EXACT EXPRESSION FOR THE THERMODYNAMICAL POTENTIAL OF A PARABOLIC QUANTUM WIRE

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The exact formula is obtained for the thermodynamical potential of a parabolic quantum wire directed perpendicular to the impressed magnetic field.

The purpose of the present paper is to receive the exact formula for the thermodynamical potential of a parabolic quantum wire (QW) which axis direct perpendicular to the impressed magnetic field. Gazeau et. all [1] considered the analogous problem for QW directed parallel to magnetic field.

All the calculations in this paper are made in the basis of coherent state [2], as the coherent-state method is the most simple and convenient way of solving the problem. The derivation of the thermodynamical potential (Ω) is based on residue series in the complex plane, like that in [1]. The expression for Ω, derived in this paper, will be used in future for calculation the exact formulae of different physical values (for example, the thermoelectromotive force and the magnetic moment).

Let us consider a quantum wire (QW) in uniform stationary magnetic field. We choose the vector potential in the form $\vec{A}=(0,xH,0)$ which corresponds to the magnetic field H, parallel to the z axis. The QW is directed along the y axis and characterized by parabolic confinements in the plane (x,z).

The Hamiltonian of the problem under consideration is

$$\aleph=\frac{1}{2m}\left[p_x^2+\left(p_y+m\omega_c x\right)^2+p_z^2\right]+\frac{1}{2}m\omega_0^2\left(x^2+z^2\right) \tag{1}$$

where x is the usual canonical coordinate, p_x is its conjugate momentum, $\omega_c=eH/mc$ is the cyclotron frequency, c is the velocity of light in vacuum, m is electron mass, e is the absolute value of its charge and ω_0 characterizes the parabolic potential of the QW for electron in conduction band.

Since $\aleph$ is independent of y it is possible to replace $p_y \to p_y$ everywhere. The Hamiltonian (1) can be now written as

$$\aleph=\aleph_1+\aleph_2+\aleph_3 \tag{2}$$

where

$$\aleph_1=\frac{1}{2m}\left[p_x^2+m^2\omega^2\left(x-x_0\right)^2\right] \tag{3}$$

$$x_0=-\left(\frac{\omega_c}{\omega}\right)^2\frac{cp_y}{eH} \tag{4}$$

$$\omega^2=\omega_c^2+\omega_0^2 \tag{5}$$

$$\aleph_2=\frac{1}{2m}\left(p_z^2+m^2\omega_0^2 z^2\right) \tag{6}$$

$$\aleph_3=\left(\frac{\omega_0}{\omega}\right)^2\frac{p_y^2}{2m} \tag{7}$$

$\aleph_1$ and $\aleph_2$ are two independent harmonic oscillator Hamiltonians. It is known [2], [3] that the Hamiltonian and wave function for harmonic oscillator in the coherent- state (CS) representation can be written in the form:

$$\aleph_1=\hbar\omega\left[A_\alpha^+A_\alpha^-+\frac{1}{2}\right] \tag{8}$$

$$A_\alpha^-=\frac{1}{\sqrt{2\hbar}}e^{i\omega t}\left[\sqrt{m\omega}\left(x-x_0\right)+\frac{ip_x}{\sqrt{m\omega}}\right] \tag{9}$$

$$\left|\alpha\right\rangle=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left[-\left(\sqrt{\frac{m\omega}{2\hbar}}\left(x-x_0\right)-\alpha e^{-i\omega t}\right)^2+\frac{\left(\alpha e^{-i\omega t}\right)^2}{2}-\frac{\left|\alpha\right|^2}{2}\right] \tag{10}$$

$$\aleph_2=\hbar\omega_0\left(A_\gamma^+A_\gamma^-+\frac{1}{2}\right) \tag{11}$$

$$A_\gamma^-=\frac{1}{\sqrt{2\hbar}}e^{i\omega_0 t}\left(\sqrt{m\omega_0}\,z+\frac{ip_z}{\sqrt{m\omega_0}}\right) \tag{12}$$

$$|\gamma\rangle = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left[-\left(\sqrt{\frac{m\omega_0}{2\hbar}}z - \gamma e^{-i\omega_0 t}\right)^2 + \frac{\left(\gamma e^{-i\omega_0 t}\right)^2}{2} - \frac{|\gamma|^2}{2}\right] \tag{13}$$

where α and γ are the arbitrary complex numbers.

