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DENSITY MATRIX OF THE SYSTEM OF IDENTICAL PARTICLES, INTERACTING VIA OSCILLATOR FORCES

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The exact expression for N-particles density matrix is obtained for D-dimensional system of identical particles, connected by oscillator forces. This expression is presented as a product of the ideal gas density matrix with the renormalized mass and a factor, which does not depend on statistics and depicts only the character of interparticle interaction.

1. Introduction

The quantum mechanical problem of description of the system of identical particles interacting via forces proportional to their displacement from the equilibrium position (we shall call them oscillator forces) is one of the basic problems in theoretical physics. Due to the symmetry of wave functions this problem is not trivial. It was considered in [1, 2], where the wave function and the ground state energy of the system of Bose-particles were found. It turned out that the question of extracting of the center of mass keeping the antisymmetry of wave function in case of many-fermion system was not simple. Some results are presented in monograph by D. Thouless [3].

Let's consider the system of N identical particles with mass m and coordinates $\mathbf{r}_1, ..., \mathbf{r}_N$ in D-dimensional space of volume V with the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2 + \Phi,$$

were the potential energy reads

$$\Phi = \frac{K}{4}\sum_{i=1}^{N}\sum_{j=1}^{N}|\mathbf{r}_i - \mathbf{r}_j|^2.$$

This is the potential energy of particles, connected by oscillator forces. We shall be interested in the total N-particle density matrix

$$R_N(\mathbf{r}_1, \ldots, \mathbf{r}_N|\mathbf{r}'_1, \ldots, \mathbf{r}'_N) = \sum_{\alpha}\Psi^*_\alpha(\mathbf{r}'_1, \ldots, \mathbf{r}'_N)e^{-\beta\hat{H}}\Psi_\alpha(\mathbf{r}_1, \ldots, \mathbf{r}_N), \quad (1.1)$$

where Ψ_α is the complete system of wave functions, symmetrized in accordance to statistics, which the particles obey, $T = 1/\beta$ is the temperature.

Our task is calculation of the matrix R_N. With this aim we apply method proposed former for calculating of density matrix of liquid ^4He [4, 5]. It is important that treating this oscillator model we are able to observe a set of interesting details during calculations, and also to affirm some conclusions, made by us for ^4He without enough basis.

2. Basic statements

Let's choose as the complete system of functions the symmetrized product of plane waves:

$$\Psi_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\sum_Q (\pm)^Q \frac{1}{\sqrt{V^N}} \exp(i\sum_{j=1}^N \mathbf{k}_j \mathbf{r}_{Qj}), \qquad (2.1)$$

were the sum over Q means the sum over different permutations of particle coordinate indices; "+" is used for Bose statistics and "–" for Fermi one, $\alpha = (\mathbf{k}_1,\ldots,\mathbf{k}_N)$ is the set of wave vectors, components of which take integer values multiplied by $2\pi/V^{1/D}$. The sum over different quantum numbers α in (1.1) means sum over $\mathbf{k}_1,\ldots,\mathbf{k}_N$ with factor $1/N!$, which takes into account that permutations of the wave vectors indices in the wave function do not give new states. In thermodynamical limit $N\to\infty$, $V\to\infty$, $N/V = const$ the sum over $\mathbf{k}$ turns into integral with the factor $V/(2\pi)^D$.

Let's carry the wave function Ψ_α (2.1) in (1.1) to the left hand side through the operator $\exp(-\beta\hat{H})$. Then momentum operators $\mathbf{p}_j = -i\hbar\nabla_j$ are to be substituted by quantities $\hbar\mathbf{k}_j$, the expression for the density matrix can be represented in the following form:

$$R_N(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_N) =$$

$$= \frac{1}{(N!)^2 V^N}\sum_Q\sum_{Q'}(\pm)^{Q+Q'}\sum_{\mathbf{k}_1}\cdots\sum_{\mathbf{k}_N}\exp\left(-\beta\sum_{j=1}^N\frac{\hbar^2 k_j^2}{2m}+\right.$$

