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Abstract

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On the Application of Zubarev' s Method of Additional Variables to Statistical Physics

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As is well known, the problem of investigating the physical properties of dynamical systems consisting of a large number of interacting particles is very complicated. In 1953 D. N. Zubarev, in connection with the problem of elementary excitations in a real Fermi gas, developed the method of additional variables and applied it to the calculation of the energy spectrum of these excitations.

In the present note the method of additional variables is applied to the calculation of the statistical sum of a system of N interacting particles. The statistical sum Z_N is the trace of the operator $e^{-\beta\hat{H}}$, where $\beta = \frac{1}{kT}$, and $\hat{H}$ is the Hamiltonian of the system.

For definiteness, let us consider Fermi particles (the consideration of Bose particles is entirely analogous) in a volume V, interacting by means of a two-particle central potential $W_{ij} = W(|\mathbf{x}_i - \mathbf{x}_j|)$. The Hamiltonian of the system is represented in the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{1}$$

where

$$\hat{H}_0 = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m}, \qquad \hat{H}_1 = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \hat{W}_{ij}.$$

We now introduce additional operators* $\hat{Q}_{\mathbf{k}}$ ($|\mathbf{k}| < k_0$, $\mathbf{k} \neq 0$, $\hat{Q}_{\mathbf{k}}^{+} = \hat{Q}_{-\mathbf{k}}$, $+$ denotes Hermitian conjugation). The state vector of the system satisfies the additional conditions

$$\hat{Q}_{\mathbf{k}} |\Psi\rangle = 0 \qquad (|\mathbf{k}| < k_0). \tag{2}$$

We have

$$Z_N = S_\Psi \langle \Psi | e^{-\beta \hat{H}} | \Psi \rangle = S_\Phi \langle \Phi | e^{-\beta \hat{H}'} | \Phi \rangle, \tag{3}$$

where

$$|\Phi\rangle = \hat{U}|\Psi\rangle, \qquad \hat{H}' = \hat{U}\hat{H}\hat{U}^{-1}, \qquad \hat{U}^+ = \hat{U}^{-1}.$$

We take

$$\hat{U} = \exp\left\{ -\frac{i}{\hbar} \sum_{|\mathbf{k}|<k_0}{}' \hat{P}_\mathbf{k} \hat{\rho}_\mathbf{k} \right\}. \tag{4}$$

* We use the Hermitian variant of Zubarev' s method ([1]).

$\sum'$ denotes summation over $\mathbf{k} \neq 0$; $\hat{P}_\mathbf{k}$ is the operator canonically conjugate to $\hat{Q}_\mathbf{k}$;

$$\hat{\rho}_\mathbf{k} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\mathbf{k}\hat{\mathbf{x}}_j}, \qquad \hat{\rho}_\mathbf{k} = \hat{\rho}_\mathbf{k}^R + i\hat{\rho}_\mathbf{k}^I.$$

The vectors $|\Phi\rangle$ satisfy the conditions

$$(\hat{Q}_\mathbf{k} - \hat{\rho}_\mathbf{k})|\Phi\rangle = 0 \qquad (|\mathbf{k}| < k_0). \tag{5}$$

The Hamiltonian is

$$\hat{H}' = \hat{H}_0' + \hat{H}_{osc}' + \hat{H}_I', \tag{6}$$

where

$$\hat{H}_0' = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m}$$

is the Hamiltonian of "free" fermions;

$$\hat{H}_{osc}' = \frac{1}{2m} \sum_{|\mathbf{k}|<k_0}{}' k^2 \hat{P}_\mathbf{k} \hat{P}_{-\mathbf{k}} + \frac{N}{2V} \sum_{|\mathbf{k}|<k_0}{}' W_k \hat{Q}_\mathbf{k} \hat{Q}_{-\mathbf{k}}.$$

is the Hamiltonian of "free" oscillators, whose vibration frequencies are

$$\omega_k = \sqrt{\frac{1}{m}\frac{N}{V}\,k^2 W_k}, \qquad W_k = \int W(|\mathbf{x}|)e^{-i\mathbf{k}\mathbf{x}}\,d^3x;$$

$\hat{H}_I'$ contains the interaction terms between fermions, between oscillators, and between fermions and oscillators ([1]).

