"One-dimensional" coherent states and oscillation effects in metals in a magnetic field

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Using the "one-dimensional" coherent electron states in a quantizing magnetic field the oscillating part of the electron density of states for a metal, which determines the physical nature for the oscillations of the thermodynamic and kinetic metal characteristic in magnetic field, is calculated. The physical reason of the significant simplification of the mathematical procedure is that the coherent states are most adequate to describe the quantum macroscopic phenomena such as the Shubnikov - de Haas and the de Haas - van Alphen effects in metals.

Keywords: Shubnikov - de Haas effect; macroscopic quantum phenomena in magnetic field.

Usando los estados electrónicos coherentes "unidimensionales" en un campo magnético cuantizador, se calcula la parte oscilatoria de la densidad de estados electrónicos en un metal, la cual determina la naturaleza física de las oscilaciones de las características termodinámicas y cinéticas de un metal en un campo magnético. Físicamente la razón de la gran simplificación que se obtiene mediante este procedimiento matemático, es que los estados coherentes usados en el proceso de cálculo son los más adecuados para describir los fenómenos cuánticos macroscópicos, tales como los efectos Shubnikov - de Haas y de Haas-van Alphen en metales.

Descriptores: Efecto de Shubnikov - de Haas; fenómenos cuánticos macroscópicos.

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1. Introduction

In 1963, R.J. Glauber [1,2] introduced the concept of a coherent state $|\alpha\rangle$ as an eigenstate of a non-hermitian annihilation operator $\hat{a}$ of excitations of the boson type ($\hat{a}|\alpha\rangle=\alpha|\alpha\rangle$). The Schrödinger equation for a charge in a constant uniform magnetic field is reduced to the Schrödinger equation for a one-dimensional displaced harmonic oscillator. The use of coherent states significantly simplifies mathematical calculations of the oscillating part of the thermodynamic characteristics. Coherent states are eigenstates of a non-hermitian operator and are not orthogonal, i.e. transitions between different coherent states can occur spontaneously. The Shubnikov-de Haas and de Haas-van Alphen effects are not only quantum effects, they are also macroscopic effects, and in these respects (the quantum character and macroscopic scale, simultaneously) they are related to such phenomena as superconductivity, weak-link superconductivity (Josephson effects), laser radiation, and von Klitzing's effect (the quantum Hall effect). Our aim is not only to demonstrate the mathematical advantage of using the method of coherent states, combined with a universal approach to the thermodynamic and kinetic effects in metals in a constant uniform magnetic field, but also to establish the physical reasons why the mathematical description is adequate for the physics of the quantum oscillation effects. The physical nature of the oscillations of the kinetic coefficients of a metal in a magnetic field (Shubnikov-de Haas effect) as well of the oscillations of the thermodynamic potentials and their derivatives has been established on the basis of Landau's theory of diamagnetism. The oscillations are governed by two factors: the presence of the Fermi surface and the radical change in the density of states $\rho(\varepsilon)$ in a quantizing magnetic field [3]. Turning on a constant uniform magnetic field $\mathbf{H}$ parallel to the z-axis makes the motion of a current-carrying particle quasi-one dimensional and the density of states changes from $\rho_{3D}(\varepsilon)\propto\sqrt{\varepsilon}$ to $\rho_{1D}(\varepsilon)\propto 1/\sqrt{\varepsilon}$ (for the three- and one-dimensional systems, respectively). Due to the Landau quantization of the electron energy spectrum, this inverse square-root singularity of $\rho(\varepsilon)$ is repeated many times in the energy interval $0\leq+\varepsilon\leq\mu$ (μ is the chemical potential), when the condition $\mu\gg\hbar\omega_H$ is satisfied (where $\omega_H{=}eH/mc$ is the cyclotron frequency; m, e is the effective mass and the charge of the current carrier, respectively, and c is the light velocity in the vacuum. For energies $\varepsilon\approx\mu$ near the Fermi surface the density of states $\rho(\varepsilon)$ is an almost-periodic function of the magnetic field. This is the reason of the oscillatory character of the magnetic field dependence of both the thermodynamic quantities ("linear" with respect to $\rho(\varepsilon)$) and the kinetic coefficients ("quadratic" with respect to $\rho(\varepsilon)$). The oscillation period is the same for both types of quantities and is equal to the oscillation period of $\rho(\varepsilon)$.

