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The role of angular momentum conservation law in statistical mechanics

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Within the limits of Khinchin ideas [A.Y. Khinchin, Mathematical Foundation of Statistical Mechanics. NY, Ed. Dover, 1949] the importance of momentum and angular momentum conservation laws was analyzed for two cases: for uniform magnetic field and when magnetic field is absent. The law of momentum conservation does not change the density of probability distribution in both cases, just as it is assumed in the conventional theory. It is shown that in systems where the kinetic energy depends only on particle momenta canonically conjugated with Cartesian coordinates being their diagonal quadric form,the angular momentum conservation law changes the density of distribution of the system only in case the full angular momentum of a system is not equal to zero. In the gas of charged particles in a uniform magnetic field the density of distribution also varies if the angular momentum is zero [see Dubrovskii I.M., Condensed Matter Physics, 2206, **9**, 23]. Two-dimensional gas of charged particles located within a section of an endless strip filled with gas in magnetic field is considered. Under such conditions the angular momentum is not conserved. Directional particle flows take place close to the strip boundaries, and, as a consequence, the phase trajectory of the considered set of particles does not remain within the limited volume of the phase space. In order to apply a statistical thermodynamics method, it was suggested to consider near-boundary trajectories relative to a reference system that moves uniformly. It was shown that if the diameter of an orbit having average thermal energy is much smaller than a strip width, the corrections to thermodynamic functions are small depending on magnetic field. Only the average velocity of near-boundary particles that form near-boundary electric currents creating the paramagnetic moment turn out to be essential.

Key words: *phase space, invariant set, integral of motion, angular momentum, electron gas, magnetic field*

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1. Introduction

Much attention has been focused on the investigation of two-dimensional electronic gas properties lately. All these investigations are based on a conventional postulate of statistical physics, namely: statistical set distribution density (statistical operator in quantum theory) depends only on Hamiltonian of the system under consideration. This postulate leads to two paradoxical effects in case the gas of the charged particles described by classical mechanics is exposed to a uniform magnetic field. Firstly, the average magnetic moment of gas $\langle M\rangle$ is equal to zero (Bohr – van Leeuwen theorem). However, direct calculations of magnetic moment for several charged particles results in $\langle M\rangle = -E/B$, where E is the energy of the orbital motion of particles and B is magnetic field induction. Secondly, as it follows from distribution density, the gas of charged particles uniformly fills all the available area. It is well-known that two-dimensional gas of charged particles is held by uniform magnetic field perpendicular to the plane. Noninteracting particles move in fixed circular orbits. The collisions are also incapable of leading to diffusive gas expansion since new orbits of colliding particles pass through a collision point and the total area of orbits is conserved. It can be shown that Coulomb repulsion does not cause an unlimited gas expansion [1]. If the area boundaries are located far enough from the gas centre of mass, its equilibrium density should be axial-symmetric and decrease exponentially at large distances from the centre of mass. As it was shown in [2], these paradoxes also take place in quantum statistical mechanics. Quantum mechanical average value of magnetic moment in a stationary state with energy ϵ_n is

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equal to $-\epsilon_n/B$. Therefore, quantum-statistical average value of the magnetic moment of gas of particles filling these states cannot be determined by small corrections after replacing summation by integration. Eigenfunctions of stationary states, which are also eigenfunctions of the angular momentum operator, are localized if there is no boundary. Hence, the gas density should be also localized.

As shown in [1,2] the statistical mechanics of charged particles gas in magnetic field can be formulated without paradoxes if the density of distribution (or the statistical operator in quantum theory) is considered to be also dependent on the angular momentum. The role of various motion integrals in determining the probability distribution density of a state in phase space was subjected to rigorous treatment in monograph [3]. The existence of an area in the phase space that occupies a finite volume and transforms into itself according to Hamilton equations is a necessary condition of the stationary equilibrium state of an isolated system. This area is said to be an invariant set. The phase trajectory of the system, whose initial point is located in the mentioned area, indefinitely remains in it. As it follows from the definition of an invariant set, the motion integrals, i. e., the functions of dynamic variables remaining constant along the phase trajectory, should be constant in it. If these conservation laws determine the area of finite volume in the phase space, this area is an invariant set. The energy of an isolated system is always a motion integral. If an external field (for example, container walls) or interaction of particles prevents the unlimited expansion of a system, the law of energy conservation describes a closed hypersurface in the phase space. Then the invariant area of the phase space should be a thin layer ΔE near the hyper-surface of constant energy or its subset. Besides the energy, the system can have other motion integrals. As shown in monograph [3] (p. 37) the conservation of complementary controllable motion integrals should be taken into account in order to determine the invariant area over which the averaging is performed. Motion integral is said to be controllable if it has a physical sense, i. e., if it is single-valued, can be measured and preset by external conditions. If the system possesses a proper symmetry, such integrals are components of total momentum and total angular momentum about the centre of mass (see monographs [4,5]). Conservation equations for these integrals cannot determine an invariant area of finite volume on their own. They separate some subset of the set determined by energy conservation. But further in monograph [3], it is assumed that the energy is the only controllable integral of motion. Considering the ideal gas as an example (p. 68, 78), the effect of conservation of momentum and angular momentum is not taken into consideration without any substantiation.

It is assumed that the probability of detecting an isolated system at any point of invariant set Σ does not depend on point coordinates (see monograph [3], p. 49). Outside the invariant set, this probability, obviously, is equal to zero. This postulate can be expressed by a formula:

$$\mathrm{d}P(\mathbf{R}) = \frac{\varphi_\Sigma(\mathbf{R})\mathrm{d}\Gamma}{\Omega_\Sigma}\,. \tag{1}$$