We shall be interested in the approximation in which the term $\hat{H}_I'$ is neglected.*

To compute the trace in formula (3), we put

$$|\Phi\rangle = \sum_{x,Q} \langle x, Q|\Phi\rangle |x, Q\rangle, \tag{7}$$

where

$$|x, Q\rangle \equiv \prod_{m=1}^{N} |x_m\rangle \prod_{|\mathbf{k}|<k_0}'' |Q_\mathbf{k}\rangle^{**}$$

is a common eigenvector of the operators $\hat{\mathbf{x}}_1, \dots, \hat{\mathbf{x}}_N$ and $\hat{Q}_\mathbf{k}$ ($|\mathbf{k}| < k_0$).

On the basis of (5),

$$(\hat{Q}_\mathbf{k} - \hat{\rho}_\mathbf{k})|\Phi\rangle \equiv \sum_{x,Q} \langle x, Q|\Phi\rangle (Q_\mathbf{k} - \rho_\mathbf{k}(\mathbf{x}_1, \dots, \mathbf{x}_N))|x, Q\rangle = 0, \tag{8}$$

whence

$$\langle x, Q|\Phi\rangle (Q_\mathbf{k} - \rho_\mathbf{k}(\mathbf{x}_1, \dots, \mathbf{x}_N)) = 0. \tag{9}$$

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* Usually, in the method of elementary excitations, it is assumed that this approximation is good at low temperatures. But at low temperatures an approximation to the Hamiltonian is good in which the lowest energy levels are well approximated. It is accepted without proof that the approximation under consideration has this property. This observation is due to Prof. R. S. Ingarden, to whom we express our gratitude.

** $|Q_\mathbf{k}\rangle = |Q_\mathbf{k}^R\rangle|Q_\mathbf{k}^I\rangle$, $\hat{Q}_\mathbf{k} = \hat{Q}_\mathbf{k}^R + i\hat{Q}_\mathbf{k}^I$; $\prod''$ means that the product is taken over $\mathbf{k}$ ($\mathbf{k} \neq 0$) lying in a hemisphere, since $Q_{-\mathbf{k}}^R = Q_\mathbf{k}^R$, $Q_{-\mathbf{k}}^I = -Q_\mathbf{k}^I$.

Therefore an arbitrary vector $|\Phi\rangle$, satisfying the supplementary conditions (5), can be expanded in the complete system of vectors of the type $|x, Q = \rho(x)\rangle$, and

$$\underset{\Phi}{\mathrm{S}}\langle\Phi|\ldots|\Phi\rangle = \underset{x}{\mathrm{S}}\langle x, Q=\rho(x)|\ldots|x, Q=\rho(x)\rangle. \tag{10}$$

For the statistical sum in the approximation under consideration we have

$$Z_N^0 = \int d^3x_1\ldots d^3x_N \langle x|e^{-\beta\hat{H}_0'}|x\rangle\langle Q=\rho(x)|e^{-\beta\hat{H}_{osc}'}|Q=\rho(x)\rangle \tag{11}$$

and after carrying out the calculations we obtain

$$Z_N^0 = \left(\frac{1}{N!}\right)^2 V^{-N}\sum_{f_1}\ldots\sum_{f_N}\exp\left\{-\beta\sum_{j=1}^{N}\varepsilon_{f_j}\right\}\int d^3x_1\ldots d^3x_N\left\|e^{i\mathbf{f}_a\mathbf{x}_b}\right\|^2\times$$

$$\times\prod_{|\mathbf{k}|<k_0}^{\prime\prime}\sum_{m_k=0}^{\infty}\sum_{l_k=0}^{\infty}e^{-2\beta\hbar\omega_k(m_k+l_k+1)}\left|\chi_{m_k}(\rho_k^R(x))\right|^2\left|\chi_{l_k}(\rho_k^I(x))\right|^2; \tag{12}$$

here $\varepsilon_f = \mathbf{f}^2/2m$; $\left\|e^{i\mathbf{f}_a\mathbf{x}_b}\right\|^2$ is the square of the modulus of the determinant $(a, b = 1, \ldots, N)$;

$$\chi_m(y) = \frac{1}{\sqrt{c}}\,e^{-\frac{1}{2}\left(\frac{y}{c}\right)^2}\,\mathcal{H}_m\left(\frac{y}{c}\right)$$

$$\left(c = \sqrt{\frac{1}{\hbar}}\sqrt[4]{\frac{1}{m}\frac{V}{N}\frac{k^2}{W_k}},\quad \mathcal{H}_m(y) = \frac{(-1)^m}{\sqrt{2^m m!\sqrt{\pi}}}\,e^{y^2}\frac{d^n}{dy^n}e^{-y^2}\ \text{—normalized Hermite polynomial}\right).$$