$$\left.+i\sum_{j=1}^N \mathbf{k}_j(\mathbf{r}_{Qj}-\mathbf{r}'_{Q'j})\right)\exp\left(-\beta\hat{H}+\frac{\hbar^2\beta}{m}i\sum_{j=1}^N \mathbf{k}_{Qj}\nabla_j\right);$$

here operator exponent acts only to itself. Let's present the results of this action as

$$\exp\left(-\beta\hat{H}+\frac{\beta\hbar^2}{m}i\sum_{j=1}^N \mathbf{k}_{Qj}\nabla_j\right) = \exp(U),$$

where $U = U(\mathbf{k}_1,\ldots,\mathbf{k}_N;\mathbf{r}_1,\ldots,\mathbf{r}_N;\beta)$ is the function of coordinates and momenta of particles and inverse temperature β.

Differentiating with respect to β the both sides of this equation, we find the equation for U:

$$-\frac{\partial U}{\partial\beta} = -\sum_{j=1}^N\left\{\frac{\hbar^2}{2m}\nabla_j^2 U + \frac{\hbar^2}{2m}(\nabla_j U)^2 + i\frac{\hbar^2}{m}(\mathbf{k}_{Qj}\nabla_j)U\right\} + \Phi \qquad (2.2)$$

with condition $U = 0$ for $\beta = 0$.

Note that for $k_1 = k_2 = \ldots = k_N = 0$ one comes to the known equation that was obtained by I.R. Yukhnovskii within collective variables and displacements method. The examining of this method and its applications in different problems of statistical physics was subject of a serious investigations performed in Lviv school of theoretical physics in mid 60-ies — 70-ies. At that time Prof. I.R. Yukhnovskii was at the head of Theoretical Physics Chair in Lviv University.

So, for the density matrix we have

$$R_N(\mathbf{r}_1, \ldots, \mathbf{r}_N | \mathbf{r}'_1, \ldots, \mathbf{r}'_N) = \tag{2.3}$$

$$= \frac{1}{(N!)^2 V^N} \sum_Q \sum_{Q'} (\pm)^{Q+Q'} \sum_{\mathbf{k}_1} \ldots \sum_{\mathbf{k}_N} \exp\left(-\beta \sum_{j=1}^N \frac{\hbar^2 k_j^2}{2m} + \right.$$

$$\left. + i \sum_{j=1}^N \mathbf{k}_j (\mathbf{r}_{Qj} - \mathbf{r}'_{Q'j}) + U \right).$$

If interaction is excluded, then $U = 0$, and we get the density matrix of ideal quantum gas which after integration over momenta $\mathbf{k}_1, \ldots, \mathbf{k}_N$ is represented in the well known form, if one takes into consideration, that double sum over permutations in (1.1) reduces to simple sum with a factor:

$$R_N^0(\mathbf{r}_1, \ldots, \mathbf{r}_N | \mathbf{r}'_1, \ldots, \mathbf{r}'_N) = \tag{2.4}$$

$$= \frac{1}{N!} \left(\frac{m}{2\pi\beta\hbar^2} \right)^{\frac{DN}{2}} \sum_Q (\pm)^Q \exp\left(-\frac{m}{2\beta\hbar^2} \sum_{j=1}^N (\mathbf{r}_j - \mathbf{r}'_{Qj})^2 \right).$$

