A NEW METHOD IN STATISTICAL PERTURBATION THEORY

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A new variant of the statistical perturbation theory is presented, which consists in the setting up of a model of a dynamical system whose Hamiltonian contains the inverse temperature in parametric form. It is shown that for this dynamical system the perturbation theory is equivalent to the ordinary statistical perturbation theory and is much more convenient for practical calculation.

According to the principles of statistical physics, the thermodynamic properties of systems in thermal equilibrium can be determined by the sum of states. In quantum statistics the latter is usually represented as (in the case of a grand canonical ensemble)

$$\Xi = \mathrm{Sp}\,(e^{-\beta H + \alpha N}), \qquad (1)$$

where $\beta = 1/\Theta$; Θ is the temperature in energy units; $\alpha = \beta\mu$; μ is the chemical potential.

Taking into account the formal similarity between the statistical operator of a canonical ensemble and the operator describing the time sequence of a dynamical system, a number of authors have developed several variants of the statistical perturbation theory in analogy with the corresponding formalism in contemporary quantum field theory.[1] The fact that only slight practical results have been obtained in this direction is connected in large measure with new difficulties of calculation. Thus, for example, instead of the averaging of the quantum amplitudes over a real vacuum, we deal here with an averaging over the canonical ensemble of free particles; inasmuch as we have the quantity $i\beta$ in place of the time variable t, integration always extends from zero to some finite value. It must be noted that in the researches of Bogoliubov, Zubarev, and Tserkovnikov[2,3] the statistical perturbation theory supplemented by the method of canonical transformations is successfully applied to the exact calculation of thermodynamic functions of some model problems in the theory of superfluidity and superconductivity. We now consider a new version of statistical perturbation theory, which consists in the setting up of a model dynamical system, the determination of the ground-state energy of which makes it possible to compute the change in the thermodynamic potential of the system upon inclusion of the interaction for a given temperature β.

Keeping in mind the description with the aid of the grand canonical ensemble, we represent the Hamiltonian of the system under consideration as

$$H = H_0 + V, \quad H_0 = \sum_{ks} (E(k) - \mu)\, a_{ks}^{+} a_{ks} + \sum_{q} \omega(q) b_q^{+} b_q, \qquad (2)$$

where a_{ks}^{+}, a_{ks}, b_q^{+}, b_q are the Fermi and Bose amplitudes; $E(k)$ and $\omega(q)$ are the eigen energies of the fermions and bosons with quantum numbers k, s, and q, respectively; μ is the chemical potential, determined from the condition of the equality of the average number of fermions with the actual number of fermions in the system; V is the Hermitian form of a_{ks}^{+}, a_{ks} and b_q^{+}, b_q.

We introduce these statistical sum Ξ and the thermodynamic potential

$$\Psi = -\beta^{-1} \ln \Xi = -\beta^{-1} \ln [\mathrm{Sp}\, e^{-\beta H}].$$

We then have the very well-known relations (reference 1, see also reference 4):

$$\Xi/\Xi_0 = \ll \mathfrak{S} \gg = \exp \ll \mathfrak{S} \gg_{\text{coup}}, \qquad \Psi = \Psi_0 - \beta^{-1} \ll \mathfrak{S} \gg_{\text{coup}}, \qquad (3)$$

where

$$\Psi_0 = -\beta^{-1} \ln \Xi_0 = -\beta^{-1} \ln [\mathrm{Sp}\, e^{-\beta H_0}],$$

$$\mathfrak{S} = e^{\beta H_0} e^{-\beta H}, \quad \ll A \gg = \Xi_0^{-1} \mathrm{Sp}\,[e^{-\beta H_0} A].$$

the index "coup" means that in each term of the expansion all the intermediate states are coupled together by the matrix elements of V.

To obtain an explicit form of the expansion of $\mathfrak{S}$ in V, we assume a new much simpler method in place of the ordinary formalism of time sequence according to the temperature variable, since the finite limit of integration brings about an appreciable complication.

We introduce the Laplace transform of the statistical operator[1]

$$e^{-\beta H} = \frac{1}{2\pi i} \int_\Gamma e^{-\beta z} \frac{1}{z-H} dz;$$

$(z-H)^{-1} = (z-H_0)^{-1} + (z-H_0)^{-1} R(z) (z-H_0)^{-1}$, $R(z) = V + V(z-H_0)^{-1} V + \ldots$ [the contour Γ proceeds downward, parallel to the imaginary axis, to the left of all singularities of the function $(z-H)^{-1}$].