2. Some thermodynamic relations

The thermodynamic potential $\Omega_H{=}F_H{-}\mu N$ is defined by the expression [4]

$$\Omega_H = -T\sum_{\nu}\ln\left[1+e^{(\mu-\varepsilon_\nu)/T}\right]. \tag{1}$$

In the integral form it may be written as

$$\Omega_H = -T \int_0^{\infty} d\varepsilon \rho(\varepsilon) \ln \left[1 + e^{(\mu - \varepsilon)/T} \right]. \tag{2}$$

The density of states $\rho(\varepsilon)$ is given by

$$\rho(\varepsilon) = \sum_{\nu} \delta(\varepsilon - \varepsilon_{\nu}) = Tr\delta(\varepsilon - \hat{\mathcal{H}}), \tag{3}$$

where F_H is the free energy, N is the total number of particles, T is the temperature (in energy units), ν is the set of all the quantum numbers characterizing a single-particle state and $\hat{\mathcal{H}}$ is the single particle Hamiltonian. For the thermodynamic potential derivatives we have

$$N = -\left(\frac{\partial \Omega_H}{\partial \mu}\right)_{T,V,H}, \quad M = -\left(\frac{\partial \Omega_H}{\partial H}\right)_{T,V,\mu},$$
$$C = -T\left(\frac{\partial^2 \Omega}{\partial T^2}\right)_{V,\mu,H}, \tag{4}$$

where M is the magnetic moment and C is the heat capacity. We calculate the density of states from Eq.(2) at $T = 0$ for simplicity. Then the $\rho(\varepsilon)$ is being transformed into $\rho(\mu)$ and is connected with Ω_H by the expression

$$\rho(\mu) = -\left(\frac{\partial^2 \Omega_H}{\partial \mu^2}\right)_{V,H,T=0}. \tag{5}$$

We can easily see from Eq.(5), that the density of states $\rho(\mu)$ at the Fermi surface is not exclusively related to the observable quantities presented in Eq.(4). Its oscillatory part $\tilde{\rho}(\mu)$ contains the period of the oscillations, which in turn, through the Lifshitz-Onsager relation, determines the area of the extremal sections of the Fermi surface by a plane perpendicular to $\mathbf{H}$. The oscillatory part $\tilde{\rho}(\varepsilon)$ of the density of states also answers the question about the physical nature of the oscillations of the kinetic coefficients in a magnetic field. As is well known from the theory of the Shubnikov-de Haas effect, the nonzero current in the direction of the electric field $\mathbf{E}||\mathbf{x}$ is attributable to the electron scattering, which under the conditions of the Shubnikov-de Haas effect can be assumed to be elastic [3, 5]. The fact that $\rho(\varepsilon)$ in Eq.(3) is represented in the form of Tr makes it possible to employ any complete set of wave functions in the computational procedure. Oscillatory wave functions (which are eigenfunctions of the operator of the number of the boson excitations $\hat{a}^{+}\hat{a}|n\rangle = n|n\rangle$) do not carry any information about the presence of the Fermi surface, while for the coherent states $|\alpha\rangle$ (which are eigenfunctions of the operator $\hat{a}(\hat{a}|\alpha\rangle = \alpha|\alpha\rangle)$) the average number of the particles is equal to

$$\langle\alpha|\hat{a}^{+}\hat{a}|\alpha\rangle = \bar{n}_{\alpha} \simeq \frac{\mu}{\hbar\omega_H}. \tag{6}$$

In addition, the coherent states are characterized by a well-defined phase [2,6]. This is connected with the existence of a phase characteristic (cyclotron period) of the oscillation phenomena under study. It suggests that we use coherent states for our problem.