3. Solution of the equation for function U

Let's pass to the solving of the equation (2.2) for U. Simple analysis of this equation, with accounting of the explicit form of potential Φ shows, that U must be the quadratic function of $\mathbf{r}_1, \ldots, \mathbf{r}_N$ and $\mathbf{k}_1, \ldots, \mathbf{k}_N$. Let's represent it in the next form:

$$U = a_0 + a_{11} \sum_{j=1}^N \mathbf{k}_j^{*2} + i a_{12} \sum_{j=1}^N \mathbf{k}_j^* \mathbf{r}_j^* + a_{22} \sum_{j=1}^N \mathbf{r}_j^{*2}, \tag{3.1}$$

where

$$\mathbf{r}_j^* = \mathbf{r}_j - \frac{1}{N} \sum_{j=1}^N \mathbf{r}_j, \qquad \mathbf{k}_j^* = \mathbf{k}_{Qj} - \frac{1}{N} \sum_{j=1}^N \mathbf{k}_j.$$

The system of equations for unknown quantities a_0, a_{11}, a_{12}, a_{22} is found from the equation (2.2), equating, after the substitution of the expression (3.1), in it left hand side and right hand side, coefficients near the corresponding powers of $\mathbf{k}_j$ and $\mathbf{r}_j$:

$$\frac{da_0}{d\beta} = \frac{\hbar^2}{m} D(N-1) a_{22},$$

$$\frac{da_{11}}{d\beta} = -\frac{\hbar^2}{2m}a_{12}^2 - \frac{\hbar^2}{m}a_{12},$$

$$\frac{da_{12}}{d\beta} = \frac{\hbar^2}{m}2a_{12}a_{22} + \frac{\hbar^2}{m}2a_{22},$$

$$\frac{da_{22}}{d\beta} = \frac{\hbar^2}{m}2a_{22}^2 - \frac{KN}{2},$$

and $a_0 = a_{11} = a_{12} = a_{22} = 0$ for $\beta = 0$.

Omitting the details of not difficult calculations, we present the solution of these equations:

$$a_0 = -\frac{D}{2}(N-1)\ \ln(\cosh(\beta\hbar\omega)),$$

$$a_{11} = \frac{\hbar}{2m\omega}(\beta\hbar\omega - \tanh(\beta\hbar\omega)),$$

$$a_{12} = \frac{1}{\cosh(\beta\hbar\omega)} - 1,$$

$$a_{22} = -\frac{m\omega}{2\hbar}\tanh(\beta\hbar\omega),$$

where frequency is defined by

$$\omega = \sqrt{\frac{KN}{m}}.$$

It is clear that we have found the exact solution for function U due to the fact that the potential energy Φ is the quadratic function of coordinates of particles. In general case it is impossible to solve the equation (2.2). However, one can propose the perturbation theory for arbitrary Φ by expanding function U into a series in the powers of $\mathbf{k}_j$. We do not discuss here the meaning of approximations and the effectiveness of such perturbation theory. We only note, that such approach was realized by us in [4, 5] for many-boson system.

Obviously, the density matrix R_N by definition, should be a symmetrical function with respect to primed and non-primed variables. But from the expression (2.3) this property of R_N matrix is not obvious. The problem of conserving of the symmetry is one of the main in calculation of density matrix by perturbation theory.

4. Results and discussion

The next step consists in integration over wave vectors $\mathbf{k}_j$ in the expression (2.3) taking into consideration the explicit form of function U. Because in the integrand the exponent contains the quadratic function over wave vectors, this integration reduces to the product of Poisson integral

$$R_N(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_N) =$$

$$= \frac{1}{(N!)^2}\left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{D}{2}}\left[\frac{m\omega}{2\pi\hbar\,\sinh(\beta\hbar\omega)}\right]^{\frac{D}{2}(N-1)}\times$$

$$\times\sum_Q\sum_{Q'}(\pm)^{Q+Q'}\exp\left(\frac{a_{22}\sum_{j=1}^{N}\mathbf{r}_j^{*2}-\sum_{j=1}^{N}(\mathbf{r}_{Qj}-\mathbf{r}'_{Q'j}+a_{12}\mathbf{r}^*_{Qj})^2}{4\left(\beta\frac{\hbar^2}{2m}-a_{11}\right)}+\right.$$

$$\left.+\frac{a_{11}\left[\sum_{j=1}^{N}(\mathbf{r}_j-\mathbf{r}'_j)\right]^2}{4N\beta\frac{\hbar^2}{2m}\left(\beta\frac{\hbar^2}{2m}-a_{11}\right)}\right).$$