Here $\mathbf{R}$ is the many-dimensional vector defining a point of the phase space, $\mathrm{d}P(\mathbf{R})$ is a probability to detect the system in this point, Ω_Σ is the volume of invariant set, $\varphi_\Sigma(\mathbf{R})$ is the characteristic function of invariant set Σ which is equal to one if the point $\mathbf{R}$ belongs to this set, and is equal to zero in all other points of the phase space, $\mathrm{d}\Gamma = \prod_{i=1}^{N} \mathrm{d}\mathbf{p}_i \mathrm{d}\mathbf{r}_i$ is phase space volume element, N is number of particles. If the system can be divided into two subsystems described by non-overlapping groups of phase variables, so that $\Sigma = \Sigma_1 \otimes \Sigma_2, \quad \mathbf{R} = \mathbf{R}_1 + \mathbf{R}_2$, then

$$\begin{gathered} \Omega_\Sigma = \Omega_{\Sigma_1} \cdot \Omega_{\Sigma_2}, \quad \varphi_\Sigma(\mathbf{R}) = \varphi_{\Sigma_1}(\mathbf{R_1}) \cdot \varphi_{\Sigma_2}(\mathbf{R_2}), \\ \mathrm{d}P(\mathbf{R}) = \mathrm{d}P_1(\mathbf{R_1}) \cdot \mathrm{d}P_2(\mathbf{R_2}) = [\varphi_{\Sigma_1}(\mathbf{R_1})/\Omega_{\Sigma_1}] \cdot [\varphi_{\Sigma_2}(\mathbf{R_2})/\Omega_{\Sigma_2}] \cdot \mathrm{d}\Gamma_1 \mathrm{d}\Gamma_2. \end{gathered} \tag{2}$$

Considering the fact that density of distribution for a system is equal to the product of densities of distribution for subsystems, a conclusion is drawn in monograph [4] (p. 24) that the density of distribution logarithm should be an additive integral of motion and, hence, it should be a linear combination of the additive controllable integrals of motion, such as energy, momentum and angular momentum. As it follows from formula (2) this is incorrect for microcanonical distribution, since the characteristic function logarithm is meaningless.

In the second section of this paper, the laws of conservation of momentum and angular momentum are taken into account in order to calculate the volume of invariant set for the system with kinetic energy of standard form of hypersphere in the momentum subspace of the phase space. The application of this consideration to two-dimensional gas of charged particles in magnetic field (2DGMF) proves the correctness of density of distribution obtained in [1]. It is shown that 2DGMF density of distribution depends only on the energy if the shape and position of the boundaries violate the conservation of the angular momentum.

In the third section statistical mechanics is studied in detail for 2DGMF in a strip segment. Two parallel straight lines are the reflecting boundaries of the segment. The contribution is estimated of the special states with circular orbits intersecting the boundaries into thermodynamic functions and magnetic moment density per unit length of the strip.

2. Calculation of the invariant set volume with regard to the complementary integrals of motion

The method of statistical mechanics is applicable to the systems consisting of a great number of identical subsystems (particles). If the phase space points are represented by Cartesian coordinates of particles and corresponding momenta, the kinetic energy in most cases is a positive definite quadratic form of momenta of the particles forming the system and does not depend on coordinates. (Charged particles in a magnetic field which are considered in [1] and in the present work, as well as quasi-particles in a deformed solid for which the effective mass depends on coordinates are exceptions). To ensure that the energy conservation equation describes a closed hypersurface everywhere in phase space, energy should include the potential energy U depending on particle coordinates which holds particles in the bounded area. If the forces of interaction of particles manifest themselves only at a distance considerably smaller than the average distance between particles, interaction energy of particles is essential only in a small fraction of volume of invariant area. Therefore, the interaction of particles can be neglected in calculating the volume of invariant area. Interactions (collisions) cause a chaotic motion of the system. If particles interact by long-range force, this interaction needs to be considered using a mean field method. This is a model of ideal gas under external field. In this case the system Hamiltonian can be presented as the sum of identical terms, each of which depends on the coordinates and momenta of a single particle. Such a phase function is said to be a summatory function. It is postulated that a system distribution law, i.e. probability to find a system in some subset of invariant set, is equal to a ratio of the volume of this subset to the total volume (see formula (1)). Statistical properties of the system are fully determined by the dependence of the volume of invariant set on the energy, as well as, possibly, on the values of other controllable integrals of motion and external parameters.

To calculate the volume of invariant set, some integral formulae are required. Integrand function of these formulae contains characteristic function of a phase space points set for which function $A(\mathbf{R})$ is equal to a. Let us denote this set by Σ_A^a, its characteristic function by $\varphi_A^a(\mathbf{R})$, and volume by $\Omega_A(a)$. It is supposed that this volume is limited and is not equal to zero.

$$\int \varphi_A^a(\mathbf{R})\mathrm{d}\Gamma = \Omega_A(a),$$

$$\int \varphi_A^a(\mathbf{R})f[\mathbf{R}, A(\mathbf{R})]\mathrm{d}\Gamma = \int \varphi_A^a(\mathbf{R})f[\mathbf{R}, a]\mathrm{d}\Gamma. \tag{3}$$

Here integration is carried out over the whole phase space, but actually, owing to properties of the characteristic function, over set Σ_A^a.

$$\int_{\mathrm{A}} F(a)\int \varphi_A^a(\mathbf{R})\mathrm{d}a\mathrm{d}\Gamma = \int_{\mathrm{A}}\int \varphi_A^a(\mathbf{R})F[A(\mathbf{R})]\mathrm{d}a\mathrm{d}\Gamma = \int F[A(\mathbf{R})]\mathrm{d}\Gamma. \tag{4}$$

Here A is the range of values of function $A(\mathbf{R})$.

It is possible to express the properties of integrals (3) and (4) by unified method if we change a characteristic function $\varphi_A^a(\mathbf{R})$ for δ-function $\delta[A(\mathbf{R}) - a]$ in their integrands. Formulae of this type are widely used in physics, for example, while calculating the dependence of X-ray scattering intensity on direction (see monograph [6]). Then, if energy is the only controllable integral of motion of the system,

$$\Omega(E) = \Delta E \int \delta\left(\sum_{i=1}^{N}\left(\frac{1}{2m}\sum_{\nu=1}^{3} p_{\nu,i}^2 + U(\mathbf{r}_i)\right) - E\right)\mathrm{d}\Gamma. \tag{5}$$

Here m is particle mass, $p_{\nu,i}$ is ν-component of momentum of i-th particle, $\mathbf{r}_i$ is its radius-vector. In monograph [3], $\Omega(E)$ is calculated using the probability theory method. In this case it is essential that the invariant set should be determined by the only controllable integral, namely, by energy. To generalize for a case when other controllable integrals of motion also exist, we use a method proposed by Yu.A. Krutkov in [7] and [8]. This method uses the fact that the argument of δ-function in formula (5) depends on a summatory function for which the range of values is a positive semiaxis. Then Laplace transform of function $\Omega(E)$

$$\Phi(\beta) = \int_0^\infty \Omega(E)\exp(-\beta E)\mathrm{d}E \tag{6}$$

is represented as a product of Laplace transforms of corresponding functions for identical subsystems the Hamiltonians of which are terms of a summatory function. It enables one to calculate Laplace reconversion using the quickest decent method at a great number of subsystems, for example, the particle forming gas.

