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Functional methods in the theory of magnetoimpurity states of electrons in quantum wires

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Abstract
Functional methods are used to study magnetoimpurity states of electrons in nanostructures. The Keldysh formalism is applied to these states. The theory is illustrated using a quantum wire sample with impurity atoms capable of localizing electrons in a magnetic field. The characteristics of magnetoimpurity states of electrons in the wire are calculated using the model of a Gaussian separable potential.

1. Introduction

Impurity states of electrons (local and resonant) in alloyed metals and semiconductors have been known of for a long time (see, for instance, [1–4]). It is well known, in particular, that a shallow and narrow impurity potential well in a three-dimensional conductor cannot localize an electron. In one-dimensional and two-dimensional cases localization is possible with any well intensity [5].

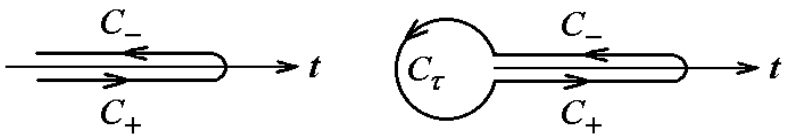
In the presence of a quantizing magnetic field the situation changes. The motion of an electron in a massive conductor in a magnetic field is similar to a one-dimensional case, and in the one-dimensional case the electron is localized in a potential well of any degree of intensity [5]. The spatial inhomogeneity of the alloyed conductor results in removal of the degeneracy of the Landau levels over the position of the 'Landau oscillator'. Impurity levels split off from every Landau level. Levels split off from the lower Landau level are local and levels split off from the higher levels fall within an area of the continuous spectrum and are resonant [6, 7]. Such levels caused by mutual influences of donor impurity atoms and magnetic fields on electrons are called magnetoimpurity levels, and the respective states of electrons are called magnetoimpurity states.

The magnetoimpurity states of electrons create the beats in the de Haas–van Alfven [6, 7] and in the Shubnikov–de Haas effects and they cause the linear growth of magnetic resistance of metals with closed Fermi surfaces along with the growth of the magnetic field [8, 9]. These states result in the appearance of new branches of collective modes in massive and low dimensional conductors: electromagnetic [10–12], sound [13], magnetoplasma [14], and electronic spin waves [15].

The existing methods for studying impurity states are based on Schrödinger's equation and on the quantum Green's functions. In the meantime, functional methods derived in quantum field theory are widely adopted in solid state theory [16, 17]. In conjunction with the Keldysh technique [18, 19] they become a powerful tool of research in condensed matter physics [17, 20, 21]. Here we will specify how the methods of functional differentiation and integration using Grassmann variables can be used to calculate the characteristics of magnetoimpurity states of electrons in massive conductors and nanostructures. The formalism set out in section 2 and a model presented in section 3 are used in section 4 to calculate the characteristics of magnetoimpurity states of electrons in quantum wires.

2. Formalism

The functional approach to the Keldysh formalism has recently been the subject of a comprehensive monograph [17] including applications in disordered conductors. As far as the authors are aware, the potential of functional methods in the theory of magnetoimpurity states of electrons in conductors [6, 11] has not been studied yet. In this section, we will describe how the formalism of the works [17, 22] is applied to arbitrary magnetic field and magnetoimpurity states of electrons on isolated impurity atoms. This theory is applicable to solid conductors and two-dimensional electron gas. The general theory of magnetoimpurity states of electrons in two-dimensional electron systems has been developed in a series of works by Azbel, Gredeskul, Avishai and others (see review [23]) using



(a) (b)

Figure 1. Keldysh–Schwinger time contour (a) and extended contour (b).

a different method of calculation. The advantage of functional methods compared with standard methods consists in the fact that transformation from operators to classical objects allows us to simplify and to speed up calculations and to make them more visual. The universal language of the functional approach permits us to describe a lot of phenomena in equilibrium and non-equilibrium systems using the unique method. In particular, the Keldysh formalism permits us to study the influence of magnetoimpurity states of electrons upon non-equilibrium system properties.

Let us write the Hamiltonian of the electrons as $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ accounts for the magnetic field, and $\hat{V}$, the interaction with a random external field. Like in the works [17, 22], we consider that it is switched 'on' at the initial time $t = -\infty$, when the system of electrons was still in the equilibrium state. Then the matrix function of the Green electrons [17, 22] can be written as

$$\mathrm{i}G_{12} = \left\langle T_{C_\mathrm{t}} \left(\hat{\psi}_{1\mathrm{H}} \hat{\psi}^+_{2\mathrm{H}} \right) \right\rangle, \tag{1}$$

where indices 1 and 2 correspond to variables $\mathbf{r}, \alpha, t$ ($\mathbf{r}$ is a position vector, $\alpha = \pm 1$ a spin variable, t time), $\hat{\psi}_{1\mathrm{H}}$ and $\hat{\psi}^+_{2\mathrm{H}}$ are Heisenberg operators of destruction and creation of electrons, T_{C_t} is the symbol of chronological ordering of operators along the Keldysh–Schwinger time contour of $C_\mathrm{t} = C_+ + C_-$ (figure 1(a)), the angle brackets indicate Gibbs averaging with the Hamiltonian $\hat{H}_0$. The reduced Planck constant is set to unity. In equation (1) the matrix indices $\pm$ in two-dimensional Keldysh space are omitted. In component form the Green function (1) is

$$G_{12} = \begin{pmatrix} G^{++}_{12} & G^{+-}_{12} \\ G^{-+}_{12} & G^{--}_{12} \end{pmatrix}. \tag{2}$$