3. Coherent states of a charged particle in a constant uniform magnetic field

Coherent states appear when one solves a problem for a linear oscillator. Some physical phenomena (superconductivity, Shubnikov - de Haas, de Haas-van Alphen effects) are quantum in their physical nature and macroscopic in their scale. The macroscopic scale indicates a possibility of an almost classical description of such phenomena. The coherent states are much more convenient to describe a field phase and amplitude simultaneously, and to show a connection between the classical and quantum field description. Historically, L.D. Landau was the first to show that the Schrödinger equation for the eigenfunctions and eigenvalues of a charge in a constant magnetic field has the form of the Schrödinger equation for the one-dimensional linear oscillator. Coherent states have been used to redefine in new terms the theory of Landau dimagnetism and the theory of the de Haas-van Alphen effects for free electron gas.

The achievements of the physics of coherent states have not been sufficiently extended to oscillation effects in metals with an arbitrary dispersion relation for electrons, or to numerous other quantum physical phenomena observed in metals in a magnetic field.

We will introduce the coherent states for a charge in a constant magnetic field $\mathbf{H}||\mathbf{z}$ and the Hamiltonian [7]

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^{\mathbf{2}} + \hat{\mathcal{H}}_{\sigma} = \hat{\mathcal{H}}_{\perp} + \hat{\mathcal{H}}_{\mathbf{z}} + \hat{\mathcal{H}}_{\sigma}, \tag{7}$$

$$\hat{\mathcal{H}}_z = \frac{\hat{p}_z^2}{2m}, \qquad \hat{\mathcal{H}}_{\sigma} = -\frac{g}{2}\mu_B \sigma_z H, \qquad \sigma_z = \pm 1, \tag{8}$$

where $\hat{\mathbf{p}}$ is the momentum operator, m is the bare electron mass, g^* is the effective spectroscopic splitting factor, and μ_B is the Bohr magneton.

We choose the vector potential $\mathbf{A}$ of the magnetic field in the Landau-gauge [7] as follows:

$$\mathbf{A} = \mathbf{A}(-yH, 0, 0), \quad \mathbf{H} = \nabla \times \mathbf{A}. \tag{9}$$

In this case $\hat{\mathcal{H}}_{\perp}$ corresponds to a one-dimensional oscillator along the y axis

$$\hat{\mathcal{H}}_{\perp} = \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega_H^2 (y - y_0)^2, \tag{10}$$

(where $y_0 = -cp_x/eH$). Instead of two coupled oscillators in the gauge $\mathbf{A} = (1/2)[\mathbf{H} \times \mathbf{r}]$. It gives us a possibility to avoid using "two-dimensional" coherent states (see Ref. 8). In dimensionless coordinates

$$\eta = \frac{y - y_0}{l_H}, \quad l_H = \left(\frac{\hbar}{m\omega_H}\right)^{1/2}, \tag{11}$$

the Hamiltonian $\hat{\mathcal{H}}_{\perp}$ takes the form

$$\hat{\mathcal{H}}_{\perp} = \frac{1}{2}\hbar\omega_H (\hat{p}_{\eta}^2 + \eta^2), \tag{12}$$

$\hat{p}_\eta = -i\nabla_\eta$. We introduce the operators $\hat{a}$ and $\hat{a}^+$

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\eta + \frac{\partial}{\partial\eta}\right), \quad \hat{a}^+ = \frac{1}{\sqrt{2}}\left(\eta - \frac{\partial}{\partial\eta}\right) \tag{13}$$

$[\hat{a}, \hat{a}^+] = 1$. Then $\hat{H}_\perp$ results in

$$\hat{H}_\perp = \hbar\omega_H\left(\hat{a}^+\hat{a} + \frac{1}{2}\right), \tag{14}$$

and

$$\hat{H} = \hbar\omega_H\left(\hat{a}^+\hat{a} + \frac{1}{2}\right) + \frac{\hat{p}_z^2}{2m} - \frac{g^*}{2}\mu_B\sigma_B H, \tag{15}$$

where μ_B is the Bohr's magneton and σ_B is the Pauli matrix.