The total momentum and the full angular momentum of particle system are also summatory functions. Correlation between the values of these terms at different instants decays fast with time interval increase due to a large number of particle collisions. It is proved in monograph [3] (p. 46) that for such functions the time-average value over the phase trajectory is approximately equal to the average value over the invariant set. If the invariant set is determined by the energy conservation law only, then the average value of phase function over this set is a function of energy value. However, controllable integral of motion value can be specified irrespectively of energy value. Hence, this value should generally define some subset of the hypersurface of constant energy which is an invariant set of the system with several integrals of motion. The volume of invariant set is determined by an integral of the product of Dirac δ- functions fixing controllable values of integrals taken over the whole phase space of a system (see monograph [4] p. 26).

If gas is held by external potential field, uniformity of space is violated and the law of momentum conservation should not be taken into account. However, potential field in many cases is essential only within a thin layer near the boundary. The sum of momenta of colliding particles is conserved. The total momentum of gas and a vessel containing this gas is conserved. It can be taken equal to zero. Then fluctuations of total momentum of gas close to zero value are small and symmetrical. One can concede that zero value of momentum of gas is approximately conserved. Details of interaction of particles with boundary can be neglected and potential field can be replaced by finite limits of integration over space coordinates (see monograph [3], p. 68). Then function $\Omega(E)$ takes a form:

$$\Omega(E) = \Delta E\Delta\mathbf{P} \int \delta\left(\sum_{i=1}^{N}\left(\frac{1}{2m}\sum_{\nu=1}^{3} p_{\nu,i}^2 + U(\boldsymbol{r}_i)\right) - E\right)\prod_{\nu=1}^{3}\delta\left(\sum_{i=1}^{N} p_{\nu,i}\right)\mathrm{d}\Gamma. \tag{7}$$

For short, let us consider conservation of one component of the momentum and omit index ν. Integrating over p_1, we obtain:

$$\Omega(E) = \Delta E\Delta\mathbf{P} \int \delta\left(\frac{1}{2m}\left(\sum_{i=2}^{N} p_i^2 + \left(\sum_{i=2}^{N} p_i\right)^2\right) + \sum_{i=1}^{N} U(\boldsymbol{r}_i) - E\right)\mathrm{d}\Gamma_1. \tag{8}$$

Here $\mathrm{d}\Gamma_1 = \mathrm{d}\Gamma/\mathrm{d}p_1$. Function $\Omega(E)$ is a functional of a non-summatory function. To reduce formula (8) to a form similar to formula (5), let us perform quadratic form diagonalization. The characteristic equation is:

$$\det[1 + (1-\lambda)\delta_{ik}] = (1-\lambda)^{N-2}(N-\lambda) = 0. \tag{9}$$

One of coefficients of the diagonal quadratic form is equal to N, and remaining $N-2$ are equal to one. Hence, if conservation of momentum is taken into account, $\Phi(\beta)$ is a product of $(N-1)$ identical factors f_0 and one factor is equal to $N^{-1/2}$. If conservation of momentum is not taken into account, N identical factors f_0 are obtained. As shown in monograph [8], such differences are insignificant for $\Phi(\beta)$ calculation. The reason for it is the fact that $\ln[\Phi(\beta)]$ has got a physical sense, while the correction to it is relatively small. New integration variables are not the momenta of separate particles here, but rather their linear combinations. This violates a derivation of canonical distribution as well as the averaging of summatory functions. Therefore, it is necessary to prove that these changes are not essential. Expansion coefficients of new variables in terms of separate particles momenta are components of eigenvectors of the quadratic form matrix. $N-2$ eigenvectors for degenerate eigenvalue 1 have one component equal to 1 and all remaining are equal to $-(N-2)^{-1}$. These small components can be neglected. Then $N-2$ integration variables remain invariable. As it follows from this analysis, the momentum conservation law being taken into consideration does not result in any essential changes.

Let us consider the gas having a conserved angular momentum $\mathbf{L_0}$. For this purpose it is necessary that the potential energy should be axially symmetric and the particles should interact by central forces. This is convenient to be considered using circular cylindrical coordinates with the axis parallel to $\mathbf{L_0}$. The angular momenta of particles are l_i and $L_0 = \sum_{i=1}^{N} l_i$. Then there is a term depending on the angular momenta of particles in typical kinetic energy. This term is a diagonal quadratic form of l_i with coefficients $(2mr_i^2)^{-1}$. Here r_i is the particle radial coordinate.

Function $\Omega(E)$ with regard to angular momentum conservation takes form:

$$\Omega(E, L_0) = \Delta E \Delta \mathbf{L} \int \delta\left(\frac{1}{2m}\sum_{i=1}^{N}\left(p_{z,i}^2 + p_{r,i}^2 + \frac{l_i^2}{r_i^2}\right) + \sum_{i=1}^{N} U(r_i) - E\right)\delta\left(\sum_{i=1}^{N} l_i - L_0\right)\mathrm{d}\Gamma. \quad (10)$$

Here $\mathrm{d}\Gamma = \prod_{i=1}^{N} \mathrm{d}p_{z,i}\mathrm{d}p_{r,i}\mathrm{d}l_i\mathrm{d}z_i\mathrm{d}r_i\mathrm{d}\varphi_i$, $p_{r,i}$ is a radial momentum of a particle, the integrations over l_i are performed in infinite limits. After integrating over l_1 one can obtain a quadratic form $Q(l_2,\ldots,l_N)$:

$$Q(l_2,\ldots,l_N) = \sum_{i=2}^{N}\frac{l_i^2}{r_i^2} + r_1^{-2}\left(\sum_{i=2}^{N} l_i - L_0\right)^2. \quad (11)$$

