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Broadening of electron states in a quantum dot with a rough boundary in an external magnetic field

L A Falkovsky† and S Klama‡

† L D Landau Institute for Theoretical Physics, Russian Academy of Sciences, Kosygina Street 2, 117 334 Moscow, Russia

‡ Ferromagnetics Laboratory, Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17/19, 60-179 Poznań, Poland

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Abstract. We investigate the influence of the quantum-dot rough boundary on its electronic energy spectrum in an external magnetic field. The case in which roughness amplitude a is small in comparison to the quantum-dot radius R is considered. We show that the ratio of damping edge states to their energy level separation is dependent on binary roughness correlation function and changes in a linear or quadratic way with respect to a/R.

1. Introduction

Recently several papers have been devoted to the calculation of the electronic energy spectrum (EES) of two-dimensional (2D) limited systems in connection with technical applications of quantum-dot (QD) structures (see e.g. Merkt (1990) and references cited therein). One of the frequently investigated models is an electron gas with boundary simulated by a parabolic potential with the characteristic frequency ω_0. Increase in ω_0 corresponds to a decrease in linear dimension of the QD. This model is interesting because one can get simple analytical results even in the presence of a perpendicular magnetic field (Rössler 1990). It is worth noting that the model with parabolic potential has some drawbacks: for instance, there are no edge states and the analysis of its dynamic conductivity in terms of ω_0 meets certain difficulties (Merkt *et al* 1989). In addition to the model with parabolic potential, another one with the 2D region bounded by an infinite potential barrier is studied. As there is no possibility to get an exact analytical result for the latter model with an external magnetic field, one applies numerical methods (Robnik 1986, Lent 1991) or a quasi-classical approach (Klama and Rössler 1992).

The main purpose of this paper is to find out, using the quasi-classical method, how a boundary of form different from a circle affects the EES of the QD.

We shall use a set of random functions to define the deviation of the considered boundary from a circle. A similar approach was applied to the study of the EES in a rough semispace (Falkovsky 1970) and a thin film (Falkovsky and Klama 1987).

2. The basic equations

We consider a bound state of the electron in a circular QD, situated in the xy-plane, with a rough boundary in an external magnetic field $H = (0, 0, H)$. We assume a parabolic

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dispersion law for the electrons and apply the effective-mass approximation. The electron energy spectrum is determined by the poles of the Green function (GF) fulfilling the following equation

$$[\mathcal{H}(\rho) - \epsilon]G(\rho, \rho') = -\delta(\rho - \rho') \qquad \rho \in [0, \infty) \tag{1}$$

where $\rho = (\rho, \varphi)$, $\varphi \in [-\pi, \pi]$. We consider the retarded GF assuming that the variable ϵ has an infinitely small positive imaginary part: $\epsilon \to \epsilon + \mathrm{i}0$. The Hamiltonian of equation (1) has the following form:

$$\mathcal{H}(\rho) = \frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)\right] + \left[\frac{1}{2}\left(\frac{\rho}{l}\right)^2 - 2\left(\frac{l}{\rho}\right)^2\frac{\partial^2}{\partial\varphi^2} - 2\mathrm{i}\frac{\partial}{\partial\varphi}\right]\frac{\hbar\omega}{4} \tag{2}$$

where $l = (\hbar c/eH)^{1/2}$, $\omega = eH/\mu c$.

We will write down the equation of the QD boundary in the form

$$\rho = R + \eta(\varphi) \tag{3}$$

where the amplitude of the random function $\eta(\varphi)$ is assumed to be small in comparison to R. With the postulate that on the boundary (3) there exists an infinite potential barrier, we can write down the boundary condition for $G(\rho, \rho')$ as follows:

$$G(\rho, \rho') = 0 \qquad \text{at} \qquad \rho = R + \eta(\varphi) \text{ or } \rho' = R + \eta(\varphi'). \tag{4}$$

If we assume that the function $G(\rho, \rho')$ as a function of ρ varies slowly at a distance $\rho - R \simeq \eta(\varphi)$, then the boundary condition (4) can be approximated by the truncated series with respect to $\eta(\varphi)$ at $\rho = R$:

$$G(R, \varphi; \rho') + \eta(\varphi)(\partial/\partial R)G(R, \varphi; \rho') = 0. \tag{5}$$

The GF $G(\rho, \rho')$ may be expanded in a double Fourier series with respect to φ and φ':

$$G(\rho, \rho') = \sum_{m,m'=-\infty}^{\infty} G(\rho, m; \rho', m') \exp[\mathrm{i}(m\varphi - m'\varphi')]. \tag{6}$$

We rewrite the boundary condition (5) and equation (1) in terms of the Fourier transforms, getting:

$$G(R, m; \rho', m') + \sum_{m_1=-\infty}^{\infty} \eta(m - m_1)\frac{\partial}{\partial R}G(R, m_1; \rho', m') = 0 \tag{7}$$

and

$$[\mathcal{H}(\rho; m) - \epsilon]G(\rho, m; \rho', m') = -\delta(\rho - \rho') \tag{8}$$

where

$$\mathcal{H}(\rho; m) = -\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)\right] + \left[\frac{1}{2}\left(\frac{\rho}{l}\right)^2 + 2m^2\left(\frac{l}{\rho}\right)^2 + 2m\right]\frac{\hbar\omega}{4}. \tag{9}$$