Thus, the partial motion of an electron in a magnetic field in the xy plane is described by the Eq. (14), which contains the operators $\hat{a}$, $\hat{a}^+$ [defined in Eq.(13)], satisfying the Bose commutation relations. With the help of the operators $\hat{a}$, $\hat{a}^+$, we determine the states:

a) the vacuum state $|0\rangle$ such that $\hat{a}|0\rangle = 0$;

b) the Fock (after V.A. Fock) state $|n\rangle$, which is an eigenstate of the operator $\hat{n} = \hat{a}^+\hat{a}$:

$$\hat{n}|n\rangle = n|n\rangle, \; |n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle; \tag{16}$$

c) the "one-dimensional" coherent state $|\alpha\rangle$, which is an eigenstate of the operator $\hat{a}$

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle. \tag{17}$$

The coherent state $|\alpha\rangle$ can also be obtained with the help of the displacement operator $\hat{D}(\alpha)$

$$|\alpha\rangle = \hat{D}(\alpha)|0\rangle, \tag{18}$$

where

$$\hat{D}(\alpha) = e^{\alpha\hat{a}^+ - \alpha^*\hat{a}} = e^{-|\alpha|^2/2}e^{\alpha\hat{a}^+}e^{-\alpha^*\hat{a}}. \tag{19}$$

Thus, we have a complete normalized set of wave functions which are the eigenfunctions of non-Hermitian operator, and for this reason are not orthogonal.

It should be specially noted, however, that the partial motion of a fermion (electron) in the xy plane in the magnetic field **H** is described with the help of boson operators.

4. Oscillations of the electron density of states

We can employ the following complete normalized set of wave functions to calculate $\rho(\mu)$ of a metal in a quantizing magnetic field:

$$|\sigma_z, p_z; \alpha\rangle = L_z^{-1/2}e^{(ip_z z/\hbar)}\chi|\alpha\rangle, \tag{20}$$

where

$$\hat{\sigma}_z\chi = \sigma_z\chi, \quad \sigma_z = \pm 1, \tag{21}$$

L_z is the normalization length, and $\hat{\sigma}_z$ is the Pauli matrix.

Taking the trace in Eq. (3) and using Eq. (20), we obtain

$$\rho(\mu) = \sum_{p_z,\sigma_z}\int\frac{d^2\alpha}{\pi}\langle\alpha; P_z, \sigma_z|\delta(\mu - H)|\sigma_z, p_z; \alpha\rangle$$
$$= \frac{L_z}{\pi(2\pi\hbar)^2}\sum_{\sigma_z}\int_{-\infty}^{\infty}dp_z\int d^2\alpha\int_{-\infty}^{\infty}dt$$
$$\times\langle\alpha; p_z, \sigma_z|e^{i(\mu-\hat{H})t/\hbar}|\sigma_z, p_z; \alpha\rangle, \tag{22}$$

where $d^2\alpha = d(Re\,\alpha)d(Im\,\alpha)$. In the operator $\hat{H}$ all three terms commute with each other. We obtain the following relations:

$$\sum_{\sigma_z=\pm1} e^{i(t/\hbar)(g^*/2)\mu_B H} = 2\cos\left(\frac{g^*\mu_B H}{2\hbar}t\right); \tag{23}$$

$$\int_{-\infty}^{\infty}dp_z e^{(-itp_z^2/2m\hbar)} = \left(\frac{2\pi\hbar m}{|t|}\right)^{1/2}e^{-i\frac{\pi}{4}sign\,t}; \tag{24}$$

$$\langle\alpha \mid e^{-it\omega_H\hat{a}^+\hat{a}}|\alpha\rangle = \sum_{n=0}^{\infty}\langle\alpha \mid e^{-it\omega_H\hat{a}^+\hat{a}}|n\rangle\langle n|\alpha\rangle$$
$$= \sum_{n=0}^{\infty}e^{-it\omega_H n}|\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2\left(1-e^{-it\omega_H}\right)}. \tag{25}$$