Here G^{+-}_{12}, for instance, indicates that $t_1 \in C_+$ and $t_2 \in C_-$. It is convenient to rewrite the operators $\hat{\psi}_{1\mathrm{S}}$ and $\hat{\psi}^+_{2\mathrm{S}}$ in equation (1) in the Schrödinger representation. Then,

$$\mathrm{i}G_{12} = \left\langle T_{C_\mathrm{t}} \left(\hat{\psi}_{1\mathrm{S}} \hat{\psi}^+_{2\mathrm{S}} \hat{U} \right) \right\rangle, \tag{3}$$

where

$$\hat{U}(t, t_0) = T_{C_\mathrm{t}} \exp\left[-\mathrm{i} \int_{t_0}^{t} \mathrm{d}t' \hat{H}(t') \right]$$

is the evolution operator along the contour C_t.

By using the standard procedure [16, 17], let us present the Green function (3) as a path integral along Grassmann fields ψ_1, ψ^*_2, associated with the field operators. For that we introduce a Gibbs exponent $\exp(-\beta\hat{H}_0)$ (β: reverse temperature) under the chronological product operator. This is achieved by using extended contour $C = C_\mathrm{t} + C_\tau$ (figure 1(b)) and the time-ordering operator T_C along this contour. It is assumed that on the part of the contour C_τ the Hamiltonian of electrons is equal to $\hat{H}_0$. Thus the Green function (3) looks as follows:

$$\mathrm{i}G_{12} = \int \mathrm{D}\psi^* \int \mathrm{D}\psi\ \psi_1 \psi^*_2 \exp\left\{ \mathrm{i} \oint_C \mathrm{d}t \left[\sum_\alpha \int \mathrm{d}\mathbf{r}\, \psi^*_\alpha(\mathbf{r}, t) \times \mathrm{i}\frac{\partial}{\partial t} \psi_\alpha(\mathbf{r}, t) - H\left(\psi^*, \psi\right) \right] \right\}. \tag{4}$$

Function $H(\psi^*, \psi)$ is derived from the operator $H(\hat{\psi}^+, \hat{\psi})$ by replacing the field operators with the Grassmann variables.

The Green functions can be derived by functional differentiation of the generating functional

$$Z\left[J, J^*\right] = \int \mathrm{D}\psi^* \int \mathrm{D}\psi\ \exp\left\{ \mathrm{i} \oint_C \mathrm{d}t \left[\sum_\alpha \int \mathrm{d}\mathbf{r}\, \psi^*_\alpha(\mathbf{r}, t) \times \mathrm{i}\frac{\partial}{\partial t} \psi_\alpha(\mathbf{r}, t) - H\left(\psi^*, \psi\right) + \sum_\alpha \int \mathrm{d}\mathbf{r}\, \psi^*_\alpha(\mathbf{r}, t)\, J_\alpha(\mathbf{r}, t) + \sum_\alpha \int \mathrm{d}r\, J^*_\alpha(\mathbf{r}, t)\, \psi_\alpha(\mathbf{r}, t) \right] \right\} \tag{5}$$

with sources J, J^* of the Fermi field. In particular, function (4) is equal to

$$\mathrm{i}G_{12} = \left(\frac{\delta^\mathrm{L}}{\mathrm{i}\delta J^*_1} \frac{\delta^\mathrm{R}}{\mathrm{i}\delta J_2} W\left[J, J^*\right] \right)_{\substack{J=0 \\ J^*=0}}, \tag{6}$$

where $W = \ln Z$ is the generating functional for connected Green functions, indices L and R mark the left and right functional derivatives over the Grassmann variables J^*, J.