Let us now introduce the Green function $G_\infty(\rho, \rho')$ defined everywhere in space. This function fulfils equation (1) for $\rho, \rho' \in [0, \infty)$ and depends on $(\varphi - \varphi')$, so it can be expanded in a Fourier series

$$G_\infty(\rho, \rho') = \sum_{m=-\infty}^{\infty} G_\infty(\rho, \rho'; m) \exp[im(\varphi - \varphi')]. \tag{10}$$

The Fourier transform $G_\infty(\rho, \rho'; m)$ fulfils the following equation:

$$[\mathcal{H}(\rho, m) - \epsilon]G_\infty(\rho, \rho'; m) = -\delta(\rho - \rho') \tag{11}$$

for $\rho, \rho' \in [0, \infty)$, $m = 0, \pm 1, \pm 2, \ldots$.

We will look for the solution of the boundary-value problem in the form:

$$G(\rho, \rho') = G_\infty(\rho, \rho') + \int_{-\pi}^{\pi} \frac{d\varphi''}{2\pi} G_\infty(\rho; R, \varphi'')\mu(R, \varphi''; \rho') \tag{12}$$

while equation (8) will be automatically fulfilled for $\rho, \rho' \in [0, R)$ and the function $\mu(R, \varphi''; \rho')$ is determined by the boundary condition (5). The equation (12) in terms of the Fourier transforms has the form:

$$G(\rho, m; \rho', m') = G_\infty(\rho, \rho'; m)\delta_{m,m'} + G_\infty(\rho, R; m)\mu(R, m; \rho', m') \tag{13}$$

where $\delta_{m,m'}$ is the Kronecker symbol.

On insertion of (13) into the boundary condition (7) we get

$$G_\infty(R; \rho' m)\delta_{m,m'} + G_\infty(R, R; m)\mu(R, m; \rho', m') + \eta(m - m')G'_\infty(R, \rho'; m') + \sum_{m_1=-\infty}^{\infty} \eta(m - m_1)G'_\infty(R, R; m_1)\mu(R, m_1; \rho', m') = 0 \tag{14}$$

where

$$G'_\infty(R, \rho'; m) = \lim_{\rho \to R-0} \frac{\partial}{\partial \rho} G_\infty(\rho, \rho'; m). \tag{15}$$

After making the following substitution in (14):

$$\mu(R, m_1; \rho', m') = (\nu(R, m_1; \rho', m') - G'_\infty(R, \rho'; m')\delta_{m',m_1})/G'_\infty(R, R; m) \tag{16}$$

we obtain the following equation for the function $\nu(R, m; \rho', m')$ introduced by way of equation (16)

$$\frac{\nu(R, m; \rho', m')}{\Phi(m)} = \Psi(m)\delta_{m,m'} + \sum_{m_1=-\infty}^{\infty} \eta(m - m_1)\nu(R, m_1; \rho', m') \tag{17}$$

where

$$\begin{aligned} \Phi(m) &= -G'_\infty(R, R; m)/G_\infty(R, R; m) \\ \Psi(m) &= G_\infty(R, \rho'; m) + \Phi^{-1}(m)G'_\infty(R, \rho'; m). \end{aligned} \tag{18}$$

3. The Green function of the circular quantum dot

We solve equation (17) by an iteration method applying the averaging procedure on each step of the iteration (see appendix 1). We consider $\eta(\varphi)$ as a random function and averaging is carried out on products of different numbers of functions $\eta(\varphi)$. In the zeroth-order approximation we get

$$\nu(R, m; \rho', m') = \nu_0(R, \rho'; m)\delta_{m,m'} \qquad \nu_0(R, \rho'; m) = \Phi(m)\Psi(m). \quad (19)$$

On insertion of (19) into (16) and (13) we obtain the GF

$$G(\rho, m; \rho', m') = [G_\infty(\rho, \rho'; m) - G_\infty(\rho, R; m)G_\infty(R, \rho'; m)/G_\infty(R, R; m)]\delta_{m,m'} \quad (20)$$

which fulfils the specular boundary condition

$$G(\rho, \rho'; m) = 0 \qquad \text{at} \qquad \rho(\text{or } \rho') = R. \quad (21)$$

Note that the poles of the first term in square brackets of expression (20) determine the EES of the unbounded space at non-zero magnetic field, i.e. the Landau levels. The poles (zeros of $G_\infty(R, R; m)$) of the second term in the expression (20) determine the EES of the boundary-value problem.