It is known[5] that the matrix element $R(z)$ and the function $(z-H)^{-1}$ are analytic as functions of the complex variable z if we make a cut along the real axis beginning at some point up to $+\infty$. For a finite volume of the system, the singularities are densely-located poles.

We can then write (3) in the form

$$\Psi = \Psi_0 - (\beta \Xi_0)^{-1} \frac{1}{2\pi i} \int_\Gamma e^{-\beta z} \operatorname{Sp} [(z-H_0)^{-2} R(z)_{\text{coup}}] \, dz$$

$$= \Psi_0 - \beta^{-1} \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon \int_\Gamma d\zeta \, \frac{e^{-\zeta\beta}}{\zeta^2} \ll \delta(\varepsilon - H_0) R(\zeta + \varepsilon)_{\text{coup}} \gg .$$

making use of the invariance of the trace relative to a cyclic permutation of the cofactors, it is easy to establish that

$$\frac{1}{2\pi i} \int_\Gamma d\zeta \, \zeta^{-2} e^{-\zeta\beta} \ll \delta(\varepsilon - H_0) R(\zeta + \varepsilon)_{\text{coup}} \gg$$

$$= -\beta \ll \delta(\varepsilon - H_0) R(\varepsilon)_{\text{coup}} \gg .$$

In this case all terms containing $(\epsilon - E_p')^{-2}$ (where E_p' is the energy of any intermediate state) cancel each other. Thus, we are led to the very useful expression of statistical permutation theory first obtained by Bloch.[1]

$$\Psi = \Psi_0 + \int_{-\infty}^{\infty} d\varepsilon \ll \delta(\varepsilon - H_0) R(\varepsilon)_{\text{coup}} \gg . \tag{4}$$

The basic idea of the present paper consists of the fact that the second term in (4) can be replaced by the change in energy of the ground state of any model of the dynamic system upon inclusion of the interaction. In the Hamiltonian of this model system (we shall call it the statistical model Hamiltonian), β entered as a numerical parameter.

Let us prove the fundamental theorem, following the scheme of Bloch.[1] Let A be the product of the Fermi and Bose amplitudes; then we have the equality

$$\ll A \gg = \langle \Phi_F | A | \Phi_F \rangle \equiv \langle A \rangle , \tag{5}$$

where $|\Phi_F\rangle$ is the vacuum state of the new Fermi and Bose amplitudes determined by the relations

$$a_{ks}^+ = (1-f_k)^{1/2} c_{ks}^+ + f_k^{1/2} b_{ks}, \quad a_{ks} = (1-f_k)^{1/2} c_{ks} + f_k^{1/2} b_{ks}^+ ,$$
$$c_{ks} | \Phi_F \rangle = b_{ks} | \Phi_F \rangle = 0. \tag{6}$$
$$b_q = (1+h_q)^{1/2} \eta_{q0} + h_q^{1/2} \eta_{q1}^+ , \quad b_q^+ = (1+h_q)^{1/2} \eta_{q0}^+ + h_q^{1/2} \eta_{q1} ,$$
$$\eta_{q0} | \Phi_F \rangle = \eta_{q1} | \Phi_F \rangle = 0 ,$$

where f_k and h_q upon determination are equal to the mean occupation number of the fermion state k, s and the boson state q

$$f_k \equiv \ll a_{ks}^+ a_{ks} \gg = (1 + e^{\beta(E(k)-\mu)})^{-1} ,$$
$$h_q \equiv \ll b_q^+ b_q \gg = (e^{\beta\omega(q)} - 1)^{-1}. \tag{7}$$

We now prove the theorem by induction. First we note that $\ll A \gg$ differs from zero only when A consists of the aggregate of pairs of creation and annihilation operators of the boson or the fermion relative to one and the same individual state. Since $\exp(-\beta H_0)$ has been factored, it then suffices to exhibit this theorem for any given state k. If all the pairs in A refer to different states, then the theorem is identical with the determination of f_k and h_q, since

$$f_k \equiv \ll a_{ks}^+ a_{ks} \gg = \langle a_{ks}^+ a_{ks} \rangle ,$$
$$h_q \equiv \ll b_q^+ b_q \gg = \langle b_q^+ b_q \rangle . \tag{8}$$

In the case of the presence of several pairs with the same index, the problem reduces to the proof of the following two assertions:

(a) If $\ll A a_{ps}^+ a_{ps} B \gg = \langle A a_{ps}^+ a_{ps} B \rangle$ and $\ll AB \gg = \langle AB \rangle$, then $\ll A a_{ps} a_{ps}^+ B \gg = \langle A a_{ps} a_{ps}^+ B \rangle$.