Let us transform equation (5) into a (κ, α, t)-representation (κ is a set of orbital quantum electron numbers in the magnetic field) and calculate the free generating functional in the magnetic field and field of sources:

$$Z_0\left[J, J^*\right] = \int \mathrm{D}a^* \int \mathrm{D}a \exp\left\{ \mathrm{i} \oint_C \mathrm{d}t \times \sum_{\kappa\alpha} \left[a^*_{\kappa\alpha}(t) \left(\mathrm{i}\frac{\partial}{\partial t} - \varepsilon_{\kappa\alpha} \right) a_{\kappa\alpha}(t) + J^*_{\kappa\alpha}(t) a_{\kappa\alpha}(t) + a^*_{\kappa\alpha}(t) J_{\kappa\alpha}(t) \right] \right\}. \tag{7}$$

Here $a_{\kappa\alpha}$, $a^*_{\kappa\alpha}$, $J_{\kappa\alpha}$, $J^*_{\kappa\alpha}$ are expansion coefficients of Grassmann variables ψ, ψ^*, J, J^* over the Landau basis, $\varepsilon_{\kappa\alpha}$ is the energy of the electron in the magnetic field, calculated

from the chemical potential. The functions $a(t)$ and $a^*(t)$ meet boundary conditions:

$$\begin{aligned} a_+(\infty) &= a_-(\infty), & a_+^*(\infty) &= a_-^*(\infty), \\ a_-(-\infty) &= a_\tau(0), & a_-^*(-\infty) &= a_\tau^*(0), \\ a_+(-\infty) &= -a_\tau(\beta), & a_+^*(-\infty) &= -a_\tau^*(\beta). \end{aligned} \tag{8}$$

Indices $+, -, \tau$ are associated with the parts C_+, C_-, C_τ of the expanded contour C.

In equation (7) let us split the coefficients $a = a_0 + a'$, $a^* = a_0^* + a'^*$, where a_0 and a_0^* are such that the linear terms over Grassmann variables a', a'^* in the exponent index drop out. Therefore it is necessary that the functions a_0^+, a_0^-, a_0^τ satisfy the system of equations

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \varepsilon\right) a_0^+ = -J^+, \qquad \left(\mathrm{i}\frac{\partial}{\partial t} - \varepsilon\right) a_0^- = J^-,$$
$$\left(\frac{\partial}{\partial \tau} + \varepsilon\right) a_0^\tau = 0, \tag{9}$$

and conditions (8). We placed $J = J^+$ on the part of the contour C_+ and $J = -J^-$ on C_-. Variables t and τ are related as $\tau = \mathrm{i}t$.

The solution of the system of equations (9) can be written as

$$a_{\kappa\alpha}^0(t) = -\int_{-\infty}^{\infty} \mathrm{d}t' \overset{0}{G}_{\kappa\alpha}(t - t') J_{\kappa\alpha}(t'),$$

where $\overset{0}{G}$ is a matrix Green function of electrons in the magnetic field. Its components are equal to

$$\overset{0}{G}{}_{\kappa\alpha}^{++}(t) = \mathrm{i}\left[\Theta(t)(f_{\kappa\alpha} - 1) + \Theta(-t) f_{\kappa\alpha}\right] \exp(-\mathrm{i}\varepsilon_{\kappa\alpha} t),$$

$$\overset{0}{G}{}_{\kappa\alpha}^{+-}(t) = \mathrm{i} f_{\kappa\alpha} \exp(-\mathrm{i}\varepsilon_{\kappa\alpha} t),$$

$$\overset{0}{G}{}_{\kappa\alpha}^{-+}(t) = \mathrm{i}(f_{\kappa\alpha} - 1) \exp(-\mathrm{i}\varepsilon_{\kappa\alpha} t),$$

$$\overset{0}{G}{}_{\kappa\alpha}^{--}(t) = \mathrm{i}\left[\Theta(t) f_{\kappa\alpha} + \Theta(-t)(f_{\kappa\alpha} - 1)\right] \exp(-\mathrm{i}\varepsilon_{\kappa\alpha} t),$$

where Θ and f are the Heaviside and the Fermi functions respectively.

The path integral (7) over the Grassmann variables a'^*, a' is the Gaussian integral. It can be calculated according to the rule [16, 17]

$$\int \mathrm{D}a'^* \int \mathrm{D}a' \exp\left(-a'^* A a'\right) = \det A,$$

where A is a non-singular matrix, irrelevant for our derivation. An important factor in the generating functional (7) is equal to

$$Z_0\left[J, J^*\right] = \exp\left(-\mathrm{i}\sum_{12} J_1^* \overset{0}{G}_{12} J_2\right). \tag{10}$$

Here $1 = (\kappa_1, \alpha_1, t_1)$, $\sum_1 = \sum_{\kappa_1\alpha_1} \int_{-\infty}^{\infty} \mathrm{d}t_1$. The summation symbol over the Keldysh indices $\pm$ in equation (10) is omitted.

The following Hamiltonian $\hat{V}$ accounts for the interaction of electrons with impurity atoms randomly distributed in a sample:

$$\hat{V} = \sum_{\kappa_1\kappa_2\alpha} \langle\kappa_1| u |\kappa_2\rangle \hat{a}_{\kappa_1\alpha}^+ \hat{a}_{\kappa_2\alpha},$$

where $\hat{a}_{\kappa\alpha}$ and $\hat{a}_{\kappa\alpha}^+$ are destruction and creation operators of electrons in state (κ, α), u is the energy of an electron in the field of impurity atoms. Since $V = 0$ on a part of the contour C_τ, the integral in the exponent index (5) is equal to

$$\oint_C \mathrm{d}t\, V\left(a^*, a\right) = \sum_{12} U_{12} a_1^* \sigma_3 a_2, \tag{11}$$

where $U_{12} = \langle\kappa_1|u|\kappa_2\rangle \delta_{\alpha_1\alpha_2} \delta(t_1 - t_2)$, σ_3 is the third Pauli matrix.