The GF $G_\infty(\rho, \rho'; m)$ can be expressed in terms of two linearly independent particular solutions of the homogeneous equation corresponding to equation (11). We denote these solutions by $R_1(\rho, m)$ and $R_2(\rho, m)$ and assume that: $R_1(\rho, m)$ is regular at $\rho \to 0$ and $R_2(\rho, m)$ is regular at $\rho \to \infty$. The required representation for the Green function has the following form:

$$G_\infty(\rho, \rho'; m) = -\frac{2\mu}{\hbar^2}\frac{1}{W(\rho')}\begin{cases} R_1(\rho; m)R_2(\rho'; m) & \text{for } \rho < \rho' \\ R_1(\rho'; m)R_2(\rho; m) & \text{for } \rho > \rho' \end{cases} \quad (22)$$

where $W(\rho)$ is the Wronskian of the particular solutions R_1 and R_2, which are expressed in terms of Kummer's functions F and U (see Abramowitz and Stegun 1964, ch 13)

$$R_1(\rho; m) = f(\xi)\xi^{(\bar\gamma-\gamma)/2}F(\bar\alpha, \bar\gamma, \xi) \quad (23a)$$

$$R_2(\rho; m) = f(\xi)U(\alpha, \gamma, \xi) \quad (23b)$$

where

$$f(\xi) = \xi^{(\gamma-1)/2}\exp(-\xi/2) \qquad \xi = (\rho/l)^2/2$$
$$\gamma = 1 + m \qquad \bar\gamma = 1 + |m| \qquad \alpha = \gamma/2 - \lambda \qquad \bar\alpha = \bar\gamma/2 - \lambda \quad (24)$$
$$2\lambda = 2\epsilon/\hbar\omega - m.$$

By applying the well known expression for the Wronskian of the functions F and U we obtain the Wronskian of our solutions R_1 and R_2:

$$W(\rho) = -(2/\rho)\Gamma(\bar\gamma)/\Gamma(\bar\alpha) \quad (25)$$

where $\Gamma(x)$ is the Γ function.

For further calculations it is convenient to apply the quasi-classical representation of the solutions R_1 and R_2. With the aim to obtain this representation we write the Schrödinger equation of the considered problem in the form

$$d^2u(\kappa)/d\kappa^2 - \lambda^2 q(\kappa)u(\kappa) = 0 \tag{26}$$

where

$$\begin{aligned} &u(\kappa) = (2\lambda\kappa)^{1/2}R(\rho; m) \\ &q(\kappa) = 1 - 2/\kappa + \kappa_0/\kappa^2 \qquad \kappa = (\rho/r_c)^2/2 \qquad r_c = l(2\lambda)^{1/2} \\ &\kappa_0 = C/\lambda^2 \qquad C = (m^2-1)/4. \end{aligned} \tag{27}$$

Since $q(\kappa) \propto \kappa^{-2}$ at $\kappa \to 0$, the correct function of the quasi-classical approximation can be obtained if in the expression for C we omit the term $(-1/4)$, i.e. we put $C = m^2/4$ for $m \neq 0$ (see e.g. Nikiforov and Uvarov 1984). Making use of the well known rules for matching wavefunctions at the turning points $\kappa_1 = 1 - (1-\kappa_0)^{1/2}$ and $\kappa_2 = 1 + (1-\kappa_0)^{1/2}$ we obtain the following expressions for the functions u_1 and u_2:

$$u_1(\kappa) = \begin{cases} \dfrac{B}{q^{1/4}(\kappa)} \exp\left(-\lambda \displaystyle\int_{\kappa}^{\kappa_1} d\kappa [q(\kappa)]^{1/2}\right) & \text{for } 0 < \kappa < \kappa_1 \qquad (28a) \\ \dfrac{2B}{|q(\kappa)|^{1/4}} \cos\left(\lambda \displaystyle\int_{\kappa_1}^{\kappa} d\kappa [|q(\kappa)|]^{1/2} - \pi/4\right) & \text{for } \kappa_1 < \kappa < \kappa_2 \qquad (28b) \\ \dfrac{B}{q^{1/4}(\kappa)}\Bigg[\exp\left(-\lambda \displaystyle\int_{\kappa_2}^{\kappa} d\kappa [q(\kappa)]^{1/2}\right) \\ \quad \times \sin\left(\lambda \displaystyle\int_{\kappa_1}^{\kappa_2} d\kappa [|q(\kappa)|]^{1/2}\right) \\ \quad +2\exp\left(\lambda \displaystyle\int_{\kappa_2}^{\kappa} d\kappa [q(\kappa)]^{1/2}\right) \\ \quad \times \cos\left(\lambda \displaystyle\int_{\kappa_1}^{\kappa_2} d\kappa [|q(\kappa)|]^{1/2}\right)\Bigg] & \text{for } \kappa > \kappa_2 \qquad (28c) \end{cases}$$

$$u_2(\kappa) = \begin{cases} \dfrac{A}{q^{1/4}(\kappa)} \exp\left(-\lambda \displaystyle\int_{\kappa_2}^{\kappa} d\kappa [q(\kappa)]^{1/2}\right) & \text{for } \kappa > \kappa_2 \qquad (29a) \\ \dfrac{2A}{|q(\kappa)|^{1/4}} \cos\left(\lambda \displaystyle\int_{\kappa_2}^{\kappa} d\kappa [|q(\kappa)|]^{1/2} + \pi/4\right) & \text{for } \kappa_1 < \kappa < \kappa_2 \qquad (29b) \\ \dfrac{A}{q^{1/4}(\kappa)}\Bigg[2\exp\left(\lambda \displaystyle\int_{\kappa}^{\kappa_1} d\kappa [q(\kappa)]^{1/2}\right) \\ \quad \times \cos\left(\lambda \displaystyle\int_{\kappa_1}^{\kappa_2} d\kappa [|q(\kappa)|]^{1/2}\right) \\ \quad +\exp\left(-\lambda \displaystyle\int_{\kappa}^{\kappa_1} d\kappa [q(\kappa)]^{1/2}\right) \\ \quad \times \sin\left(\lambda \displaystyle\int_{\kappa_1}^{\kappa_2} d\kappa [|q(\kappa)|]^{1/2}\right)\Bigg] & \text{for } 0 < \kappa < \kappa_1. \qquad (29c) \end{cases}$$