In the last equation we have used the condition

$$\sum_{n=0}^{\infty}|n\rangle\langle n| = 1 \tag{26}$$

of the completeness of the set of the Fock states. The result for the scalar product of the Fock and coherent states is as follows:

$$\langle n|\alpha\rangle = \left\langle n\left|e^{-|\alpha|^2/2}e^{\alpha\hat{a}^+}\right|0\right\rangle$$
$$= \frac{\alpha^n}{\sqrt{n!}}e^{-|\alpha|^2/2}. \tag{27}$$

The density of states $\rho(\mu)$ at the Fermi surface results in the form of a single integral

$$\rho(\mu) = \frac{L_Z\Phi m^{1/2}}{(2\pi\hbar)^{3/2}\Phi_0}$$
$$\times\int_{-\infty}^{\infty}dt\frac{e^{i\left(\frac{\mu t}{\hbar} - \frac{\pi}{4}sign\,t\right)}\cos\left(\frac{g^*\mu_B H}{2\hbar}t\right)}{i|t|^{1/2}\sin(t\omega_l)},$$
$$\Phi = L_x L_y H, \quad \Phi_0 = \frac{ch}{e}. \tag{28}$$

It is calculated with the help of the residue theorem by integrating along the contour shown in Fig. 1.

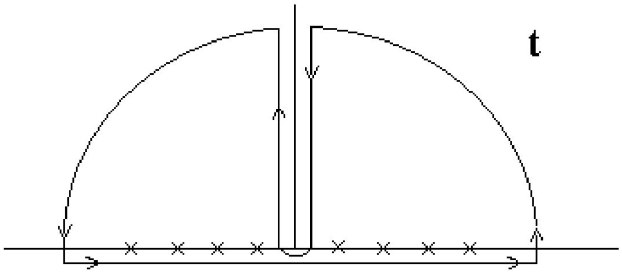

FIGURE 1. The integration contour in the complex plane t for the calculation of the integral Eq. (28).

The oscillating part of the density of states $\tilde{\rho}(\mu)$ is determined by the contribution the integral of the poles located on the real axis at the points

$$t_k = \frac{2\pi}{\omega_H} K, \quad K = \pm 1, \pm 2, \pm 3, \dots \tag{29}$$

and has the form

$$\tilde{\rho}(\mu) = \frac{mV}{\pi^2 \hbar^2} \left(\frac{eH}{c\hbar}\right)^{1/2} \sum_{K=1}^{\infty} K^{-1/2} \times \cos\left(\frac{\pi g^* m}{2m_0} K\right) \cos\left(2\pi K \frac{\mu}{\hbar\omega_H} - \frac{\pi}{4}\right), \tag{30}$$

which contains a period of the oscillations

$$\Delta\left(\frac{1}{H}\right) = \frac{e\hbar}{mc\mu}. \tag{31}$$

5. Conclusion

Our approach to the analysis of oscillation effects in metals in a magnetic field makes it possible not only to substantially simplify the mathematical procedure as compared with the traditional method of analyzing these phenomena, but also to study in a universal manner both the thermodynamic and kinetic effects. This permit us to easily extend the analysis to the case of current carriers with an arbitrary energy spectrum and nonzero temperature, and to include the effect of scattering on the form of the oscillation dependence.

We introduced a vector potential $\mathbf{A}$ of the magnetic field in the Landau-gauge that allows to use a simplified method for the one-dimensional coherent state representation. The end result is that boson operators can describe the partial motion of fermions (electrons) in the xy plane in the magnetic field.

The physical reason for the simplification achieved in the mathematical procedure is that the coherent state employed in the calculations describes quantum macroscopic phenomena, and therefore also quasi-classical phenomena, which are the Shubnikov-de Haas and de Haas-van Alphen effects in metals, semimetals and degenerate semiconductors.

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