integration over temperatures of $\bar{\mathcal{H}}(\beta, \mu)$, the ensemble average of \mathcal{H} :

$$\Omega(\beta, \mu) = \bar{\mathcal{H}}(\infty, \mu) + \frac{1}{\beta} \int_{\infty}^{\beta} d\beta' \left[\bar{\mathcal{H}}(\beta', \mu) - \bar{\mathcal{H}}(\infty, \mu) \right] . \quad (\text{II-3})$$

An alternative and more common method is to find Ω in terms of an integration of the potential energy over the coupling constant.

The quantity $\bar{\mathcal{M}}(\beta, \mu)$ we express in the form

$$\bar{\mathcal{M}}(\beta, \mu) = \frac{1}{2} \int \frac{d^3 p}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega \left(\omega + \frac{p^2}{2m} - \mu \right) A(\underline{p}, \omega) f(\omega) , \quad (\text{II-4})$$

where

$$f(\omega) = \left[e^{+\beta\omega} \mp 1 \right]^{-1} . \quad (\text{II-5})$$

(The \pm refers to bosons and fermions, respectively.) The spectral function $A(\underline{p}, \omega)$ is a function of β and μ , and is given in terms of the Fourier transform of the single-particle Green's function $G(\underline{p}, \omega)$ by

$$A(\underline{p}, \omega) = - \frac{1}{2} \text{Im} G(\underline{p}, \omega) . \quad (\text{II-6})$$

The Green's function G is related to the free-particle Green's function G_0 and the self-energy operator $\Sigma(\underline{p}, \omega)$ via the Dyson equation:

$$G(\underline{p}, \omega) = G_0(\underline{p}, \omega) \left[1 + \Sigma(\underline{p}, \omega) G(\underline{p}, \omega) \right] , \quad (\text{II-7})$$

where

$$G_0(\underline{p}, \omega) = \left(\omega + i\epsilon - \frac{p^2}{2m} + \mu \right)^{-1} . \quad (\text{II-8})$$

All of the above is well known and can be found derived, for example, in reference 7.

The calculation of thermodynamic properties is thus reduced to a calculation of the self-energy operator $\Sigma(\underline{p}, \omega)$. The rules for calculating Σ in

perturbation theory follow. To find the n th-order contribution to $\Sigma(\underline{p}, \omega)$:

1. Construct a graph by drawing n horizontal dashed lines at different levels representing the potential and by joining their $2n$ ends with solid lines representing particles or holes, and having arrows to indicate direction, in such a way that one directed line enters and one leaves each end of a dashed line (e.g., Fig. 1). Have one solid line leave the graph going up and one solid line enter the graph from the downward direction (the "external lines") -- all other solid lines must connect ends of dashed lines. In particular, it is acceptable to connect an end of a dashed line to itself (e.g., Fig. 2a), or one end of a dashed line to its opposite end (e.g., Fig. 2b). Draw only graphs in which there are no unlinked parts and only graphs that cannot be disconnected into two pieces by cutting one solid line, but draw all graphs consistent with these rules. In n th order, each topographically distinct diagram for Σ will yield $n!$ different diagrams corresponding to the $n!$ possible orderings of the vertices from top to bottom. Assign a distinct momentum, \underline{p}_i , to each solid line and momentum \underline{p} to the external lines.

2. To compute the contribution of the graph, associate with each line of momentum \underline{p}_i directed upward a factor $\left[1 \pm f\left(\frac{p_i^2}{2m} - \mu\right)\right]$, and with each line of momentum \underline{p}_j directed downward a factor $\pm f\left(\frac{p_j^2}{2m} - \mu\right)$. Do not assign such factors to the external lines. A line joining a dashed line to itself is considered as directed downward. With each dashed line, associate a factor $V(\underline{p}_i, \underline{p}_j, \underline{p}_k, \underline{p}_l)$, where \underline{p}_i and \underline{p}_j are the momenta of the directed lines leaving the vertex on the left and right, respectively, and \underline{p}_k and \underline{p}_l are the momenta of the directed lines entering the vertex on the left and right, respectively. The factor $V(\underline{p}_i, \underline{p}_j, \underline{p}_k, \underline{p}_l)$ is just the matrix element of the two-body potential. Each of the $(n - 1)$ intervals between vertices