The expressions (28) and (29) hold under the following condition:

$$(d/d\kappa)\{\kappa[(\kappa-\kappa_1)(\kappa_2-\kappa)]^{-1/2}\} \ll \lambda.$$

We find the coefficients A and B by comparing the expressions (28) and (29) with the already known asymptotic formulae for Kummer's functions F and U at large values of their arguments:

$$\begin{aligned} A &= \exp[-\lambda(1-\ln\lambda)] \\ B &= (|m|!/2\pi)\Gamma(1-\bar{\alpha})\exp[\lambda(1-\ln\lambda)]. \end{aligned} \tag{30}$$

In the quasi-classical expressions (28*c*) and (29*c*) there exist not only large terms but also small ones. Leaving them there makes sense only when the coefficients of the large terms disappear, i.e. at

$$\lambda \int_{\kappa_1}^{\kappa_2} \mathrm{d}\kappa[|q(\kappa)|]^{1/2} = \pi(N+1/2) \qquad N = 0, 1, 2, \ldots. \tag{31}$$

In such a case we have to put in the small terms $(-1)^N$ instead of

$$\sin\left(\lambda \int_{\kappa_1}^{\kappa_2} \mathrm{d}\kappa[|q(\kappa)|]^{1/2}\right). \tag{32}$$

The case of $m = 0$ has to be considered separately. In such a case there is only one turning point $\kappa_2 = 2$ ($\kappa_0 = 0$). Let us start with the wavefunction $u_2(\kappa)$. The range (29*c*) does not exist and at $\kappa > \kappa_2$ the expression (29*a*) is used. In the range of the small ξ values and large negative α values (see (23) and (24)) an asymptotic representation of Kummer's function U (see Abramowitz and Stegun 1964) defining the function u_2 is known (see (27) and (23*b*)):

$$\begin{aligned} U(1/2-\lambda, 1, \xi) \simeq \Gamma(\lambda+1/2)\mathrm{e}^{\xi/2}\{&\cos[\pi(\lambda-1/2)]J_0(2(\lambda\xi)^{1/2}) \\ &+ \sin[\pi(\lambda-1/2)]Y_0(2(\lambda\xi)^{1/2})\} \end{aligned} \tag{33}$$

where J_0, Y_0 are Bessel functions. The condition for the applicability of the quasi-classical approximation (29*b*) in the range of small κ

$$2\lambda(2\kappa)^{1/2} \gg 1 \tag{34}$$

means that the argument of the Bessel functions occurring in (33) is large. It comes out from the expression (23*b*) that in this range the representations (33) and (29*b*) match with each other and the formula (29*b*) is applicable in the interval $1/8\lambda^2 \ll \kappa < \kappa_2$. If $\kappa < 1/8\lambda^2$ the quasi-classical approximation (29*b*) is inapplicable and the behaviour of the wavefunction (27) with $R(\rho; m) = R_2(\rho; m)$ (see (23*b*)) is determined by the expansion of the Bessel functions occurring in (33) in a series with respect to the small values of the argument. In this range the function Y_0 has a logarithmically increasing asymptotic representation. Disappearance of the term with Y_0 is prevented by the vanishing of the coefficient in front of Y_0 in expression (33). The condition $\lambda - 1/2 = N$ determines the Landau levels in the unbounded 2D space.

For the function $u_1(\kappa)$ at $m = 0$, the interval $\kappa > \kappa_2$ remains (see (28*c*)), and the interval $0 < \kappa < \kappa_1$ (see (28*a*)) disappears. For all that in the expressions (28*b*, *c*) we may put $\kappa_1 = 0$, since in the quasi-classical approximation the leading contribution to the integral occurring in the arguments of the sine and cosine functions comes from the range described by (34). The expression (28*b*) is applicable (at $m = 0$) in the interval $1/8\lambda^2 \ll \kappa < \kappa_2$.

For the small $\kappa(\kappa < 1/8\lambda^2)$ we can use the well known asymptotic representation (see e.g. Abramowitz and Stegun 1964)

$$F(\alpha, 1, \xi) \simeq e^{\xi/2} J_0(2(\lambda\xi)^{1/2})$$

which goes over into expression (28*b*) in the quasi-classical range (34) and gives a bounded solution in the interval $0 < \kappa < 1/8\lambda^2$. The coefficients A and B maintain their form (30) also for $m = 0$.