Terms proportional to the first power of the angular momenta of particles are eliminated by transformation:

$$l_i = \tilde{l_i} + L_0 r_i^2\left(\sum_{j=1}^{N} r_j^2\right)^{-1}. \quad (12)$$

Thus, we obtain:

$$Q(\tilde{l_2},\ldots,\tilde{l_N}) = \sum_{i=2}^{N}\frac{\tilde{l}_i^2}{r_i^2} + r_1^{-2}\left(\sum_{i=2}^{N}\tilde{l_i}\right)^2 + L_0^2\left(\sum_{j=1}^{N} r_j^2\right)^{-1}. \quad (13)$$

The term $L_0^2\left(2m\sum_{j=1}^{N} r_j^2\right)^{-1}$ in the argument of δ-function which is generated by the energy conservation law in formula (10) makes it impossible for attracting particles to collapse if the total angular momentum of the isolated system is not equal to zero. This term also makes it impossible to use the Khinchin [3] or Krutkov [8] method to calculate $\Omega(E, L_0)$ function, because $Q(\tilde{l_2},\ldots,\tilde{l_N})$ (see (13)) cannot be converted into summatory function.

Let us consider the gas having the total angular momentum equal to zero. If it is held by a vessel which does not have axial symmetry, fluctuations of the total angular momentum near zero value are small and symmetrical. One can concede that zero value of total angular momentum of gas is approximately conserved. The quadratic form $Q(l_2,\ldots,l_N)$ at $L_0 = 0$, does not contain linear terms, and can be made diagonal. The characteristic equation takes the form:

$$\det[r_1^{-2} + (r_i^{-2} - \lambda)\delta_{ij}] = \prod_{i=2}^{N}(r_i^{-2} - \lambda)\left(\sum_{j=2}^{N}\frac{r_1^{-2}}{r_j^{-2} - \lambda} + 1\right) = 0. \tag{14}$$

The Laplace transform of function $\Omega(E, 0)$ over E takes the form:

$$\Phi(\beta) = \Delta E\Delta\mathbf{L}\int\exp\left[-\frac{\beta}{2m}\left(\sum_{j=1}^{N}(p_{z,i}^2 + p_{r,j}^2) + \sum_{j=2}^{N}\frac{\bar{l}_j^2}{a_j^2} + 2m\sum_{j=1}^{N}U(r_j)\right)\right]\prod_{j=2}^{N}\mathrm{d}\bar{l}_j\mathrm{d}\acute{\Gamma}. \tag{15}$$

Here $\mathrm{d}\acute{\Gamma} = \mathrm{d}\Gamma/\prod_{i=1}^{N}\mathrm{d}l_i$, all $\bar{l}_j$ are linear combinations of l_i which are obtained at diagonalization of the quadratic form $Q(l_2, \ldots, l_N)$, and all a_j^{-2} are coefficients of the obtained diagonal quadratic form. These coefficients are the roots of equation (14). They depend on the radial variables $a_j^{-2} = a_j^{-2}(r_1, \ldots, r_N)$. The product of these quantities is equal to the absolute term of the equation (14):

$$\prod_{j=2}^{N}a_j^{-2} = \left\{\det[r_1^{-2} + (r_i^{-2} - \lambda)\delta_{ij}]\right\}_{\lambda=0} = \prod_{i=1}^{N}r_i^{-2}\left(\sum_{j=1}^{N}r_j^2\right). \tag{16}$$

Let us integrate in the formula (15) over all variables $\bar{l}_j$ between $-\infty$ and ∞. Then we should obtain:

$$\Phi(\beta) = \Delta E\Delta\mathbf{L}(\pi)^{\frac{N-1}{2}}\int\exp\left[-\frac{\beta}{2m}\left(\sum_{j=1}^{N}(p_{z,j}^2 + p_{r,j}^2) + 2m\sum_{j=1}^{N}U(r_j)\right)\right]\left(\sum_{j=1}^{N}r_j^2\right)^{-\frac{1}{2}}$$
$$\times\prod_{i=1}^{N}\mathrm{d}p_{z,i}\mathrm{d}p_{r,i}\mathrm{d}z\mathrm{d}\varphi_i r_i\mathrm{d}r_i. \tag{17}$$

Let us remove $\left(\sum_{j=1}^{N}r_j^2\right)^{-\frac{1}{2}}$ from under integration over all variables r_j for average value of these variables $\bar{r}$. It is easy to show that $\bar{r} = 2^{-1/2}R_0$, where R_0 is a boundary circle radius, taking into account that almost everywhere in the phase space any term in this sum is considerably less than the sum itself. Hence, the result differs from the one obtained without regard for conservation of zero value of the angular momentum by the factor $R_0^{-1}(2/N\pi)^{1/2}$. This factor is inessential. To prove that the replacement of the angular momenta by their linear combination is insignificant, let us put all $r_j = \bar{r}$ in characteristic equation (14). We obtain the equation identical to the one obtained in the case of the momentum conservation being taken into account. Hence, transformation of the angular momenta is not essential.

We have shown that conservation of zero values of complementary controllable integrals of motion does not change the volume of the invariant set and, hence, does not change the density of distribution, if the gas kinetic energy is of a standard form.

Let us now turn our attention to considering the 2DGFM statistical mechanics. Hamiltonian in this case takes the form:

$$H = \sum_{i=1}^{N}h_i = \frac{1}{2m}\sum_{i=1}^{N}\left[\left(p_{x,i} - \frac{m\omega}{2}y_i\right)^2 + \left(p_{y,i} + \frac{m\omega}{2}x_i\right)^2 + 2mU(r_i)\right]. \tag{18}$$

Here $\omega = eB/m$ is cyclotron frequency, $-e$ is particle charge, and B is magnetic field induction. Vector potential is chosen in the form $\mathbf{A} = (-By/2, Bx/2, 0)$. The potential energy includes interaction of a particle with mean field which is formed by all other particles. For this mean field and the potential energy as a whole to be axially symmetrical, an external potential field and a vessel containing the gas should be absent or axially symmetrical. If the vessel is considered as limits of integration over the radial coordinates of particles, this Hamiltonian does not describe the phenomenon of a current which is generated by reflection of particles from the boundary.