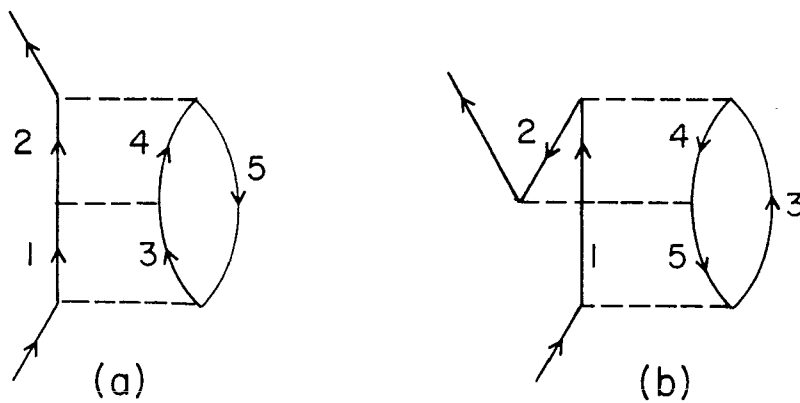


Fig. 1



Fig. 2

contributes a factor that is the inverse of the sum of

(a) $p_i^2/2m$ for each downward-going line of momentum \underline{p}_i crossing the interval,

(b) $-p_j^2/2m$ for each upward-going line of momentum \underline{p}_j crossing the interval,

(c) ω if both external lines do not cross the interval,

(d) $-\omega$ if both external lines cross the interval, or

(e) 0 if only one crosses.

Multiply all the above factors together along with an additional $(-1)^{\ell + 1}$, where ℓ is the number of closed loops formed by solid lines representing fermions. Finally integrate over all \underline{p}_i with a factor $(2\pi)^{-3}$ for each three-dimensional momentum integration.

The potential $V(\underline{p}_i, \underline{p}_j, \underline{p}_k, \underline{p}_\ell)$ is simply expressed in terms of the Fourier transform of a local two-body spin-independent potential $v(r)$ by

$$V(\underline{p}_i, \underline{p}_j, \underline{p}_k, \underline{p}_\ell) = (2\pi)^3 \delta(\underline{p}_i + \underline{p}_j - \underline{p}_k - \underline{p}_\ell) v(\underline{p}_i - \underline{p}_k) \quad , \quad (\text{II-9})$$

where

$$v(\underline{p}) = \int e^{-i\underline{p} \cdot \underline{r}} v(r) d\underline{r} \quad . \quad (\text{II-10})$$

For particles with spin, one must include the spin dependence of V and also sum over spins of internal lines -- exactly as one does in ground-state perturbation theory.

2. Example

As an illustration of the rules, we evaluate the contribution for fermions of the two third-order diagrams of Fig. 1:

$$\Sigma^{(a)}(\underline{p}, \omega) = \int \left\{ [1-f_1][1-f_3]f_5[1-f_2][1-f_4](-1)^3 d\underline{p}_1 d\underline{p}_2 d\underline{p}_3 d\underline{p}_4 d\underline{p}_5 v(\underline{p}_1 - \underline{p})v(\underline{p}_2 - \underline{p}_1)v(\underline{p} - \underline{p}_2) \right. \\ \left. \times (2\pi)^9 \delta(\underline{p}_1 + \underline{p}_3 - \underline{p} - \underline{p}_5) \cdot \delta(\underline{p}_2 + \underline{p}_4 - \underline{p}_1 - \underline{p}_3) \cdot \delta(\underline{p} + \underline{p}_5 - \underline{p}_2 - \underline{p}_4) \right\} / (\omega - \epsilon_1 - \epsilon_3 + \epsilon_5)(\omega - \epsilon_2 - \epsilon_4 + \epsilon_5) (2\pi)^{15}$$

and

(II-11)