As already mentioned, the EES of the QD is determined by the poles of the second term in equation (20), i.e. by equation $G_\infty(R, R; m) = 0$. The latter in the quasi-classical approximation leads us, with (22), (27) and (28), (29) taken into account, to the QD EES for arbitrary values of the parameters of the system. The form of the functions u_1 and u_2 (cf (28), (29)) enables us to perform this task separately for each range of κ_R values. In the range $\kappa_R < \kappa_1$ the energy levels do not exist. At $\kappa_R > \kappa_2$ confinement does not play an essential role and the energy spectrum of the corresponding electronic states is of Landau type. The energy spectrum of these states is calculated on applying (28*c*). We arrive at the condition $u_1(\kappa_R) = 0$, leading to

$$\epsilon \simeq [N + (|m| + m + 1)/2]\hbar\omega + (\hbar\omega/2\pi)e^{-2J(\lambda)} \tag{35}$$

where

$$J(\lambda) = \lambda \int_{\kappa_2}^{\kappa_R} d\kappa [q(\kappa)]^{1/2}. \tag{36}$$

The integral in (36) should be calculated at a value of the variable ϵ which is determined by the first term of the RHS of expression (35). It is clear that the last term of the RHS of (35) accounts for the influence of the QD boundary on the Landau levels. The condition $\kappa_R > \kappa_2$ means that the QD radius is sufficiently large, i.e.

$$R > \sqrt{2}l\{1 + m + 2N + [(2N + 1)(2N + 2m + 1)]^{1/2}\}^{1/2}.$$

If the condition

$$R \gg 2l\{2N + m/2 + [N(N + m)]^{1/2}\}^{1/2} \tag{36a}$$

is fulfilled, then $J(\lambda) = \lambda\kappa_R = (R/2l)^2$.

In the interval $\kappa_1 < \kappa_R < \kappa_2$ there appear edge states (arising due to interaction of an electron with the QD boundary). On applying (22) and (28) we obtain the following equation for the spectrum of the edge states in the quasi-classical approximation

$$\lambda \int_{\kappa_1}^{\kappa_R} d\kappa [|q(\kappa)|]^{1/2} = \pi(N + 3/4). \tag{37}$$

After performing the integration in (37) we arrive at the expression describing the spectrum of the edge states:

$$\lambda \left[\frac{\pi}{2}(1 - \kappa_0^{1/2}) + (2\kappa_R - \kappa_R^2 - \kappa_0)^{1/2} + \sin^{-1}\left(\frac{\kappa_R - 1}{(1 - \kappa_0)^{1/2}}\right) - \kappa_0^{1/2} \sin^{-1}\left(\frac{\kappa_R - \kappa_0}{\kappa_R(1 - \kappa_0)^{1/2}}\right)\right] = \pi(N + 3/4) \tag{38}$$

$$\kappa_0 = C/\lambda^2 = m^2/4\lambda^2 \qquad \kappa_R = (R/r_c)^2/2 \qquad r_c = l(2\lambda)^{1/2}. \tag{39}$$

In general, the transcendental equation (38) can be treated numerically. Its analytical solution can be found in the particular case $\kappa_0 \ll \kappa_R \ll 1$ and $\kappa_0 \ll 1$. In this case the power series expansion of the LHS of equation (38) leads to

$$\lambda[2(2\kappa_R)^{1/2} - \pi\kappa_0^{1/2}]$$

and we obtain

$$\epsilon = (N + \tfrac{1}{2}|m| + \tfrac{3}{4})^2\hbar\omega_R + \tfrac{1}{2}m\hbar\omega \qquad \omega_R = \pi^2\hbar/(2\mu R^2). \tag{40}$$

The requirements imposed on κ_0 and κ_R determine the conditions of the applicability of the expression (40): $N \gg |m|$, $R \ll Nl$. It follows that the formula (40) holds in the weak magnetic field region.

4. The influence of the quantum-dot boundary roughness on broadening of the electron states

Let us consider the influence of the QD boundary roughness on the behaviour of EES. In the model under consideration reflections of the electron occur at a rough QD boundary. The time averaging of the electron motion will be replaced by averaging over an ensemble of random rough boundaries of the QD of equal mean radii R (for details, see Ziman (1970), section 3.2). We admit that a rough QD boundary is described by a random function $\eta(\varphi)$ (cf (3)). A further assumption says that the ensemble of random functions is normal. It follows that this ensemble is made entirely precise by fixing the mean value of η (assumed to be zero since the radius R of the QD (see (4)) can be defined by the condition $\langle\eta(\varphi)\rangle = 0$) and the binary correlation function. Hence the mean value of the product of an even number of functions η falls into a sum of products of binary correlation functions (see appendix 1). The binary correlation function in (ρ, φ) space depends only on the difference $(\varphi - \varphi')$, i.e.

$$\langle\eta(\varphi)\eta(\varphi')\rangle = \eta_2(\varphi - \varphi'). \tag{41}$$

The Fourier transform of the binary correlation function has the form

$$\langle\eta(m)\eta(m')\rangle = \eta_2(m)\delta_{m,-m'} \tag{42}$$

$$\eta_2(m) = \int_{-\pi}^{\pi} \frac{d\varphi}{2\pi}\eta_2(\varphi)e^{-im\varphi}. \tag{43}$$

Averaging the Green function over the ensemble $\{\eta(\varphi)\}$ reduces to averaging of the function ν occurring in (17). The latter leads with the help of (16) to the desired averaged Green function. On performing the averaging procedure described in appendices 1 and 2 we get

$$\langle\nu(R, m; \rho', m')\rangle = \nu(R, \rho'; m)\delta_{m,m'} \tag{44}$$

$$\nu(R, \rho'; m) = \nu_0(R, \rho'; m) + \nu(R, \rho'; m)\Phi(m)\sum_{m_1=-\infty}^{\infty} \frac{\nu(R, \rho'; m_1)}{\Psi(m_1)}\eta_2(m - m_1). \tag{45}$$