If conditions of the angular momentum conservation are satisfied, this Hamiltonian can be transformed to the polar coordinates:

$$H = \frac{1}{2m} \sum_{i=1}^{N} \left[\left(p_{r,i}^2 + \frac{l_i^2}{r_i^2} \right) + \left(\frac{m r_i \omega}{2} \right)^2 + m\omega l_i + 2mU(r_i) \right]. \tag{19}$$

Let us substitute Hamiltonian (19) in expression (10) at $L_0 = 0$ instead of Hamiltonian of unbound particles:

$$\Omega(E, 0) = \Delta E \Delta \mathbf{L} \int \delta \left(H_{\mathrm{ef}} + m\omega \sum_{i=1}^{N} l_i - E \right) \delta \left(\sum_{i=1}^{N} l_i \right) \prod_{i=1}^{N} \mathrm{d}p_{r,i} \mathrm{d}l_i \mathrm{d}r_i \mathrm{d}\varphi_i, \tag{20}$$

where

$$H_{\mathrm{ef}} = \frac{1}{2m} \sum_{i=1}^{N} \left[p_{r,i}^2 + \frac{l_i^2}{r_i^2} + \left(\frac{m r_i \omega}{2} \right)^2 + 2mU(r_i) \right] \tag{21}$$

is Hamiltonian of the ideal the gas particles of which have potential energy $\frac{1}{8} m(r\omega)^2 + U(r)$. Hence, it follows that for $L_0 = 0$, microcanonical density of distribution of 2DGMF coincides with the density of distribution of the gas with Hamiltonian H_{ef}. Otherwise, the angular momentum conservation law should not be considered. Thus, the theory that was deduced for physical reasons in [1] is proved mathematically.

Let us pay attention to a peculiarity of the derivation of the canonical density of distribution from microcanonical one for 2DGMF case. Usually it is assumed at this derivation that a system under consideration is a spatially separated part of a big system which is described by microcanonical density of distribution. The complementary subsystem of the big system is a thermostat. Any subsystem of the canonically distributed system is also distributed canonically. 2DGMF under consideration cannot be spatially divided into subsystems with similar densities of distribution. The parabolic potential energy in the density of distribution is centered in the centre of mass of the whole 2DGMF system which coincides with the centre of symmetry of external field and a vessel at the equilibrium state. Long-range interaction and the phenomenon of the near-boundary current also keep the system away from space sectioning into similar subsystems. For the same reason, only the system of other kind occupying the same volume can be considered as a thermostat.

It may appear that the choice of the angular momentum as a complementary controllable integral of motion is arbitrary. If the vector potential is chosen in the form $\mathbf{A} = (-By, 0, 0)$, Hamiltonian of a particle will take the form:

$$h = (2m)^{-1} \left[(p_x - m\omega y)^2 + p_y^2 \right] + U(\sqrt{x^2 + y^2}). \tag{22}$$

Thus, the angular momentum $l = xp_y - yp_x$ is not a motion integral. Let us show that in this case another integral of motion exists, consideration of which leads to the same results. Hamiltonian in the form of formula (22) can be obtained from formula (18) using canonical transformation, which has the course-of-value function:

$$F = \acute{p}_x x + \acute{p}_y y - \frac{1}{2} m\omega xy. \tag{23}$$

Then

$$p_x = \acute{p}_x - \frac{1}{2} m\omega y, \qquad p_y = \acute{p}_y - \frac{1}{2} m\omega x, \qquad \acute{x} = x, \qquad \acute{y} = y. \tag{24}$$

By transforming l to new variables we obtain a new expression for the motion integral:

$$\acute{l} = \acute{x}\acute{p}_y - \acute{y}\acute{p}_x - \frac{1}{2} m\omega \left(\acute{x}^2 - \acute{y}^2 \right). \tag{25}$$

The summatory function $\acute{L} = \sum_{i=1}^{N} \acute{l}_i$ is the integral of motion of the system, Hamiltonian of which is the sum of one-particle Hamiltonians (22). If these expressions for Hamiltonian and controllable integral of motion $\acute{L}$ are substituted into formula (20), the changes will be reduced to the changes of integration variables under formulae (24).

The controllable integrals of motion which should be taken into account in order to determine the invariant set are objectively determined by the symmetry of the system under consideration. The problem concerning a degree of correspondence of a real system properties to those for the idealized symmetrical system is complex and should be considered in each special case.

3. Statistical thermodynamics of charged particles gas located in strip in magnetic field

Let us consider 2DGMF which uniformly fills an endless strip restricted by two parallel lines as an example of a system for which the angular momentum is not conserved. The statistical thermodynamics should be formulated for the particles filling a segment of a strip, and the rest of the strip serves as a thermostat and a reservoir for a grand canonical distribution. As a whole, the strip is a translation invariant system, and one-particle Hamiltonian should be taken in the form of formula (22). Strip boundaries are supposed to be mirror reflecting ones. Segment boundaries which are perpendicular to the strip axis are conditional. This means that particles freely traverse these boundaries in any direction, and the particle flow across any macroscopic boundary segment should be equal to zero in average.

The fulfillment of the latter condition requires that special cares should be taken in the case of 2DGMF. If the distance of an orbit centre from reflecting boundary d is less than the orbit radius ρ ("near-boundary area"), then, as a result of reflecting, the center moves by jumps along the boundary in the direction that is determined by a direction of particle velocity at the moment of colliding with the wall. If mirror reflection takes place, average velocity of this motion is:

$$v = \frac{\omega\sqrt{\rho^2 - d^2}}{\arccos(d/\rho)}\,. \tag{26}$$

It is accepted here that $d < 0$ if the centre is located within the strip, otherwise $d > 0$. Particles which appear on these trajectories are not orbiting in a circle but are moving in a chain of arcs along the strip boundary. This motion generates a particle flow and electric current which, in turn, generates a paramagnetic moment which is proportional to the segment area. This is often considered as an explanation of the fact that the magnetic moment according to Bohr – van Leeuwen theorem is equal to zero (see, for example, monograph [9]). It is implicitly suggested therewith that the orbits of particles in internal areas are fixed, like atoms in a crystal, and their position averaging is not performed. In such a case, the orbits in internal area generate a diamagnetic moment which is compensated by the moment of near-boundary current. This is incorrect because in the area where the density of the centers of orbits is uniform, their position averaging leads to a zero value of current density elsewhere as it was shown by van Vleck in monograph [10]. If the density near the walls does not change, the current generated in this area by orbital motion also vanishes, but a current exists which is generated by jump-wise motion of centers of near-boundary orbits. Kinetic energy of this motion is equal to zero. Therefore, this current and magnetic moment which is generated by it cannot be obtained within the limits of statistical mechanics if the density of distribution depends on energy only.