It is easy to check that $|\alpha\rangle$ and $|\gamma\rangle$ satisfies all necessary requirements of the CS.

For example, in the case of $|\alpha\rangle$:

1) $|\alpha\rangle$ is eigenstate of boson annihilation operator and integral of motion A_α^-:

$$A_\alpha^-|\alpha\rangle = \alpha|\alpha\rangle \tag{14}$$

$$\left[i\hbar\frac{\partial}{\partial t} - \aleph_1, A_\alpha^\pm\right] = 0 \tag{15}$$

$$\left[A_\alpha^-, A_\alpha^+\right] = 1 \tag{16}$$

2) $|\alpha\rangle$ is known to comply with normalization condition

$$\langle\alpha|\alpha\rangle = 1 \tag{17}$$

The wavefunctions $|\alpha\rangle$ form a complete system, but they are not orthogonal.

3) $|\alpha\rangle$ can be created from the ground state $|0\rangle$ for which

$$A_\alpha^-|0\rangle = 0 \tag{18}$$

From the foregoing it transpires that one should present the solution of the wave equation of the problem (2)

$$\left(i\hbar\frac{\partial}{\partial t} - \aleph\right)\psi = 0 \tag{19}$$

in the form

$$\psi = |\alpha\rangle|\gamma\rangle|k_y\rangle \tag{20}$$

where $|k_y\rangle = e^{ik_y y}$, $\hbar k_y = p_y$.

Let us calculate the thermodynamical potential Ω for the case under consideration. In Fermi- Dirac statistics Ω is given by

$$\Omega = -\frac{1}{\beta} Tr \ln\left(1 + e^{-\beta(\aleph - \xi)}\right) \tag{21}$$

with $\beta = 1/k_B T$, T is temperature, k_B is the Boltzmann contact, ξ is the chemical potential of the conductivity electrons.

We consider the case of physical interest:

$$\aleph - \xi > 0 \tag{22}$$

Let us prove that

$$\ln\left[1 + e^{-\beta(\aleph-\xi)}\right] = \int_{-\infty}^{+\infty} \frac{e^{-(il+1)(\aleph-\xi)\beta/2}}{2(il+1)\cos h(\pi l/2)} dl \tag{23}$$

much as [1].

It is necessary for that to reduce the right hand members to the left- hand side using the contour integration.

In accordance with the Jordan lemma we take an integration path at $\aleph - \xi > 0$ lying in the lower halt- plane, where the integrand under consideration has only simple poles:

$$l = l_0^{(n)} = -i(2n+1), \quad n = 0,1,2,... \tag{24}$$

Using residue theorems we get the right hand members in the form

$$\sum_{n=0}^{\infty} (-1)^n (n+1)^{-1} e^{-\beta(n+1)(\aleph-\xi)}. \tag{25}$$

The application of the formula (1.511) from [4] to the series (25) finishes our proof.

Taking into account the expression (23) we transform formula (21) to the following form:

$$\Omega = -\frac{1}{\beta}\int_{-\infty}^{+\infty} \frac{e^{(il+1)\xi\beta/2}}{2(il+1)\cosh(\pi l/2)}\theta(l) dl \tag{26}$$

where $\theta(l)$ is the function

$$\theta(l) = Tr\, e^{-(il+1)\aleph\beta/2} \tag{27}$$

Now we shall calculate $\theta(l)$ in the basis of CS.