From equation (5) it is clear that the full generating functional can be derived from the free functional (10) by operator action:

$$\exp\left(-\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t\, V\right),$$

obtained from equation (11) as a result of the replacement

$$a_{\kappa\alpha}^*(t) \to \frac{\delta^{\mathrm{R}}}{\mathrm{i}\delta J_{\kappa\alpha}(t)}, \qquad a_{\kappa\alpha}(t) \to \frac{\delta^{\mathrm{L}}}{\mathrm{i}\delta J_{\kappa\alpha}^*(t)}.$$

Consequently, the generating functional (5) is equal to

$$Z\left[J, J^*\right] = \exp\left(-\mathrm{i}\sum_{12} U_{12} \frac{\delta^{\mathrm{R}}}{\mathrm{i}\delta J_1} \sigma_3 \frac{\delta^{\mathrm{L}}}{\mathrm{i}\delta J_2^*}\right)$$
$$\times \exp\left(-\mathrm{i}\sum_{34} J_3^* \overset{0}{G}_{34} J_4\right). \tag{12}$$

In exponent indices it is necessary to execute summing over the Keldysh indices. Thus, the procedure of calculation of the Green function of the system can be carried out by calculation of functional derivative in equations (6) and (12). This procedure is easier than the method of local perturbations using the operator formalism.

Equation (12) enables us to write the generating functional in the form of a series over perturbation V. Green function (6) is also presented in the form of a series which coincides with the series derived by using the diagram technique and Wick's theorem [16]. The first-order correction to the generating functional W is equal to

$$\begin{aligned} W_1\left[J, J^*\right] = &\sum_{12} U_{12}\left(\overset{0}{G}{}_{21}^{++} - \overset{0}{G}{}_{21}^{--}\right) \\ &- \mathrm{i}\sum_{12} U_{12} \sum_{34}\Big[\overset{*}{J}{}_3^+ J_4^+\left(\overset{0}{G}{}_{31}^{+-}\overset{0}{G}{}_{24}^{-+} - \overset{0}{G}{}_{31}^{++}\overset{0}{G}{}_{24}^{++}\right) \\ &+ \overset{*}{J}{}_3^+ J_4^-\left(\overset{0}{G}{}_{31}^{+-}\overset{0}{G}{}_{24}^{--} - \overset{0}{G}{}_{31}^{++}\overset{0}{G}{}_{24}^{+-}\right) \\ &+ \overset{*}{J}{}_3^- J_4^+\left(\overset{0}{G}{}_{31}^{--}\overset{0}{G}{}_{24}^{-+} - \overset{0}{G}{}_{31}^{-+}\overset{0}{G}{}_{24}^{++}\right) \\ &+ \overset{*}{J}{}_3^- J_4^-\left(\overset{0}{G}{}_{31}^{--}\overset{0}{G}{}_{24}^{--} - \overset{0}{G}{}_{31}^{-+}\overset{0}{G}{}_{24}^{+-}\right)\Big]. \end{aligned}$$

Using equation (6) we obtain the first-order corrections to the components of matrix Green function (2):

$$\begin{aligned}
{}^{1}_{}G_{12}^{++} &= \sum_{34} U_{34}\left({}^{0}_{}G_{13}^{+-}\,{}^{0}_{}G_{42}^{-+} - {}^{0}_{}G_{13}^{++}\,{}^{0}_{}G_{42}^{++}\right),\\
{}^{1}_{}G_{12}^{+-} &= \sum_{34} U_{34}\left({}^{0}_{}G_{13}^{+-}\,{}^{0}_{}G_{42}^{--} - {}^{0}_{}G_{13}^{++}\,{}^{0}_{}G_{42}^{+-}\right),\\
{}^{1}_{}G_{12}^{-+} &= \sum_{34} U_{34}\left({}^{0}_{}G_{13}^{--}\,{}^{0}_{}G_{42}^{-+} - {}^{0}_{}G_{13}^{-+}\,{}^{0}_{}G_{42}^{++}\right),\\
{}^{1}_{}G_{12}^{--} &= \sum_{34} U_{34}\left({}^{0}_{}G_{13}^{--}\,{}^{0}_{}G_{42}^{--} - {}^{0}_{}G_{13}^{-+}\,{}^{0}_{}G_{42}^{+-}\right).
\end{aligned}$$

The diagrams for these corrections are presented in [24]. They differ from the usual diagrams of the cross technique [25] by having additional indices $\pm$ at the ends of lines.