$$\Sigma^{(b)}(\underline{p}, \omega) = \int \left\{ [1-f_1][1-f_3]f_5 f_2 f_4 (-1)^5 d\underline{p}_1 d\underline{p}_2 d\underline{p}_3 d\underline{p}_4 d\underline{p}_5 v(\underline{p}_1 - \underline{p})v(\underline{p}_2 - \underline{p}_1)v(\underline{p} - \underline{p}_2) \right. \\ \left. \times (2\pi)^9 \delta(\underline{p}_1 + \underline{p}_3 - \underline{p} - \underline{p}_5) \cdot \delta(\underline{p}_2 + \underline{p}_4 - \underline{p}_1 - \underline{p}_3) \cdot \delta(\underline{p} + \underline{p}_5 - \underline{p}_2 - \underline{p}_4) \right\} / (\omega - \epsilon_1 - \epsilon_3 + \epsilon_5)(\epsilon_2 + \epsilon_4 - \epsilon_1 - \epsilon_3) (2\pi)^{15},$$

where f_i represents $f\left(\frac{p_i^2}{2m} - \mu\right)$.

3. Generalization

We can sum a large class of diagrams, namely those corresponding to the replacement of G_0 by G in all internal lines, by rules that are essentially the same as those given in Sec. II.1:

(a) Construct only irreducible graphs.

(b) Calculate the contribution of an upward directed line \underline{p}_i by assigning the factor $A(\underline{p}_i, \omega_i) [1 \pm f(\omega_i)]$ and for a downward directed line the factor $\pm A(\underline{p}_i, \omega_i) f(\omega_i)$. For the energy denominator the upward lines contribute $-(\omega_i + \mu)$ and the downward lines $(\omega_i + \mu)$. Proceed as in Sec. II.1, and finally also integrate over all ω_i as well as \underline{p}_i .

These rules are greatly more complicated, since A must be obtained self-consistently, but one diagram now includes an infinite class of the old diagrams.

III. PROOF OF RULES

The starting point from which we shall demonstrate the rules given in Sec. II.1 is the time-dependent form of the perturbation expansion for Σ . This expansion is described in detail in the appendix to reference 7. Briefly, to calculate any order of perturbation theory in the time-dependent formalism, one writes down all topologically distinct connected diagrams of that order and evaluates the diagrams by writing a G_0 for each line, and a V for each vertex as in time-dependent ground-state perturbation theory. The time integrations must be between $t = 0$ and $t = -i\beta$ in order to include correctly the periodicity boundary condition obeyed by the thermodynamic Green's functions. In listing all the distinct diagrams no attention is paid to different time orderings. The momentum parts and the numerical factors are the same as in ground-state theory.

Each n th-order diagram in this perturbation theory corresponds to $n!$ of the "ordered" diagrams one writes down according to the rules of Sec. II.1. In order to demonstrate the equivalence of those rules to the time-dependent perturbation theory, we must show how the contribution of an n th-order diagram evaluated by the time-dependent theory splits into $n!$ distinct contributions, each equal to the contribution from one ordered diagram evaluated by the rules of Sec. II.1.

Consider a diagram of n th order in V . The n vertices are labeled with n different times; to evaluate the diagram, one of these times is set equal to zero, and the remaining $n - 1$ times are integrated from $t = 0$ to $t = -i\beta$. These $n - 1$ time integrations can be split into $(n - 1)!$ different integrations corresponding to different orders of the $n - 1$ times along the line from 0 to $-i\beta$. There are only $(n - 1)!$ terms rather than $n!$ terms, since one time has been arbitrarily chosen to be zero. We shall show that each

of the $(n - 1)!$ terms equals the contribution, evaluated by the rules of Sec. II.1, of n "ordered" diagrams that differ only by a cyclic permutation of the vertices.