The particles which are located in the segment under consideration at the initial moment do not remain there for ever because there are two oppositely directed flows along the strip near boundary lines. In due time, particles leave the fixed area and are replaced by the other ones. Therefore, the invariant set does not exist in a conventionally defined phase space. In order to generalize the statistical mechanics method for this case, one should apply an artificial technique. Let us assume that $\mathbf{X}$ axis coincides with the strip axis. Then, in the upper semiplane, negatively charged particles move in positive direction as a result of reflections, and in the lower semiplane they move in negative direction. Phase space areas which contain near-boundary trajectories are separated by hypersurfaces $|d_t| = \rho$ and $|d_b| = \rho$. Here $|d_t|, |d_b|$ are distances of orbit center from top and bottom boundaries of the strip determined by the value of p_x, ρ is the radius of the orbit which is proportional to the square root of kinetic energy of a particle in this orbit. Let us determine 2DGMF phase space in such a way that near-boundary trajectories of particles are related to a reference system which moves uniformly along the strip. If velocity of this reference system V is taken equal to the jump-like velocities averaged over the near-boundary area, the phase trajectory of the system will remain in finite volume of the phase space if random exchange of particles with the reservoir through the conditional boundary is neglected.

For the near-boundary areas of the phase space not to be overlapped, it is necessary to consider only that part of phase volume, in which all orbits have diameter smaller than a strip width $2L_y$. This approximation is valid when the statistical weight of the neglected part is small. Later on we shall refine this criterion. If there is no magnetic field, Hamiltonian is not changed when transition to a moving reference system takes place, but in the case under consideration it results in the appearance of a uniform electrical field with potential $\phi = \phi_0 - (V/c)A_x = \phi_0 + VBy/c$, where c is light velocity (see monograph [11] p.79). This formula is given in Gaussian system of units where vector potential in a motionless reference system is taken in the form $\mathbf{A} = (-By, 0, 0)$. A constant ϕ_0 does not effect the dynamics of the particle, but it is essential for the calculation of invariant set volume. Product $Vy > 0$ for negatively charged particles in both near-boundary areas. Therefore, potential energy decreases as boundaries are approached. This should result in an increase of density near the boundaries. The physical reason for such a density increase lies in the fact that for the trajectory reflected from the wall, the range of y values in which this trajectory is located is smaller than the diameter. Therefore, the beginning of the density increase depends on the orbit radius, i.e. on kinetic energy. Let us change kinetic energy by its average value, determine $\rho_T = (2k_{\mathrm{B}}T)^{1/2}(m\omega^2)^{-1/2}$ and put $\phi_0 = -|V|B(L_y - 2\rho_T)/c$. Then Hamiltonian in the moving (top and bottom) reference systems in SI system of units is:

$$H = \sum_{i=1}^{N} h_i = \sum_{i=1}^{N} \left\{ \frac{1}{2m} \left[(p_x - m\omega y)^2 + p_y^2 \right] - m\omega \left[Vy - |V|(L_y - 2\rho_T) \right] \right\}. \tag{27}$$

Let us refer to the well known (see monograph [11] p.73) solution of a problem on particle motion in the crossed electric and magnetic fields expressed through constants $p_x, |V|$, and $\rho = \omega^{-1}(\sqrt{2E_{\max}/m} - |V|)$ where $E_{\max}$ is the maximal value of kinetic energy:

$$y = \rho \sin \omega t + (m\omega)^{-1}(p_x + m|V|), \qquad x = \rho \cos \omega t + X - |V|t. \tag{28}$$

Here X is determined by initial value of x-coordinate of a particle. With relation to a moving system, the center of an orbit moves in the direction opposite to jump-wise motion under the action of the electric field. The origin of longitudinal momentum is shifted by a constant value. The strip width in which particle trajectory is contained is less than the diameter which an orbit with maximal kinetic energy would have if electric field were absent. Thus, if the potential field described by formula (27) is switched on in the near-boundary area of the phase space, the current caused by reflections from boundary is compensated on the average.The system phase trajectory will remain in the limited volume of the phase space if random exchange of particles with the reservoir through the conditional boundary is neglected, and the method of grand canonical distribution is applicable here. In the system which is determined this way, the longitudinal component of the total momentum is controllable integral as well as energy. It can be shown, as it was seen in the second section, that the controllable integral being taken into account will not essentially change the volume of the invariant set. This volume is determined only by Hamiltonian, like in the conventional theory. The proposed correction consists in Hamiltonian modification in near-boundary areas. Thus, thermodynamical parameters of the system, in particular, magnetic moment, do not take into consideration the effects of near-boundary electric currents $I_b = -eN_bV$, where N_b is the average number of particles per unit length of the near-boundary area. These effects should be further considered.