Here we restrict ourselves to a selective summing of diagrams with one cross for the retarded Green's function $G = G^{++} - G^{+-}$ of electrons in a nanostructure averaged over impurity configurations. Such an approximation allows us to consider accurately the amplitude of electron scattering by isolated impurity atoms with a small concentration of such atoms. Let us choose the scattering potential in the form

$$\hat{V} = \sum_j |\eta_j\rangle\, u_0 \,\langle\eta_j|, \tag{13}$$

where $|\eta_j\rangle\langle\eta_j|$ is the projection operator on vector $|\eta_j\rangle$, u_0 is a constant, index j enumerates impurity atoms. We deem that function $\eta(\mathbf{r}) = \langle\mathbf{r}|\eta\rangle$ is equal to

$$\eta\,(r) = \left(\sqrt{\pi}a\right)^{-1}\exp\left(-\frac{r^2}{2a^2}\right),$$

where a is a constant. Transformation of equation (13) to the sum of delta functions $\upsilon_0\delta(\mathbf{r}-\mathbf{r}_j)$ is performed by making the replacement

$$4\pi \lim_{\substack{a\to 0\\ u_0\to\infty}} \left(a^2 u_0\right) = \upsilon_0.$$

In the case of potential (13) the sum of diagrams with one cross for the mean Green function in the $(\kappa, \alpha, \varepsilon)$-presentation is equal to $G = G_0 + G_0 T G_0$, where the value

$$T_\alpha\,(\varepsilon) = u_0 n_i\left(1 - u_0\sum_\kappa \frac{|\langle\kappa|\eta\rangle|^2}{\varepsilon - \varepsilon_{\kappa\alpha}}\right)^{-1} \tag{14}$$

is proportional to the scattering amplitude of electrons, n_i is the density of impurity atoms.

3. Quantum wire model

The model of a quantum wire convenient for calculations is a system of electrons in a two-dimensional conductor on which the confinement potential is placed, restricting their motion in one direction. An example of a quantum wire is a two-dimensional electron gas at the border of Si and SiO_2 in the system like a metal–dielectric–semiconductor structure or in a $GaAs/Al_xGa_{1-x}As$ heterostructure with the confinement potential created using electron beam lithography. In such systems, electrons move freely in one direction and their motion in other directions is restricted.

Let us select the vector potential of the magnetic field H perpendicular to plane (x, y) occupied by a two-dimensional electron gas in the form of $\vec{A} = (0, Hx, 0)$. The confinement potential is assumed to be parabolic, $m\omega_0^2 x^2/2$. Here m is the effective mass of the electron, ω_0 is the potential parameter. Then the orbital wavefunction of the electron's stationary state looks as usual [5]:

$$\psi_{nk_y}\,(x, y) = \left(\sqrt{\pi}2^n n!\, l\, L\right)^{-1/2}\exp\left[-\frac{1}{2}\left(\frac{x-x_0}{l}\right)^2\right] \times H_n\left(\frac{x-x_0}{l}\right)\exp\left(\mathrm{i}k_y y\right), \tag{15}$$

but its parameters are renormalized. Here n and k_y are the oscillator quantum number and the projection of the electron momentum on the wire axis y, $l = (1/m\omega)^{1/2}$, $\omega = (\omega_0^2 + \omega_c^2)^{1/2}$ is the hybrid frequency (ω_c is the electron's cyclotron frequency), $x_0 = -\omega_c k_y/(m\omega^2)$, L is the length of the wire, H_n is the Hermite polynomial. The electron's energy in state (15) is equal to

$$\varepsilon_{nk_y\sigma} = \omega\left(n + \frac{1}{2}\right) + \frac{k_y^2}{2M} + \sigma\mu_B H, \tag{16}$$

where $M = m(\omega/\omega_0)^2$, μ_B is the electron spin magnetic moment, $\sigma = \pm 1$ is the spin quantum number. The density of electron states with spectrum (16) is equal to

$$\nu_\sigma\,(\varepsilon) = \sqrt{\frac{M}{2}}\frac{L}{\pi}\sum_n \frac{\Theta\,(\varepsilon - \varepsilon_{n\sigma})}{\sqrt{\varepsilon - \varepsilon_{n\sigma}}},$$

where $\varepsilon_{n\sigma} = \omega(n + \frac{1}{2}) + \sigma\mu_B H$ are Landau levels of the electron in the wire.

4. Magnetoimpurity states of electrons in quantum wires

In quantum wires even separate impurity atoms significantly affect the properties of conduction electrons. In this section we will derive the equation of Lifshitz [26] for the spectrum of impurity states of electrons in quantum wire located in a magnetic field. We approximate the potential of an impurity atom located at the center of the coordinate system using a separable Gaussian potential (13), convenient for calculations.