This assertion is the consequence of the commutation relation for a_{ps} and a_{ps}^+, while A and B are the products of the operators a_{ks}^+, a_{ks}, b_q^+, b_q. For the case of bosons we have: if $\ll AB \gg = \langle AB \rangle$ and $\ll A b_q^+ b_q \gg = \langle A b_q^+ b_q \rangle$, then

$$\ll A b_q b_q^+ B \gg = \langle A b_q b_q^+ B \rangle .$$

(b) If in A there are n pairs of Fermi amplitudes with the index k, or m pairs of boson amplitudes with index q, we have the equalities

$$\ll a_{ks}^{+n} a_{ks}^n \gg = \langle a_{ks}^{+n} a_{ks}^n \rangle , \quad \ll b_q^{+m} b_q^m \gg = \langle b_q^{+m} b_q^m \rangle .$$

In the case of fermions, the equality is trivial since the mean value of the null operator appears on both sides. In the Bose case, writing out both sides,

$$\ll b_q^{+m} b_q^m \gg = \ll (b_q^+ b_q - m + 1)(b_q^+ b_q - m + 2) \ldots b_q^+ b_q \gg$$
$$= m! h_q^m \quad \langle b_q^{+m} b_q^m \rangle = h_q^m \langle \eta_{q1}^m \quad \eta_{q1}^{+m} \rangle = m! h_q^m .$$

(a) and (b) contain the complete proof of the theorem.

We now consider the model dynamical system with the Hamiltonian

$$H^{st} = H_0^{st} + V; \qquad H_0^{st} = \sum_{ks}(E(k) - \mu)(c_{ks}^+ c_{ks} - b_{ks}^+ b_{ks}) + \sum_q \omega(q)(\eta_{q0}^+ \eta_{q0} - \eta_{q1}^+ \eta_{q1}). \tag{9}$$

The change in the ground state energy of this system will be

$$\Delta E^{st} = \int_{-\infty}^{\infty} \langle \delta(\varepsilon - H_0^{st}) \left[V + V \frac{1}{\varepsilon - H_0^{st}} V + \dots \right]_{coup} \rangle d\varepsilon. \tag{10}$$

Applying our theorem to the expression under the integral, it is not difficult to note the identities (10) and the second term (4). Choice of H_0^{st} guarantees the averaging over the present dynamical vacuum and the correct energy gaps. Thus we obtain

$$\Psi = \Psi_0 + \Delta E^{st}, \tag{11}$$

i.e., the correction to the thermodynamical potential at a given temperature is equal to the change in the ground state energy for the dynamical system with the Hamiltonian H^{st}. This assertion completes the program outlined above.

We now proceed to a discussion of the results.

1. The physical idea which underlies the foregoing formal transformations is that the statistical average over the canonical ensemble is considered as a quantum mechanical averaging over the state $|\Phi_F\rangle$, in which the individual states are filled with the probability corresponding to their weights in the ensemble. The ordinary formalism of perturbation theory is built up relative to $|\Phi_F\rangle$. Consequently, $|\Phi_F\rangle$ is the analogue of the vacuum state of the free system at temperatures different from zero. For fermions, it is a Fermi sphere with a diffuse edge, while for bosons it is a "smeared" Bose-condensate. (The states below the condensate are filled with the probability h_k). The appearance of quasi-particles b, c, η on $|\Phi_F\rangle$ corresponds to a departure from statistical equilibrium. At zero temperature, they go over into a real perturbation: the electron-hole on the Fermi sphere and the boson on the condensate (the boson $\eta_{k_1}^+$, $\bar{\eta}_{k_1}$ does not appear at absolute zero).

2. The new formulation possesses a great advantage for practical calculations since, for the treatment of the statistical model of the Hamiltonian, we can without complication call upon the entire methodology developed for the investigation of other dynamic systems: in particular, perturbation theory and the Green's-function method of modern quantum field theory, and also the method of canonical transformations in its many versions. In particular, for consideration of phase transitions of second order and Bose-Fermi systems, we can formulate the principles of compensations of the various diagrams of Bogoliubov[6] at temperatures differing from absolute zero.

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