Let's substitute explicit expressions for a_{mn} and perform some not difficult, but rather cumbersome transformations. The main aim of these transformations is to represent the density matrix in explicitly symmetrized form with respect to primed and non-primed variables. In connection with this, these transformations are useful and instructive for solving the problem in general case as well. Finally, we get

$$R_N(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_N)= \tag{4.1}$$

$$=\left(\frac{m}{m^*}\right)^{\frac{D}{2}}R^*_N(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_N)\times$$

$$\times\exp\left(-\frac{m}{2\beta\hbar^2}\frac{x}{\tanh x}\frac{1}{2N}\sum_{i=1}^{N}\sum_{j=1}^{N}\left[(\mathbf{r}_i-\mathbf{r}_j)^2+(\mathbf{r}'_i-\mathbf{r}'_j)^2\right]+\right.$$

$$\left.+\frac{m^*}{2\beta\hbar^2}\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{r}_i-\mathbf{r}'_j)^2-\frac{m}{2\beta\hbar^2}\frac{1}{N}\left(\sum_{j=1}^{N}(\mathbf{r}_j-\mathbf{r}'_j)\right)^2\right),$$

where R^*_N matrix is the matrix of ideal gas (2.4), with changing of mass of particle m to effective mass $m^* = mx/\sinh x$, $x=\beta\hbar\omega=\beta\hbar\sqrt{KN/m}$, $R^*_N = R^0_N$ for $m\to m^*$.

We have got an important result: the density matrix is presented in a form of product of the density matrix of ideal gas of particles with renormalized mass m^* which is responsible for the particle statistics, and the factor which does not depend on statistics and expresses only the character of interaction. The latter, for diagonal elements, looks like Boltsman factor with the effective energy $\tilde{\Phi}=\Phi\tanh(x/2)/(x/2)$. For $\beta\to 0$, that is for high temperatures (classic limit), $\tilde{\Phi}=\Phi$, and for low temperatures, $\beta\to\infty$, this Boltsman factor includes in the exponent instead of temperature the quantity $T_0=\hbar\omega/2$ that is the energy of ground state oscillation.

In the limit of low temperatures (4.1) becomes of the form:

$$R_N(\mathbf{r}_1,\ldots,\mathbf{r}_N|\mathbf{r}'_1,\ldots,\mathbf{r}'_N)=$$

$$= \left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{D}{2}} e^{-\beta E_0}\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Psi_0(\mathbf{r}'_1,\ldots,\mathbf{r}'_N),$$

where the first multiplier expresses the motion in D-dimensional space and provides limit value of the matrix for $N = 1$,

$$E_0 = D(N-1)\frac{\hbar\omega}{2} = \frac{D(N-1)}{2}\hbar\sqrt{KN/m}$$

is the ground state energy for $D(N-1)$ oscillator, the wave function of ground state of which is given by

$$\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{D(N-1)}{4}} \exp\left(-\frac{m\omega}{2\hbar}\frac{1}{2N}\sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{r}_i-\mathbf{r}_j)^2\right) =$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{D(N-1)}{4}} \exp\left(-\frac{m\omega}{2\hbar}\sum_{j=1}^{N}\mathbf{r}_j^2\right)\exp\left(\frac{m\omega}{2\hbar N}\left(\sum_{j=1}^{N}\mathbf{r}_j\right)^2\right).$$

Let's note, that the system, we are considering, differs essentially from many other physical systems; the energy is not an additive quantity, $E_0 \sim N^{3/2}$, the frequency ω depends on the number of particles. If one implies the additional condition on the elasticity constant in thermodynamical limit $KN = const$ for $N \to \infty$, $V \to \infty$, $N/V = const$ then the physical model with ordinary properties is obtained. This additional condition reminds the well known model of ferromagnet with the exchange interaction "everyone with everyone" but decreased in N times, exact solution for which yields the approximation of the molecular field.