The electron scattering operator with an impurity center looks like

$$T = \frac{|\eta\rangle\, u_0\, \langle\eta|}{1 - u_0 D}, \tag{17}$$

where

$$D_\sigma\,(\varepsilon + \mathrm{i}0) = \sum_{nk_y}\frac{\left|\langle\eta|nk_y\rangle\right|^2}{\varepsilon - \varepsilon_{nk_y\sigma} + \mathrm{i}0} = F_\sigma\,(\varepsilon) - \mathrm{i}\pi\, g_\sigma\,(\varepsilon)\,.$$

The operator poles in equation (17) correspond to impurity states of electrons. Impurity levels satisfy the equation

of Lifshitz

$$1 - u_0 D_\sigma\,(\varepsilon + \mathrm{i}0) = 0. \tag{18}$$

This equation can be obtained from the formula (3.63) in [27], if one considers the self-energy function Σ, entering into this formula, in the linear approximation over n_i and takes into account multiple scattering of electrons by isolated short-range impurity atoms in a quantizing magnetic field. In this case the formula takes the following form in our notation:

$$G_\sigma\,(\kappa, \varepsilon) = \left[\varepsilon - \varepsilon_{\kappa\sigma} - \frac{n_i u_0}{1 - u_0 D_\sigma\,(\varepsilon + \mathrm{i}0)}\right]^{-1}.$$

In the linear approximation over n_i this equation implies a relation between functions G, G_0 (presented in section 2) and the multiple impurity scattering operator T. As noted in [27], this is equivalent to replacement of the amplitude of Born scattering of electrons by an isolated impurity atom in equations (3.61) and (3.67), which describe the collision frequency of electrons, by a T-matrix (see section 3.7 in [27]). The T-matrix accounts for the effects of potential and resonant electron scattering by impurity atoms. Replacing the resonant dominator $(1 - u_0 F_\sigma)^2 + (\pi u_0 g_\sigma)^2$ in function Σ by unity we obtain the Born potential scattering contribution to the electron collision frequency. Near the poles of the T-matrix satisfying equation (18) the amplitude is characterized by the Breit–Wigner resonances [5], which influence considerably the observed values [6–13, 15].

Considering (13) and (15), we derive

$$\langle \eta | n k_y \rangle = \frac{2\sqrt{\pi l}}{\sqrt{\sqrt{\pi} 2^n n!\,(\alpha+1)\,L}} \left(\frac{|\alpha - 1|}{\alpha + 1}\right)^{n/2} \times \exp\left[-\frac{1}{2} a^2 k_y^2 \left(1 + \frac{\alpha^2 \xi^2}{\alpha + 1}\right)\right] H_n\left(a k_y \xi \frac{\alpha^{3/2}}{\sqrt{|\alpha^2 - 1|}}\right),$$

where $\alpha = (l/a)^2$, $\xi = \omega_c/\omega$. As a result, equation (18) takes the form

$$1 - u_0 \frac{2l}{\alpha + 1} \sum_n \int_{-\infty}^{\infty} \mathrm{d}k_y \frac{\gamma^n}{\varepsilon - \varepsilon_{nk_y\sigma} + \mathrm{i}0} \frac{1}{\sqrt{\pi} 2^n n!} \times \exp\left[-a^2 k_y^2 \left(1 + \frac{\alpha^2 \xi^2}{\alpha + 1}\right)\right] H_n^2\left(a k_y \xi \frac{\alpha^{3/2}}{\sqrt{|\alpha^2 - 1|}}\right) = 0, \tag{19}$$

where $\gamma = |\alpha - 1|/(\alpha + 1)$. Considering the identity

$$\frac{1}{\varepsilon - \varepsilon_{nk_y\sigma} + \mathrm{i}0} = -\mathrm{i} \int_0^\infty \mathrm{d}u \exp\left[\mathrm{i}u\left(\varepsilon - \varepsilon_{nk_y\sigma} + \mathrm{i}0\right)\right]$$

and calculating the integral included in (19), equation (19) can be written as

$$1 + \mathrm{i} \frac{2^{3/2} u_0 l M^{1/2}}{\omega^{1/2} (\alpha + 1)} \int_0^\infty \mathrm{d}x \exp\left[\mathrm{i}x\left(\frac{\varepsilon}{\omega} - \frac{1}{2} - \sigma \frac{\mu_B H}{\omega} + \mathrm{i}0\right)\right] \times \left(1 - \gamma^2 \mathrm{e}^{-2\mathrm{i}x}\right)^{-1/2} \left[\mathrm{i}x + 2Ma^2\omega\left(1 + \frac{\alpha^2\xi^2}{\alpha + 1}\right) - 4Ma^2\omega \frac{\alpha^3 \xi^2}{(\alpha+1)^2} \frac{1}{\mathrm{e}^{\mathrm{i}x} + \gamma}\right]^{-1/2} = 0. \tag{20}$$