Formula ([2])

$$\sum_{m=0}^{\infty}[\chi_m(y)]^2 e^{-\alpha m} = \frac{1}{\sqrt{\pi}\,c\sqrt{1-e^{-2\alpha}}}\,e^{-\frac{1}{c^2}\,\mathrm{tgh}\,\frac{\alpha}{2}\,y^2} \tag{13}$$

allows the summations over m_k and l_k in (12) to be performed. Then

$$Z_N^0 = \exp\left\{-\beta\sum_{|\mathbf{k}|<k_0}^{\prime}\hbar\omega_k\right\}\left(\frac{1}{N!}\right)^2 V^{-N}\times$$

$$\times\sum_{f_1}\ldots\sum_{f_N}\exp\left\{-\beta\sum_{j=1}^{N}\varepsilon_{f_j}\right\}\int d^3x_1\ldots d^3x_N\left\|e^{i\mathbf{f}_a\mathbf{x}_b}\right\|^2\prod_{|\mathbf{k}|<k_0}^{\prime\prime}B_k e^{-A_k\rho_k(x)\rho_{-\mathbf{k}}(x)}, \tag{14}$$

where

$$A_k = \frac{1}{\hbar}\sqrt{m\frac{N}{V}\frac{W_k}{k^2}}\ \mathrm{tgh}\,\beta\hbar\omega_k, \qquad B_k = \frac{1}{\hbar\Pi}\sqrt{m\frac{N}{V}\frac{W_k}{k^2}\frac{1}{1-e^{-4\beta\hbar\omega_k}}}. \tag{15}$$

The calculation of the integral over $\mathbf{x}_1, \dots, \mathbf{x}_N$ is difficult. We shall calculate this integral by replacing $\left(\frac{1}{N!}\right)^2 \left\| e^{i\mathbf{f}_a \mathbf{x}_b} \right\|^2$ by unity, which corresponds to neglecting the antisymmetrization of the states. This gives an estimate of the value of Z_N^0 from above*:

$$Z_N^{0\,\max} = \sum_{f_1} \dots \sum_{f_N} \exp\left\{-\beta \sum_{j=1}^{N} \varepsilon_{f_j}\right\} R_N, \tag{16}$$

* Z. Galiasevich drew our attention to this.

where

$$R_N = \exp\left\{-\beta \sum_{|\mathbf{k}|<k_0}{}' \hbar\omega_k\right\} V^{-N} \prod_{|\mathbf{k}|<k_0}{}'' B_k \int d^3x_1 \dots d^3x_N \prod_{|\mathbf{k}|<k_0}{}'' e^{-A_k \rho_k \rho_{-\mathbf{k}}}; \tag{17}$$

this is the configurational integral.

Let us compute R_N approximately for large N, following exactly Zubarev' s method from paper ([3]). It is not difficult to verify that in this approximation

$$R_N = \exp\left\{-\beta \sum_{|\mathbf{k}|<k_0} \hbar\omega_k\right\} \prod_{|\mathbf{k}|<k_0}{}'' B_k \left(A_k + 1\right)^{-1}. \tag{18}$$

The connection of the present result with the classical case of this problem will be considered in the following paper.

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CITED LITERATURE

1 D. N. Zubarev, Candidate dissertation, Moscow, 1953; ZhETF, **25**, 548 (1953); Z. Galasiewicz, Postępy fizyki, **7**, 317 (1956). **2** E. C. Titchmarsh, *Introduction to the Theory of the Fourier Integrals*, Oxford, 1948. **3** D. N. Zubarev, DAN, **95**, 757 (1954).

Note: Figure translations are in progress. See original paper for figures.