Calculation of the volume of invariant set and statistical integral for a system in the thermostat demands calculation of the integral over the one-particle phase space:

$$f_0(\beta) = \int_{-L_x}^{L_x} \mathrm{d}x \iiint \exp\left[-\beta h(p_x, p_y, y)\right] \mathrm{d}p_x \mathrm{d}p_y \mathrm{d}y \tag{29}$$

(see “Dopolneniya redaktora” in monograph [8] as well as study [1]). The variable β in the course of further derivation of canonical density of distribution is found to be proportional to inverse temperature $\beta = (k_\mathrm{B}T)^{-1}$ (see ibid.). Integration limits over the coordinate subspace are determined by boundaries, and momenta integration is performed over the whole space. The three-dimensional area $\{p_x, p_y, y\}$ is the layer restricted by planes $y = \pm L_y$. It is divided into three parts, in which the Hamiltonian is of various forms. This is more convenient to be described introducing other variables of integration (q, ρ, y):

$$p_x = m\omega(q + y), \qquad p_y = \pm m\omega\sqrt{\rho^2 - q^2}, \qquad y = y. \tag{30}$$

Then integral (29) takes the form:

$$f_0(\beta) = 4L_x(m\omega)^2 \int_0^\infty \exp\left[-\frac{\beta m(\omega\rho)^2}{2}\right] \rho \left(\int_{S(\rho)}\int \frac{P(q, y, \rho)\mathrm{d}q\mathrm{d}y}{\sqrt{\rho^2 - q^2}}\right) \mathrm{d}\rho, \tag{31}$$

where area $S(\rho)$ on the plane $\{q, y\}$ is a rectangle $-L_y < y < L_y, \quad -\rho < q < \rho$; $P(q, y, \rho) = 1$ if the point (q, y, ρ) is located in medial area, and $P(q, y, \rho) = \exp\{\beta m\omega[Vy - |V|(L_y - 2\rho_T)]\}$ if this point is located in near-boundary areas. The separation on near-boundary and medial areas is possible only at $\rho < L_y$. In the area of the phase space where $\rho > (\beta m\omega^2/2)^{-1/2}$ the exponential factor is small. Therefore, the integration over ρ can be performed in the limits $[0, \infty)$ without changing the integrand. At $\beta = (k_\mathrm{B}T)^{-1}$, this width of peak is the orbit radius of the particle having the average kinetic energy ρ_T. The system for which $\rho_T \ll L_y$, is considered below. If the peculiarities of near-boundary trajectories are not taken into account, i.e. if we put $P(q, y, \rho) \equiv 1$, the integral $f_0(\beta)$ is found to be exactly the same as that for gas when there is no magnetic field. We will show below that the corrections to thermodynamic quantities that are caused by peculiarities of near-boundary areas are small and proportional to $b^{-1} = \rho_T L_y^{-1} = (2mk_\mathrm{B}T)^{1/2}(eBL_y)^{-1}$. For the strip 10^{-2}m in width containing non-degenerated electronic gas in the field of 10^{-1} T at room temperature, $b \approx 3000$. But this does not mean that the assertion of Bohr–van Leeuwen theorem is valid if these corrections are neglected. Let us remind that the calculation of volume of the invariant set and application of statistical thermodynamics method makes sense only under the condition of excluding the near-boundary currents by introducing a moving reference system.

Let us determine the areas of near-boundary trajectories in terms of variables (q, ρ, y). The coordinate of orbit center $y_0 = \omega^{-1}(p_x/m) = q + y$. Then, the distance of the center from the strip upper boundary $d_t = y_0 - L_y$ and the distance from the lower boundary $d_b = -y_0 - L_y$. A distance sign is negative if the orbit center is located in the strip. The points in areas S_t and S_b which are cut from the rectangle by straight lines $q + y - L_y = -\rho$ and $-q - y - L_y = -\rho$ correspond to near-boundary trajectories. The remaining medial area S_m contains phase points of circular trajectories which completely lie within the strip. Function $\rho\exp[-\beta m(\omega\rho)^2/2]$ has a maximum in the point $\rho_m = (\beta m\omega^2)^{-1/2} = 2^{-1/2}\rho_T$. Let as perform integration over ρ by removing the other factors of integrand from under integral at $\rho = \rho_m$. For simplicity, let us perform substitution $\rho_T \to \rho_m$ in all the formulae determined earlier. Then we obtain:

$$\begin{aligned} f_0(\beta) &= 8\pi m L_x L_y \beta^{-1}\left\{1 - \rho_m L_y^{-1} + \rho_V L_y^{-1}[\exp(2\rho_m\rho_V^{-1}) - \exp(\rho_m\rho_V^{-1})\mathrm{I}_0(\rho_m\rho_V^{-1})]\right\} \\ &= Z_0[1 - \rho_m L_y^{-1}] + Z_V, \end{aligned} \tag{32}$$

where $\rho_V = (\beta m\omega|V|)^{-1}$. Here Z_0 coincides with expression for $f_0(\beta)$ in ideal gas when there is no field.

The parameter $|V|$ is determined as the average value of jump-like velocity. In the case of mirror reflection, the expression (26) should be averaged over the near-boundary area of the phase space.

Since the density of distribution in the near-boundary area depends on $|V|$, the averaging leads to a self-consistent equation:

$$\int_0^{L_y} \exp\left(-\frac{\rho^2}{2\rho_m^2}\right)\rho^2 \mathrm{d}\rho \int_{-\rho}^{\rho} \frac{\mathrm{d}q}{\sqrt{\rho^2-q^2}} \int_{-q-\rho}^{0} \exp\left(\frac{\eta+2\rho_m}{\rho_V}\right)\frac{\sqrt{1-d^2/\rho^2}}{\arccos(d/\rho)}\mathrm{d}\eta = \frac{Z_V|V|}{8\omega L_x(m\omega)^2}\,. \tag{33}$$

Here $\eta = y - L_y$ and $d = q + \eta$. Let us substitute $|V| = \omega\rho_m\zeta$, integrate over ρ and we obtain the equation for ζ which does not depend on task parameters:

$$[1-\exp(-\zeta)\mathrm{I}_0(\zeta)] = \int_0^{\pi} \mathrm{d}t \exp(-\zeta\cos t)\int_t^{\pi} \mathrm{d}u \frac{\sin^2 u}{u}\exp(\zeta\cos u). \tag{34}$$

Here the variables are introduced by:

$$q + \eta = \rho\cos u, \qquad q = \rho\cos t. \tag{35}$$

In the linear approximation by ζ we obtain $\zeta = 0.38$.