Separating the real and imaginary parts in this equation, we derive functions $F_\sigma(\varepsilon)$ and $g_\sigma(\varepsilon)$. The latter is equal to

$$g_\sigma\,(\varepsilon) = \frac{2^{3/2} l\, M^{1/2}}{\alpha + 1} \sum_n \frac{\Theta\,(\varepsilon - \varepsilon_{n\sigma})}{\sqrt{\varepsilon - \varepsilon_{n\sigma}}} \frac{\gamma^n}{\sqrt{\pi} 2^n n!} \times \exp\left[-2Ma^2\,(\varepsilon - \varepsilon_{n\sigma})\left(1 + \frac{\alpha^2\xi^2}{\alpha + 1}\right)\right] \times H_n\left(\sqrt{2M} a \sqrt{\varepsilon - \varepsilon_{n\sigma}}\, \xi \frac{\alpha^{3/2}}{\sqrt{|\alpha^2 - 1|}}\right).$$

From equation (20) we understand that if $u_0 < 0$ in the spectrum of electrons, there is a system of impurity levels $\varepsilon_{n\sigma}^{(r)}$ split off from Landau levels. A level below the border of the continuous spectrum $\varepsilon_{0(-1)}$ is local; other levels are quasilocal. Their widths are equal to $\Gamma = \pi g/|F'|$, where the prime marks the derivative over energy taken at the point $\varepsilon_{n\sigma}^{(r)}$. These levels result from the mutual impact of the impurity atom and magnetic field on electrons. Therefore they are called magnetoimpurity states.

Equations (19) and (20) state that if $u_0 < 0$ then the position of the local level $\varepsilon_{l\sigma}$ in zone $\varepsilon \leqslant \varepsilon_{0\sigma}$ is the root of the equation

$$1 - \frac{4\sqrt{\pi} M l\, |u_0|}{(\alpha + 1)\, k_{0\sigma}} \exp\left(a^2 k_{0\sigma}^2 \rho^2\right) [1 - \Phi\,(a k_{0\sigma} \rho)] = 0, \tag{21}$$

where

$$k_{0\sigma} = \sqrt{2M\,(\varepsilon_{0\sigma} - \varepsilon)}, \qquad \rho = \sqrt{1 + \frac{\alpha^2 \xi^2}{\alpha + 1}},$$

where Φ is the probability integral [28]. If $a k_{0\sigma} \rho \ll 1$, from this equation we find the distance Δ_0 between the local level and the border of the continuous spectrum:

$$\Delta_0 = \varepsilon_{0\sigma} - \varepsilon_{l\sigma} = \frac{8\pi M a^2 u_0^2 \alpha}{(\alpha + 1)^2} = \begin{cases} \dfrac{4\pi u_0^2 \alpha}{\varepsilon_0}, & \alpha \ll 1, \\ \dfrac{4\pi u_0^2}{\alpha \varepsilon_0}, & \alpha \gg 1. \end{cases} \tag{22}$$

Here $\varepsilon_0 = (2Ma^2)^{-1}$. In the extreme case $a k_{0\sigma} \rho \gg 1$ from equation (21) we derive

$$\Delta_0 = \frac{2\,|u_0|\,\sqrt{\alpha}}{(\alpha + 1)\,\rho} = \begin{cases} 2\,|u_0|\,\sqrt{\alpha}, & \alpha \ll 1, \\ 2|u_0|/\alpha\xi, & \alpha \gg 1. \end{cases}$$

When $\varepsilon \to -\infty$ from equation (20) we find $\varepsilon_l = -|u_0|$.

The root of equations (19) or (20) in the zone $\varepsilon \leqslant \varepsilon_{1\sigma}$ when $u_0 < 0$ corresponds to the resonance level $\varepsilon_{r\sigma}$. Its position we derive from the equation

$$1 + \frac{8 l u_0 \alpha^3 \xi^2 \gamma}{\sqrt{\pi}\varepsilon_0\,(\alpha + 1)\,|\alpha^2 - 1|} \left\{\frac{\sqrt{\pi}}{2a\rho} - \frac{\pi k_{1\sigma}}{2} \exp\left(a^2 k_{1\sigma}^2 \rho^2\right) \times [1 - \Phi\,(a k_{1\sigma} \rho)]\right\} = 0, \tag{23}$$

where

$$k_{1\sigma} = \sqrt{2M\,(\varepsilon_{1\sigma} - \varepsilon)}.$$

From this equation we obtain that if $ak_{1\sigma}\rho \ll 1$, the resonance level exists only if $|u_0| > u_c$, where

$$u_c = \varepsilon_0 \frac{(\alpha+1)^3 \rho}{4\alpha^{7/2}\xi^2}. \tag{24}$$

Distance Δ_1 between level $\varepsilon_{1\sigma}$ and the resonance level in this case is equal to

$$\Delta_1 = \varepsilon_{1\sigma} - \varepsilon_{r\sigma} = \frac{\varepsilon_0}{\pi\rho^2}\left(1 - \frac{u_c}{|u_0|}\right)^2. \tag{25}$$