Substitute the expressions (2), (8), (11), (7) into equation (27). For further calculation we adopt the following relations according to equations (22)-(25) of [5]:

1) The trace of an arbitrary operator M equals

$$TrM = \frac{L_y}{2\pi}\int dk_y \frac{1}{\pi}\int d^2\gamma \frac{1}{\pi}\int d^2\alpha \langle\alpha|\langle\gamma|\langle k_y|M|\alpha\rangle|\gamma\rangle|k_y\rangle \tag{28}$$

where $\{\alpha,\gamma,k_y\}$ are the set of quantum numbers in the CS, $(1/\pi)d^2\alpha=(1/\pi)d(\mathbf{Re}\,\alpha)d(\mathbf{Im}\,\alpha)$ is the real element of the area in the complex plane and $(1/\pi)d^2\gamma=(1/\pi)d(\mathbf{Re}\,\gamma)d(\mathbf{Im}\,\gamma)$.

2) the identity valid for boson operators

$$\langle\alpha|\exp(\chi A^+A^-)|\alpha\rangle=\exp\left[-\left(1-e^{\chi}\right)|\alpha|^2\right] \tag{29}$$

3) the Poisson integral in the form

$$\int_{-\infty}^{+\infty}dk_y\,\mathbf{exp}\left(-bk_y^2\right)=\sqrt{\frac{\pi}{b}},\ \ \mathbf{Re}\,b>0 \tag{30}$$

4) and

$$\int d^2\alpha e^{-C|\alpha|^2}=\frac{\pi}{C},\ \ \mathrm{Re}\,C>0. \tag{31}$$

In our case

$$b=\frac{\hbar^2}{2m}\cdot\frac{\beta}{2}\left(\frac{\omega_0}{\omega}\right)^2(il+1) \tag{32}$$

$$C=1-e^{\chi} \tag{33}$$

and

$$\chi=\begin{cases}\chi_0=-(il+1)\beta\hbar\omega_0/2 & \text{at the integration over } \gamma \quad (34)\\ \dfrac{\omega}{\omega_0}\chi_0 & \text{at the integration over } \alpha \quad (35)\end{cases}$$

It is easy to check that $\mathbf{Re}\,b>0$ and $\mathbf{Re}\,C>0$ writing $l=\mathbf{Re}\,l+i\,\mathbf{Im}\,l$ and taken into account that $\mathrm{Im}\,l<0$ for the integration path lying in the lower half – plane.

Introducing the well-known function $\mathbf{sh}\,a=\left(e^a-e^{-a}\right)/2$ we finally get

$$\theta(l)=\frac{L_y}{4\hbar}\frac{\omega}{\omega_0}\sqrt{\frac{m}{\pi\beta(il+1)}}\frac{1}{\mathrm{sh}\left(\dfrac{\chi_0}{2}\right)\mathrm{sh}\left(\dfrac{\omega}{\omega_0}\dfrac{\chi_0}{2}\right)}. \tag{36}$$

The substitution of (34) - (36) into (26) leads to the following expression for Ω:

$$\Omega=\int_{-\infty}^{+\infty}\frac{N(l)}{D(l)}dl \tag{37}$$

where

$$N(l)=-\frac{L_y}{8\hbar}\sqrt{\frac{m}{\pi\beta^3}}\frac{\omega}{\omega_0}e^{(il+1)\xi\beta/2} \tag{38}$$

$$D(l)=(il+1)^{3/2}\cosh(\pi l/2)\mathrm{sh}\left[(il+1)\beta\hbar\omega_0/2\right]\mathrm{sh}\left[(il+1)\beta\hbar\omega/2\right]. \tag{39}$$

Now we shall calculate Ω for the case $\xi<0$. The integral over l can be evaluated by using residue theorems at the condition that the integrand function satisfies the Jordan lemma. The latter is valid if the integration path at $\xi<0$ lies in the lower half – plane. Observe that in the lower halt – plane the integrand function has only simple poles the same as in (24).