As it follows from formula (32):

$$f_0\left(\frac{1}{k_\mathrm{B}T}\right) \approx Z_0\left(1+\frac{5\zeta}{4b}\right) \approx Z_0\left(1+\frac{0.5}{b}\right), \tag{36}$$

where $b = L_y\rho_m^{-1}$. If the density of particles is calculated as the average of the summatory expression $n(y) = L_x^{-1}\sum_{i=1}^{N}\delta(y-y_i)$, we shall see that in the area $-L_y + 2\rho_m < y < L_y - 2\rho_m$ it is uniform and equal to $n_0(1-0.5b^{-1})$. A decrease of the number of particles per unit length which is equal to $0.5n_0\rho_m$ in the internal area is caused by the increase of the average density in the near-boundary areas $n_b \approx 1.25n_0$. If the strip is uniformly filled with a neutralizing background with a density of n_0, particles density redistribution in magnetic field would lead to generation of an essential potential difference between boundaries and the strip middle. Actually electrostatic interaction of particles should be considered sequentially using the method of self-consistent field. Obviously, this will lead to a decrease of density difference and other corrections.

Thus, at $L_y \gg \rho_m$, i.e. for the macroscopic strip in a rather strong magnetic field, the obtained statistical thermodynamics coincides, to a high degree of accuracy, with the results of the conventional theory, with the exception for phenomena connected with the near-boundary jump-wise current. This current $I_b = 2\rho_m e n_b|V|$ generates the magnetic moment in the strip. The density of this magnetic moment per area unit numerically coincides with the current and is equal to:

$$M_z = I_b = 0.95n_0(k_\mathrm{B}T)B^{-1} \approx 4\cdot 10^{-4}\mathrm{J}\cdot\mathrm{T}^{-1}\cdot\ \mathrm{m}^{-2} \tag{37}$$

at $n_0 = 10^{16}$ m^{-2},$T = 300$ K, $B = 0.1$ T. The regard for electrostatic interactions of particles can only insignificantly change the coefficient ζ. The paramagnetic moment of the strip segment $\mu_z = 4L_xL_yM_z$ within a factor of ≈ 0.95 coincides in magnitude with the diamagnetic moment of the same amount of the free gas obtained in [1]. However, in that study boundary conditions were considered for which the gas total angular momentum was conserved and there was no near-boundary current or it was very small. Therefore, the summation of these magnetic moments does not make sense. The thermodynamical diamagnetic moment which can be obtained from formula (36) is many orders of magnitude smaller than μ_z. It can be shown, just as it was made in [1] that 2DGMF energy change in the strip at magnetic field change $\delta E = -\mu_z\delta B$. This relation should be included in thermodynamics of 2DGMF in the strip.

References

1. Dubrovskii I.M., Condens. Matter Phys., 2006, **9**, 23.
2. Dubrovskii I.M., Condens. Matter Phys., 2006, **9**, 645.
3. Hinchin A.Ya. Mathematicheskie Principy Statisticheskoy Mehaniki. GITTL, Moscow-Leningrad, 1943. [Khinchin A.Y. Mathematical Foundation of Statistical Mechanics. New York, Ed. Dover, 1949].
4. Landau L.D., Lifshic E.M. Statisticheskaja fizika, Chast' I. Nauka, Moskva, 1976. [Landau L.D., Lifshitz E.M. Statistical Physics, 3rd rev., part I. Pergamon Press, New York, 1980].
5. Zubarev D.N. Neravnovesnaja statisticheskaja termodinamika. Nauka, Moskva, 1971. [Zubarev D.N., Nonequilibrium Statistical Thermodynamics. Consultant Bureau, New York, 1974].
6. Krivoglaz M.A. X-ray and Neutron Diffraction in Nonideal Crystals. Berlin, Heidelberg: Springer Verlag, 1996.
7. Krutkov Yu.A., Z. Phys., 1933, **81**, 377.
8. Krutkov Yu.A. "Dopolneniya redaktora" in monograph: Lorentz H.A., Statisticheskie teorii v termodinamike. Perevod s francuzskogo pod redakciey i s dopolneniyami Yu.A Krutkova. ONTI, Leningrad-Moskva, 1935.
9. Peierls R.E. Quantum Theory of Solids. Clarendon Press, Oxford, 1955.
10. van Vleck J.H. Theory of Electric and Magnetic Susceptibilities. Oxford University Press, 1932 [Reprinted in 1965], p. 101.
11. Landau L.D., Lifshic E.M. Teorija polja. Gosizdat fiz.-mat. lit., Moskva, 1960. [Landau L.D., Lifshitz E.M. The Classical Theory of Fields: Volume 2. Butterworth-Heinemann, 1987].

Роль закону збереження кутового моменту у статистичній механіці

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У рамках ідей Хінчина [А.Я. Хинчин, Математические принципы статистической механики. ГИТТЛ, Москва-Ленинград, 1943] розглянуто закони збереження імпульсу і кутового моменту у випадках присутності або відсутності магнітного поля. Закон збереження імпульсу не змінює розподілу густини ймовірності, як і передбачалося у загальноприйнятій теорії. Показано, що у системах, кінетична енергія яких залежить тільки від імпульсів частинок, канонічно спряжених декартовим координатам, і є діагональною квадратичною формою, закон збереження кутового моменту змінює розподіл густини ймовірності тільки, якщо повний кутовий момент системи не дорівнює нулю. Для газу заряджених частинок у магнітному полі розподіл густини ймовірності змінюється і у випадку нульового повного кутового моменту [Dubrovskii I.M., Condensed Matter Physics, 2206, **9**, 23]. Розглянуто двовимірний газ заряджених частинок, що знаходиться на відрізку необмеженої смуги, у магнітному полі. У цих умовах кутовий момент не зберігається. Поблизу границь смуги існують спрямовані потоки частинок, тому фазова траєкторія газу, що розглядається, не залишається у обмеженій області фазового простору. Щоб застосувати до цього випадку метод статистичної механіки, запропоновано розглядати траєкторії поблизу границь у системі відліку, що рівномірно рухається. При цьому виявляється, що поправки до термодинамічних функцій, що залежать від магнітного поля малі, якщо діаметр орбіти з середньою термічною енергією значно менший, ніж ширина смуги. Суттєва тільки середня швидкість частинок, що відбиваються від границь. Ці частинки утворюють поблизу границь електричний струм, що породжує магнітний момент.

Ключові слова: *фазовий простір, інваріантна множина, інтеграл руху, кутовий момент, електронний газ, магнітне поле*

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