Since in the $(n - 1)!$ terms in the time-dependent perturbation theory the integration times are ordered, one can always replace the $G_0(\underline{p}, t_i, t_j)$ that occurs in the integral by

$$G_{0,>}(\underline{p}, t_i, t_j) = \frac{1}{i} e^{-ip^2(t_i - t_j)/2m} \left[1 \pm f\left(\frac{p^2}{2m} - \mu\right) \right], \quad (\text{III-1})$$

if $t_i > t_j$, or by

$$G_{0,<}(\underline{p}, t_i, t_j) = \pm \frac{1}{i} e^{(t_i - t_j)/2m - ip^2} f\left(\frac{p^2}{2m} - \mu\right), \quad (\text{III-2})$$

if $t_i < t_j$. Thus to each $G_{0,>}$, or forward-going line, there corresponds a factor $1 \pm f$; and to each backward-going line, or $G_{0,<}$, a factor $\pm f$. There is an over-all factor of $(-1)^{2n-1}$. At each vertex (t_ℓ) , one will have a factor $e^{i\sigma_\ell t_\ell}$, where

$$\sigma_\ell = \frac{1}{2m} (p_a^2 + p_b^2 - p_c^2 - p_d^2), \quad (\text{III-3})$$

where \underline{p}_a and \underline{p}_b are the momenta of the lines leaving the vertex, and \underline{p}_c and \underline{p}_d are the momenta of the lines entering the vertex. One must therefore calculate the integral

$$I = \int_0^{-i\beta} dt_n e^{it_n \sigma_n} \int_0^{t_n} dt_{n-1} e^{it_{n-1} \sigma_{n-1}} \dots \int_0^{t_3} dt_2 e^{it_2 \sigma_2} \quad (III-4)$$

The results of the t_2 integral can be written as

$$\int_0^{t_3} dt_2 e^{it_2 \sigma_2} = \sum_{\lambda_2=0,1} \frac{i(-1)^{\lambda_2} e^{it_3 \lambda_2 \sigma_2}}{\sigma_2} \quad (III-5)$$

and it is clear that one can write I as

$$I = \prod_{i=2}^n \sum_{\lambda_i=0,1} \frac{i^{n-1} e^{\beta \Gamma_n} (-1)^{\sum_{j=2}^n \lambda_j}}{\Gamma_2 \Gamma_3 \dots \Gamma_{n-1} \Gamma_n} \quad (III-6)$$

where

$$\begin{aligned} \Gamma_k &= \sigma_k + \lambda_{k-1} \Gamma_{k-1} \\ &= \sigma_k + \lambda_{k-1} [\sigma_{k-1} + \lambda_{k-2} (\sigma_{k-2} + \lambda_{k-3} \sigma_{k-3} + \dots)] \end{aligned} \quad (III-7)$$

The sum now contains 2^{n-1} distinct terms, and we must rearrange it into n different groups of terms so that all terms in each group have a common value of $\exp(\beta \Gamma_n)$. This is done by rewriting the sum as

$$I = \sum_{k=1}^n \left[\prod_{i=2}^{k+1} \sum_{\lambda_i=0,1} \frac{i^{n-1} e^{\beta \Gamma_n} (-1)^{\sum_{j=2}^n \lambda_j}}{\Gamma_2 \Gamma_3 \dots \Gamma_{n-1} \Gamma_n} \right]_{(\lambda_n=1, \lambda_{n-1}=1, \dots, \lambda_{k+1}=1, \lambda_k=0)} \quad (III-8)$$

where the $k = 1$ term corresponds to taking all $\lambda_i = 1$.

$$I = \sum_{k=1}^n \frac{i^{n-1} (-1)^{n-k} \exp\left[\beta \sum_{j=k+1}^n \sigma_j\right]}{\binom{n}{\sum_{k+1} \sigma_j} \binom{n-1}{\sum_{k+1} \sigma_j} \cdots \binom{n-k}{\sigma_{k+1}}} \left\{ \prod_{i=2}^{k-1} \sum_{\lambda_i=0,1} \frac{(-1)^{\sum_{j=2}^{k-1} \lambda_j}}{\Gamma_k \Gamma_{k-1} \cdots \Gamma_3 \Gamma_2} \right\}_{\lambda_k=0} \quad (III-9)$$