The width of this level if $\Delta_1 \ll \omega$ is equal to

$$\Gamma = \varepsilon_0 \frac{(\alpha+1)^2}{\alpha^3\xi^2}\sqrt{\frac{\Delta_1}{\omega}}\exp\left(-\frac{\omega}{\varepsilon_0}\rho^2\right).$$

In particular, when $\alpha \gg 1$ this means that

$$\Gamma = \frac{\varepsilon_0}{\alpha\xi^2}\sqrt{\frac{\Delta_1}{\omega}}\exp\left(-\frac{\omega}{\varepsilon_0}\alpha\xi^2\right). \tag{26}$$

If $ak_{1\sigma}\rho \gg 1$, the equation (23) results in

$$\Delta_1 = \frac{2|u_0|\alpha^{7/2}\xi^2}{(\alpha+1)^3\rho} = \begin{cases} 2|u_0|\alpha^{7/2}\xi^2, & \alpha \ll 1, \\ \dfrac{2|u_0|}{\alpha\xi}, & \alpha \gg 1. \end{cases} \tag{27}$$

In an extreme case of the δ-potential $a \to 0$, $|u_0| \to \infty$, from (27) this means that

$$\Delta_1 = \frac{\omega|\upsilon_0|}{2\pi\omega_c l^2}.$$

If the parabolic potential is absent ($\omega_0 = 0$), then we get that

$$\Delta_1 = \frac{|\upsilon_0|}{2\pi l^2}$$

is the distance between the Landau level and the magnetoimpurity level split off from it in a two-dimensional electron gas. Here $l = (c/eH)^{1/2}$ is the magnetic length, $(2\pi l^2)^{-1}$ is the degeneracy order of the Landau level. The width of level (27) when $\Delta_1 \ll \omega$ is equal to

$$\Gamma = \frac{\sqrt{\pi}(\alpha+1)^{3/2}\rho\,\Delta_1^2}{\sqrt{\varepsilon_0\omega}}\exp\left(-\frac{\omega}{\varepsilon_0}\rho^2\right) = \begin{cases} \sqrt{\dfrac{\pi}{\varepsilon_0\omega}}\Delta_1^2\exp\left(-\dfrac{\omega}{\varepsilon_0}\right), & \alpha \ll 1, \\ \sqrt{\dfrac{\pi}{\varepsilon_0\omega}}\alpha^{5/2}\xi^2\Delta_1^2\exp\left(-\dfrac{\omega}{\varepsilon_0}\alpha\xi^2\right), & \alpha \gg 1. \end{cases}$$

Let us list numerical values of the functions derived here: Δ_0 (22), u_c (24), Δ_1 (25) and Γ (26) for the parameters $m = 10^{-28}$ g, $|u_0| = 0.2 \times 10^{-12}$ erg, $a = 10^{-7}$ cm, $H = 10^4$ Oe, $\omega_0 = \omega_c$, which are typical for the structures studied above. We have $\Delta_0 = 0.2 \times 10^{-14}$ erg, $u_c = 0.1 \times 10^{-12}$ erg, $\Delta_1 = 0.6 \times 10^{-16}$ erg, $\Gamma = 0.1 \times 10^{-16}$ erg, $\Gamma/\Delta_1 = 0.2$. Thus the local and the resonance levels can be detected for instance in tests aimed at measuring the absorption of electromagnetic radiation in quantum wires at low temperatures in a quantizing magnetic field.

5. Summary and conclusions

The properties of isolated impurity atoms in massive and low dimensional conductors are usually studied by the method of local perturbations or by the zero-range radius potential method [1–4, 23, 26]. Together with these methods in the theory of solid state physics, the Keldysh method [18, 19] is widely used in combination with functional methods of quantum field theory [16, 17]. In particular, this method was used recently to study properties of normal and superconducting metals with randomly distributed impurity atoms [17, 20–22]. In papers [20–22] the impurity scattering of electrons is taken into account within the Born approximation. Meanwhile in two- and one-dimensional structures the impurity donors of arbitrarily small strength are capable of forming local and resonant states of electrons. They will be formed also in massive conductors in the presence of a magnetic field [6, 7, 10, 11]. That is why it is necessary to go beyond the Born approximation and to take these states into account within the framework of the Keldysh formalism. In this paper we have shown that the characteristics of impurity states of electrons in nanostructures in a magnetic field can be evaluated by functional methods. The theory is applied to electrons in quantum wires. The model of quantum wires is the two-dimensional electron gas with a parabolic confinement potential. The impurity atom field is modeled by a Gaussian separable potential. The positions and the widths of local and resonant levels of the energy of electrons caused by the combined effect of donor impurity atoms and a magnetic field are obtained. A functional approach combined with the Keldysh formalism allows us to study the influence of magnetoimpurity states of electrons on kinetic properties of non-equilibrium conductors, taking into account the interaction of electrons among themselves and with other quasi-particles, as well as the influence on weak localization of electrons in a magnetic field.

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