The solution of equation (45) has the form

$$\nu(R, \rho'; m)/\Psi(m) = 1/[\Phi^{-1}(m) - \Sigma(m)] \tag{46}$$

where the self-energy part $\Sigma(m)$ fulfils the equation:

$$\Sigma(m) = \sum_{m'=-\infty}^{\infty} \frac{\eta_2(m-m')}{\Phi^{-1}(m') - \Sigma(m')}. \tag{47}$$

By means of the expressions (13), (16) and (46) we obtain the averaged Green function

$$\langle G(\rho, m; \rho', m') \rangle = G(\rho, \rho'; m)\delta_{m,m'} \tag{48}$$

where

$$G(\rho, \rho'; m) = G_\infty(\rho, \rho'; m) - G_\infty(\rho, R; m)G_\infty(R, \rho'; m)/(G_\infty(R, R; m) + G'_\infty(R, R; m)\Sigma(m)). \tag{49}$$

Equation (49) differs from (20) by the presence of a term with a self-energetic part in the denominator. The term proportional to $\Sigma(m)$ in the numerator of equation (49) was neglected. We based on the expansion (5), hence the contribution to (49) connected with $\Sigma(m)$ has been taken as small. This contribution has been retained in the denominator of (49) since the first term in the denominator can vanish. The zeros of the denominator of the RHS of expression (49) determine the EES of the QD in the presence of a rough boundary:

$$\epsilon = \epsilon_N(R; m) - i\Gamma(R; m) \tag{50}$$

where the energy level width $\Gamma(R; m) \propto \Sigma(m)$, and $\epsilon_N(R; m)$ describes the EES if $\Sigma(m) = 0$, i.e. in the case of an ideal QD boundary.

By means of (22) the equation describing EES can be written in the form

$$R_1(R; m) + [\partial R_1(R; m)/\partial R]\Sigma(m) = 0. \tag{51}$$

The function $R_1(R; m)$ in equation (51) depends also on the energy variable ϵ. Since $\Sigma(m)$ is considered as a small quantity one can expand, in (51), $R_1(R; m)$ in a power series in $(\epsilon - \epsilon_N(R; m))$. In $R_1(R; m)$ only the linear term is left and in the second term in (51) the zeroth-order term only. The value $\Phi^{-1}(m') = 0$ should be taken in the denominator of (47) in this approximation. The solution of (47) depends on how rapidly η_2 varies as a function of $(m - m')$. If η_2 decreases rapidly and only one term can be left in the sum over m', then

$$\Sigma(m) = i[\eta_2(m = 0)]^{1/2}. \tag{52}$$

If η_2 is a slowly varying function of $(m - m')$, i.e. if the number of terms in the sum in the RHS of (47) is large, then the summation over m' in (47) can be replaced by integration, and (47) takes the form

$$\Sigma(m) = i\pi \int_{-\infty}^{\infty} dm'\, \eta_2(m - m')\delta(\Phi^{-1}(m')) = i\pi \sum_{m'=-\infty}^{\infty} \eta_2(m - m') \left(\frac{\partial \Phi^{-1}(m')}{\partial m'}\right)^{-1}. \tag{53}$$

For qualitative estimation of the influence of the QD boundary roughness on its EES $\Gamma(R; m)$ (see (50)) should be compared with the separation between the nearest energy levels of the EES. In the case of weak magnetic field (see (40)) this separation is equal to

$$d\epsilon/dN = 2(N + |m|/2 + \tfrac{3}{4})\hbar\omega_R \tag{54}$$

and for the Landau spectrum this separation is equal to $\hbar\omega$. On the basis of equation (51) we obtain the broadening of the energy levels:

$$i\Gamma(R;m) = \left[\left(\frac{\partial R_1(R;m)}{\partial R}\right) \Big/ \left(\frac{\partial R_1(R;m)}{\partial \epsilon}\right)\right]_{\epsilon=\epsilon_N} \Sigma(m). \tag{55}$$

For a weak magnetic field we obtain

$$i\Gamma(R;m) = (2/R)\epsilon_N(H=0)\Sigma(m) = (2/R)(N+|m|/2+\tfrac{3}{4})^2\hbar\omega_R\Sigma(m) \tag{56}$$

and the ratio of the $i\Gamma(R;m)$ and the level separation (54) amounts to

$$(1/R)(N+|m|/2+\tfrac{3}{4})\Sigma(m). \tag{57}$$

For $\Sigma(m)$ the formula (52) or (53) should be taken. In the considered case the formula (53) has the form

$$\Sigma(m) = \frac{2i}{R}\sum_{m'=-\infty}^{\infty} \eta_2(m-m')(N+|m'|/2+\tfrac{3}{4}). \tag{58}$$

The effect of the QD boundary roughness on Landau-type levels is described by (55) where the derivatives should be calculated with the help of (28*c*). With the condition (36*a*) fulfilled we find

$$i\Gamma(R;m) = (\hbar\omega R/2\pi l^2)\exp(-R^2/2l^2)\Sigma(m) \tag{59}$$

where $\Sigma(m)$ is given by expressions (52) and (53). The latter expression takes the form

$$\Sigma(m) = \frac{iR}{2l^2}\exp\left(-\frac{R^2}{2l^2}\right)\sum_{m'=0}^{\infty}\eta_2(m-m'). \tag{60}$$