We now determine Ω by applying the residue theorems to (37):

$$\Omega=-2\pi i\sum_{n=0}^{\infty}\left.\frac{N(l)}{\dfrac{\partial D(l)}{\partial l}}\right|_{l=l_0^{(n)}} \tag{40}$$

Substituting (38) and (39) into (40) we find

$$\Omega=\sum_{n=1}^{\infty}\Omega_n \tag{41}$$

where

$$\Omega_n=\frac{L_y}{4\hbar}\sqrt{\frac{m}{2\pi\beta^3}}\frac{\omega}{\omega_0}\frac{(-1)^n e^{n\xi\beta}}{n^{3/2}\,\mathbf{sh}[n\beta\hbar\omega_0/2]\,\mathbf{sh}[n\beta\hbar\omega/2]} \tag{42}$$

Obraztsov [6] deduced a formula relating the thermoelectromotive force *(Q)* in a quantizing magnetic field to the entropy *(S)* of a semiconductor:

$$Q=-\frac{S}{eN} \tag{43}$$

It is known that the average number of electrons (N) is given by

$$N=-\left(\frac{\partial\Omega}{\partial\xi}\right)_{T,V} \tag{44}$$

and

$$S=-\left(\frac{\partial\Omega}{\partial T}\right)_{\xi,V} \tag{45}$$

where V is the volume.

Calculate Q stating from (41)-(45). As result we obtain:

$$Q = \frac{k_B}{e} \frac{\sum_{n=1}^{\infty} \left\{ n\beta\xi - n\frac{\hbar\omega\beta}{2}\mathbf{coth}\left(n\frac{\hbar\omega\beta}{2}\right) - n\frac{\hbar\omega_0\beta}{2}\mathbf{coth}\left(n\frac{\hbar\omega_0\beta}{2}\right) - \frac{3}{2}\right\}\Omega_n}{\sum_{n=1}^{\infty} n\Omega_n} \tag{46}$$

Put $n = 1$ and $\omega_0 = 0$ in (46). Then we derive the well known result for the thermoelectromotive force of nondegenerate electron gas [6]:

$$Q = -\frac{k_B}{e}\left(\frac{3}{2} + \frac{\hbar\omega_C\beta}{2}\coth\frac{\hbar\omega_C\beta}{2} - \beta\xi\right) \tag{47}$$

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[1] *J.P.Gazeau, P.Y.Hsiao, and A.Jellal.* Phys. Rev. B 2002, 65, p. 094427-1 – 094427-9.
[2] *I.A. Malkin and V.I. Man'ko.* Dynamic Symmetries and Coherent State of Quantum System. M., «Nauka». 1979.
[3] *R.G. Agayeva*. J. Phys. A: Math. Gen. 1980, 13, p. 1685-1699.
[4] *Gradshteyn I.S. and Ryzhik I.M.* Tables of Integrals, Sums, Series and Products. M., «Nauka». 1971.
[5] *R.G. Agayeva*. Proceeding of Third International Seminar «Group Theoretical Methods in Physics», London, «Gordon and Breach», 1984, v.2, p. 213-222.
[6] *Yu.N.Obraztsov*. FTT 1965, **7**, p. 573-581.

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PARABOLİK KVANT MƏFTİLİN TERMODİNAMİK POTENSİALI ÜÇÜN DƏQİQ İFADƏ

İstiqaməti maqnit sahəsinə perpendikulyar olan parabolik kvant məftilin termodinamik potensialı üçün dəqiq ifadə alınmışdır.

Р.Г. Агаева

ТОЧНОЕ ВЫРАЖЕНИЕ ДЛЯ ТЕРМОДИНАМИЧЕСКОГО ПОТЕНЦИАЛА ПАРАБОЛИЧЕСКОЙ КВАНТОВОЙ ПРОВОЛОКИ

Получено точное выражение для термодинамического потенциала параболической квантовой проволоки, направленной перпендикулярно к приложенному магнитному полю.

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