Call the summation in the braces S_k . Then

$$\begin{aligned} S_1 &= 1, \\ S_2 &= \sigma_2^{-1}, \\ S_3 &= \sum_{\lambda_2=0,1} \frac{(-1)^{\lambda_2}}{(\sigma_3 + \lambda_2 \sigma_2) \sigma_2} = \left[\sigma_3 (\sigma_3 + \sigma_2) \right]^{-1}, \end{aligned} \quad (III-10)$$

and in general

$$S_k = \left[\sigma_k (\sigma_k + \sigma_{k-1}) (\sigma_k + \sigma_{k-1} + \sigma_{k-2}) \cdots (\sigma_k + \sigma_{k-1} + \cdots + \sigma_3) (\sigma_k + \sigma_{k-1} + \cdots + \sigma_3 + \sigma_2) \right]^{-1}. \quad (III-11)$$

This latter result follows from a simple induction argument. Assuming the result to be true for any arbitrary set of Γ_i for $i=2,3,\dots,k-1$, we can write

$$S_k = \sum_{\lambda_2=0,1} \frac{(-1)^{\lambda_2}}{\sigma_2} \left[\prod_{i=3}^{k-1} \sum_{\lambda_i=0,1} \frac{(-1)^{\sum_{j=3}^{k-1} \lambda_j}}{\Gamma_k \Gamma_{k-1} \cdots \Gamma_3} \right]. \quad (III-12)$$

But the term in brackets is such a sum of "order" $k-1$ involving

$\bar{\sigma}_3 = \sigma_3 + \lambda_2 \sigma_2$, and hence, by the inductive hypothesis we have

$$S_k = \sum_{\lambda_2=0,1} \frac{(-1)^{\lambda_2}}{\sigma_2} \frac{1}{\sigma_k (\sigma_k + \sigma_{k-1}) \cdots (\sigma_k + \sigma_{k-1} + \cdots + \sigma_4) (\sigma_k + \sigma_{k-1} + \cdots + \sigma_4 + \bar{\sigma}_3)} \quad (\text{III-13})$$

Computation of the λ_2 summation then produces the general formula (III-11)

for S_k .

The integral I has thus been reduced to

$$I = \sum_{k=1}^n \frac{i^{n-1} (-1)^{n-k} e^{\beta(\sigma_n + \cdots + \sigma_{k+2})}}{(\sigma_n + \delta_{n-1} + \cdots + \sigma_{k+1}) (\sigma_{n-1} + \cdots + \sigma_{k+1}) \cdots \sigma_{k+1} \sigma_k (\sigma_k + \sigma_{k-1}) \cdots (\sigma_k + \cdots + \sigma_2)} \quad (\text{III-14})$$

These n terms correspond to just n cyclic permutations of a given diagram.

Let $k = n$. Then the summand is

$$\frac{i^{n-1}}{\sigma_n (\sigma_n + \sigma_{n-1}) \cdots (\sigma_n + \cdots + \sigma_3) (\sigma_n + \sigma_{n-1} + \cdots + \sigma_2)} \quad (\text{III-15})$$

The denominators clearly are the energy denominators one writes down by

following the rules in Sec. II for the original diagram. The $k = n-1$ term

$$i^{n-1} e^{\beta \sigma_n} \left[(\sigma_{n-1}) (\sigma_{n-1} + \sigma_{n-2}) \cdots (\sigma_{n-1} + \cdots + \sigma_2) (-\sigma_n) \right] \quad (\text{III-16})$$

differs from the $k = n$ term by a factor $e^{\beta \sigma_n}$, and furthermore the σ_n has become $-\sigma_n$ and each factor has been reduced by σ_n . Thus the $k = n-1$ term corresponds to the time-ordered diagram formed by moving the latest vertex n

to the earliest time (a cyclic permutation). All energy denominators will clearly be reduced by $-\sigma_n$, and the last denominator (σ_n) will change sign when it becomes the first denominator; the $e^{\beta\sigma_n}$ will change the particles into holes and vice versa at the n th vertex, since $e^{\beta\omega} f = 1 \pm f$. Thus I corresponds to the sum of all diagrams of n th order that are just cyclic permutations of a single diagram of n th order. Thus we have exhibited the correspondence between the time-dependent perturbation diagrams and the ordered diagrams as well as derived the rules of Sec. II.1. We leave it to the reader to check that the detailed numerical factors are equivalent as well as to generalize the derivation to cover the situation of Sec. II.3.

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