Physically realistic models of a non-ideal surface as well as the QD boundary as discussed in this paper call for further theoretical analysis (cf Ziman 1979) and experiments aimed at reaching information on energy level widths. The rough boundary of the QD under consideration has been described making use of the random homogeneous field defined at the circular boundary. The binary correlation function of this random field depends on the angular distance φ (see (41)) of points at the circular boundary: in general $\eta_2(\varphi) = \eta_2(\cos\varphi)$ (Koroluk *et al* 1985).

Let us consider a simple example. The roughness of the QD boundary can be characterized by the roughness amplitude a ($a^2 = \langle\eta^2(\varphi=0)\rangle$) and the correlation length φ_0; the latter represents the angular distance over which the function $\eta_2(\varphi)$ varies significantly. Let us assume that

$$\eta_2(\varphi) = a^2\cos^2(\varphi/2)\exp[-\sin^2(\varphi/2)/\varphi_0]. \tag{61}$$

The Fourier transform (see (43)) of this correlation function has the form

$$\eta_2(m) = \tfrac{1}{2}a^2\mathcal{P}(\tau;m) \qquad \mathcal{P}(m;\tau) = [I_m(\tau) + (d/d\tau)I_m(\tau)]e^{-\tau} \tag{62}$$

where $\tau = 1/2\varphi_0$ and $I_m(\tau)$ is the modified Bessel function. Now, for the model defined by (61) we shall give the expressions for $\Sigma(m)$ for rapidly (see (52)) and slowly (see (53)) varying η_2 as a function of $(m - m')$. On substituting (62) into (52) we obtain

$$\Sigma(m) = (ia/\sqrt{2})[I_0(\tau) + I_1(\tau)]^{1/2} \exp(-\tau/2) \tag{52a}$$

that is

$$\Sigma(m) \simeq ia(\varphi_0/\pi)^{1/4} \qquad \text{for } \varphi_0 \ll 1. \tag{52b}$$

A further substitution of (62) into (58) leads to

$$\Sigma(m) \simeq (ia^2/R)[2N + |m| + \tfrac{3}{2} - (N + \tfrac{3}{4})\mathcal{P}(m, \tau)]. \tag{58a}$$

The broadening of the Landau-type levels is described by (59) with $\Sigma(m)$ given by (52*a*) for the case of η_2 representing a rapidly varying function of $(m - m')$. For the case of slowly varying η_2 as a function of $(m - m')$ by substituting (62) into (60) we obtain

$$\Sigma(m) = \frac{iRa^2}{4l^2} \exp\left(-\frac{R^2}{2l^2}\right) \times \begin{cases} 1 + \displaystyle\sum_{k=1}^{m} \mathcal{P}(k;\tau) & \text{for } m > 0 \\ 1 & \text{for } m = 0 \\ 1 - \displaystyle\sum_{k=0}^{|m|-1} \mathcal{P}(k;\tau) & \text{for } m < 0. \end{cases} \tag{60a}$$

Let us note that only in the latter case does the level width depend on the sign of m.

The expressions (52*a*), (58*a*) and (60*a*) with (56) and (58) taken into account define the electron energy level widths in all the above cases for the model of a rough QD boundary with the correlation function (61).

5. Conclusions

Within the considered approximation the roughness, i.e. the amplitude a of the function η, is assumed to be small compared with the QD radius R.

We arrived at a remarkably simple result: damping of the edge states referred to separations of their levels decreases linearly (see (56) and (52)) or quadratically (see (56) and (58)) in a/R. It means that edge states in a QD do not exist if the linear dimension of the QD is comparable with the roughness amplitude. On the other hand at large roughness and strong magnetic field, i.e. if the magnetic length l is small in comparison with the QD diameter and roughness amplitude, the levels can be observed. In this case only a thin layer (of thickness l) of the cyclotron trajectories at the QD boundary is influenced by roughness, which leads to broadening of the levels corresponding to these trajectories (see (59)).

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Appendix 1

The mixed moment of the nth order of the random variables $\eta(\varphi_1), \ldots, \eta(\varphi_n)$ is determined using the characteristic function $f_n(v_1, \varphi_1; \ldots; v_n, \varphi_n)$ of the n-dimensional probability density function

$$\langle \eta(\varphi_1) \ldots \eta(\varphi_n) \rangle = \mathrm{i}^n \left[\frac{\partial^n}{\partial v_1 \ldots \partial v_n} f_n(v_1, \varphi_1; \ldots; v_n, \varphi_n) \right]. \tag{A1.1}$$

For an n-dimensional random variable distributed according to the normal law the characteristic function (at $\langle \eta(\varphi) \rangle = 0$) has the following well known form (see e.g. Gnedenko 1969)

$$f_n(v_1, \varphi_1; \ldots; v_n, \varphi_n) = \exp\left(-\tfrac{1}{2} \sum_{i,k=1}^{n} \eta_2(\varphi_i - \varphi_k) v_i v_k \right). \tag{A1.2}$$

Therefore the task of averaging the consecutive terms in the series (A2.3) (cf appendix 2) should be performed as follows: each term should first have created its corresponding characteristic function (A1.2) and then be averaged using (A1.1). It means an averaging at each step of the iteration. Of course, to make use of (A1.1) and (A1.2) one should first Fourier transform the series (A2.3).