Elsewhere we'll calculate the thermodynamic functions and density matrices, proceeding from the expression (4.1) for R_N derived by the method introduced in [7] and here we will make one more final remark.

The calculation method for N-particle density matrices was proposed and used by us in [4, 5] for investigation of the Bose-Einstein condensation point in liquid ^4He. The equation (2.2) for U function was solved by the perturbation theory method. The density matrix of liquid ^4He was obtained as a product of the density matrix of ideal Bose-gas with renormalized mass of particles and the density matrix of the ground state of the liquid. This made possible to pick out two mechanisms of the shift of the point of Bose-condensation due to the effective mass and due to the effect of the free volume. This result, derived by the perturbation theory method, is confirmed as one can see, by the exact solution of the problem for the identical particles system, interacting via oscillator forces.

References

[1] Elliot J.P., Skyrme T.H.R. Centre-of-mass effects in the nuclear shell-model. // Proc. Roy. Soc., 1955, vol. A232, No 1191, p. 561–566.

[2] Gartenhaus S., Schwartz C. Center-of-mass motion in many-particle systems. // Phys. Rev., 1957, vol. 108, No 2, p. 482–490.

[3] Thouless D.J. The Quantum mechanics of Many-Body Systems. Academic Press, New York and London, 1972, 242 p.

[4] Vakarchuk I.O. Bose-Einstein condensation in superfluid helium-4. "Physics in Ukraine"— International Conference (Kiev, 22-27 June, 1993). Proceedings Contributed Papers. "Statistical Physics and Phase Transitions". P. 145–148.

[5] Vakarchuk I.O. On the theory of λ-transition in liquid ^4He. // Visnyk Lvivs'koho Universytetu. Seriya fizychna. Vypusk 26, 1993, p. 29–38 (in Ukrainian).

[6] Yukhnovskii I.R. Statistical operator and collective variables. I. Displacement transformations. // Ukr. Fiz. Zh., 1964, vol. 9, No 7, p. 702–713 (in Ukrainian);
The quantum partition function and collective variables. II. Transition function to collective variables. // Ukr. Fiz. Zh., 1964, vol. 9, No 8, p. 827–838 (in Ukrainian);
Displacement method and collective variables. // Kiev, 1971, (Prepr. ITP: ITP-71-26R) (in Russian).

[7] Vakarchuk I.O. Density matrix of liquid He^4 at low temperatures. // Kiev, 1973, (Prepr. ITP: ITP-73-76R) (in Russian);
Density matrix of many-boson system at low temperatures. // Teor. Mat. Fiz., 1975, vol. 23, No 2, p. 260–272 (in Russian);
Irreducible cluster expansion for the logarithm of the s-particle density matrix of the many-boson system. // Teor. Mat. Fiz., 1977, vol. 32, No 2, p. 247–266 (in Russian);
Density matrix of superfluid helium-4. Part I. // Teor. Mat. Fiz., 1989, vol. 80, No 3, p. 439–451 (in Russian);
Density matrix of superfluid helium-4 . Part II. // Teor. Mat. Fiz., 1990, vol. 82, No 3, p. 438–449 (in Russian).

МАТРИЦЯ ГУСТИНИ СИСТЕМИ ТОТОЖНИХ ЧАСТИНОК, ЗВ'ЯЗАНИХ ОСЦИЛЯТОРНИМИ СИЛАМИ

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Для D-вимірної системи N тотожних частинок, зв'язаних осциляторними силами, знайдено точний вираз для повної матриці густини, яка представляється у вигляді добутку матриці густини ідеального газу з перенормованою масою частинок, на фактор, що не залежить від статистики і відображає лише характер міжчастинкової взаємодії.