

PHYSICAL REVIEW LETTERS

VOLUME 3

JULY 15, 1959

NUMBER 2

CALCULATION OF PARTITION FUNCTIONS*

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(Received June 15, 1959)

It is the purpose of this Letter to describe briefly the manner in which a transformation due to Stratonovich¹ can be used to calculate approximately the grand partition functions of some many-body systems.

Consider the grand partition function

$$Z = \text{Tr}[\exp(-\beta K - \beta V - \nu N)],$$

where

$$K = \sum_i \epsilon_i \eta_i^* \eta_i, \quad V = \frac{1}{2} \sum_{i,j,k,l} v_{ij;kl} \eta_i^* \eta_j \eta_k^* \eta_l,$$

$$N = \sum_i \eta_i^* \eta_i, \quad \beta = 1/\kappa T, \quad \nu = \mu/\kappa T,$$

(T = temperature, μ = chemical potential) and the η_i^* and η_i are the creation and destruction operators for the particles of the system; the η_i^* and η_i may have commutation relations appropriate to either Bose-Einstein or Fermi-Dirac statistics.

It should be noted that $v_{ij;kl} = v_{kl;ij}$ necessarily, so that V can be regarded as a quadratic form in the variables $\xi_{ij} = \eta_i^* \eta_j$. Bringing this quadratic form into normal form one has $V = \sum_{\alpha} \lambda_{\alpha} \rho_{\alpha}^2$, where the λ_{α} are real and the ρ_{α} are linear combinations of the ξ_{ij} . The grand partition function may now be rewritten

$$Z = \text{Tr}[\exp(-\beta K - \nu N - \beta \sum_{\alpha} \lambda_{\alpha} \rho_{\alpha}^2)]. \quad (1)$$

One can now transform this expression by making use of the identity

$$\int_{-\infty}^{\infty} \exp\{-\pi x^2 - 2\pi^{1/2} ax\} dx = \exp\{a^2\}. \quad (2)$$

This identity cannot be applied directly to (1) because of the noncommutativity of the operators involved. To overcome this difficulty one may make use of the ordering label technique of Feynman² and introduce an ordering label s to write

$$Z = \text{Tr}\{\exp[-\sum_s (K_s + \mu N_s) - \sum_{\alpha} \sum_s \lambda_{\alpha} \rho_{\alpha s}^2]\}, \quad (3)$$

where \sum_s has been written for $\int_0^{\beta} ds$; the quantities in (3) can now be handled as though they were c numbers, the ordering determined by s being restored when convenient.

Applying the identity (2) to (3) one now easily finds

$$Z = \int \exp\{-L[x_{\alpha s}]\} \prod_{\alpha s} dx_{\alpha s}, \quad (4)$$

where

$$L[x_{\alpha s}] = \pi \sum_{\alpha, s} x_{\alpha s}^2 + \beta f[x_{\alpha s}], \quad (5)$$

and

$$\exp\{-\beta f[x_{\alpha s}]\} \equiv \text{Tr} \left\{ \exp \left[-\sum_s (K_s + \mu N_s) - 2\pi^{1/2} \sum_{\alpha s} (-\lambda_{\alpha})^{1/2} x_{\alpha s} \rho_{\alpha s} \right] \right\}. \quad (6)$$

The essential feature of the transformation (4)-(6) is that the operator appearing in the exponent in (6) is only quadratic in the operators η_i^* , η_i , so that the evaluation of the indicated trace is essentially similar to the evaluation of the partition function of a system of noninteract-

ing particles moving in a field determined by the $x_{\alpha s}$. Equations (4) and (5) then express Z as a weighted average of the quantity (6) over the fields $[x_{\alpha s}]$.

In some cases the integral (4) can be conveniently evaluated by the method of steepest descents. One then finds

$$\ln Z \approx -\pi \sum_{\alpha} (x_{\alpha}^0)^2 - \beta f[x_{\alpha}^0] - \frac{1}{2} \ln[\det(L_2)_0], \quad (7)$$

where the x_{α}^0 are determined by the equation

$$(\partial L / \partial x_{\alpha s})_0 = 0 \quad (8)$$

(it can be shown that the solution $x_{\alpha s}^0$ of this equation is independent of s , hence the use of the abbreviated notation x_{α}^0 for $x_{\alpha s}^0$), while L_2 is the matrix

$$(L_2)_{\alpha s; \gamma s'} = \frac{1}{2\pi} \frac{\partial^2 L}{\partial x_{\alpha s} \partial x_{\gamma s'}}; \quad (9)$$

(\cdot)₀ means that the quantity is evaluated at $x_{\alpha s} = x_{\alpha}^0$.

Evaluation of the formulas (7)-(9) shows that (8) represents an obvious generalization to finite temperature of the ordinary Hartree self-consistent-field equations, while the first two terms of (7) represent the energy in the Hartree approximation and the last term of (7) is (at $T=0$) essentially the correlation energy calculated in the approximation of Brueckner and Gell-Mann.³

We add a few remarks concerning some of the features and the range of application of the method illustrated above.

(i) In a higher approximation Eq. (8) determining x_{α}^0 is replaced by

$$\left[\frac{\partial}{\partial x_{\alpha s}} \left\{ L[x_{\alpha s}] + \frac{1}{2} \ln \det(L_2) \right\} \right]_0 = 0. \quad (10)$$

This equation represents a generalization of the Hartree-Fock equations to include the effects of correlation in the approximation of Brueckner and Gell-Mann.³

(ii) It is possible to write V as a Hermitean form in the variables $\xi_{ij} = \eta_i \eta_j$. Writing V in this form and proceeding in the same manner as above, one obtains results formally similar to those given above but representing a different method of approximation in the calculation of Z .

(iii) In the approximation described in (ii) the equation equivalent to (8) no longer represents

the Hartree-Fock equations, but in the Fermi-Dirac case constitutes a set of equations which are generalizations of (and include) the Bardeen, Cooper, and Schrieffer equations of superconductivity.⁴

(iv) In the approximation described in (ii) the term equivalent to the last term of (7) represents (at $T=0$) the correlation energy calculated in the approximation of the Brueckner nuclear matter theory.⁵

(v) In the approximation described in (ii), the equation equivalent to (10) determines at $T=0$ a self-consistent field dependent upon the reaction matrix, of the type introduced in the Brueckner nuclear-matter theory.⁵

(vi) In some cases the solutions of (8) are degenerate in the sense that there is a continuum of solutions x_{α}^0 all yielding the same value for $L[x_{\alpha}^0]$. In this case special measures have to be taken in the application of the method of steepest descents. This situation corresponds physically to the presence of collective motions of the type illustrated by the rotational collective motion of nuclei.

(vii) In some cases there may be two or more solutions of (8) representing local minima of L . In evaluating (7) one must of course use the solution x_{α}^0 which makes L an absolute minimum. However, it may be that as β is varied the local minima change their relative positions and the absolute minimum switches at some temperature from one to another local minimum. This process presumably gives a description of some sorts of phase transition.

These remarks will be enlarged upon in a series of papers now being prepared for publication.

* This work has been supported in part by the National Science Foundation.

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