Appendix 2

The averaged Green function (13) will be calculated by a method similar to that developed in the theory of metals with a random distribution of impurities (Edwards 1958, Abrikosov *et al* 1965). In our case the averaging of the Green function reduces to averaging of the function ν given by (17).

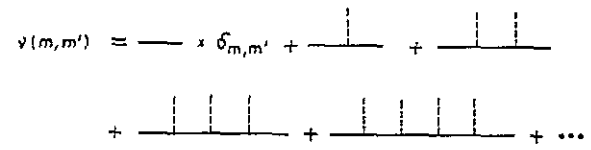
Let us introduce the following notation (cf (18), (19)):

$$\nu(R, m; \rho', m') = \nu(m, m') \qquad \Phi(m)\Psi(m) = \nu_0(m). \tag{A2.1}$$

Equation (17) can be rewritten as

$$\nu(m, m') = \nu_0(m)\delta_{m,m'} + \nu_0(m) \sum_{m_1} \frac{\eta(m - m_1)}{\Psi(m)} \nu(m_1, m'). \tag{A2.2}$$

An iteration procedure leads to the following form of (A2.2) as an infinite series:



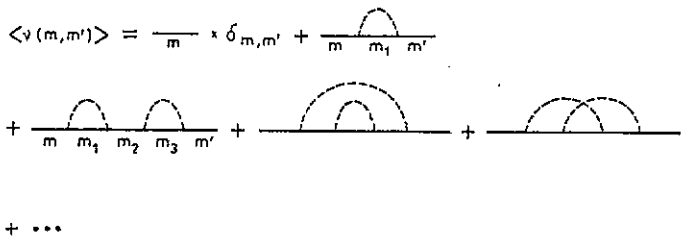
(A2.3)

The full lines in (A2.3) correspond to $\nu_0(m_i)$ ($m_i = m, m_1, \ldots, m'$) and broken lines correspond to the following factor

$$\eta(m_i^{(b)} - m_{i+1}^{(b)}) / \Psi(m_i^{(b)}) \tag{A2.4}$$

where $m_i^{(b)}$ $(= m, m_1, \ldots, m_k < m')$ labels the line (from left to right) going from the left into that vertex at the beginning of the ith broken line. Each term in the series (A2.3) is summed (from $-\infty$ to $+\infty$) over indices of the internal full lines. There is no summation over the free full lines with indices m and m'.

Let us now assume that the random variables entering the series (A2.3) have a normal distribution. Hence the mean values of the products of odd numbers of η factors vanish (cf section 4); however, the even-order moments are expressed in terms of the second moments. Each moment of order $2n$ falls into $(2n-1)!!$ terms, which in turn contain n factors (binary correlation functions) each. On taking the average of the series (A2.3) (cf appendix 1) we obtain



(A2.5)

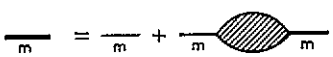
where the sum of terms with moments of the second and fourth order is explicitly shown. In (A2.5) to the mth full line there corresponds $\nu_0(m)$, and to the jth broken line there corresponds the factor

$$K_j = \frac{\eta_2(m_j^{(b)} - m_{j+1}^{(b)})}{\Psi(m_j^{(b)})\Psi(m_j^{(e)})}\delta(m_j^{(b)} - m_{j+1}^{(b)}, m_{j+1}^{(e)} - m_j^{(e)}). \tag{A2.6}$$

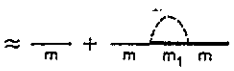
Here δ is the Kronecker symbol. By $m_j^{(b)}$ $(= m, m_1, \ldots, m_k < m')$ is denoted the index of the full line going into the vertex with outgoing jth broken line; by $m_j^{(e)}$ $(= m_1, \ldots, m_k < m')$ is denoted the index of the full line going into that vertex where the jth broken line ends. In each term in the series (A2.5) there is performed summation over the indices of the internal full lines of the diagram. On writing (A2.6) we have profited from (42). For any diagram in (A2.5) with $j \geqslant 1$ broken lines we shall write the following expression:

$$\nu_0(m)\nu_0(m')\sum_{m_1}\nu_0(m_1)\ldots\sum_{m_k}\nu_0(m_k)\prod_j K_j. \tag{A2.7}$$

It is a straightforward task to sum up the reducible diagrams and we arrive at the Dyson-type equation with the self-energy part given by the sum of irreducible diagrams:



(A2.8)



(A2.9)

where the bold line corresponds to $\nu(m)$. The approximate equation (A2.9) corresponds to the (45) in the text. It has been obtained after neglecting the contribution to the self-energy part of the irreducible diagrams with crossing broken lines which do not transform into diagrams with both free full lines after exclusion of one broken line. Such an approximation holds provided that $(2\mu\epsilon)^{1/2}|\Sigma(m)| \ll \hbar$. Also, with the latter inequality fulfilled, the perturbation method is applicable to the problem considered.

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