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DENSITY OF STATES FOR BALLISTIC ELECTRONS IN ELECTRIC AND MAGNETIC FIELDS

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The density of states for ballistic electrons in the presence of an electric field of almost arbitrary shape is calculated for one, two, and three dimensions using the semiclassical quantization in a finite sample. The semiclassical results are compared with these of the complete quantum treatment for a constant electric field. The case of crossed electric and magnetic fields is also considered and it is demonstrated that in this configuration the density of states exhibits a transition between magnetic and electric types of motion. Implications of this transition for the quantum Hall effect are mentioned.

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Density of states (DOS) in the energy space is a fundamental property of electrons in external fields. In particular, DOS characterizes dimensionality of the system. More specifically, DOS for two-dimensional (2D) structures in the presence of a magnetic field has been discussed in great detail in relation to the quantum Hall effect [1, 2]. With the advancement of modern technologies it has become possible to fabricate samples whose dimensions are smaller than the electron mean free path between scattering events. Such ballistic systems have special properties, which has been demonstrated both theoretically and experimentally [3, 4].

In the theoretical work on DOS the attention has been focused on potential wells, while non-confining potentials have not attracted much interest. In the theory of transport phenomena the electric field has been usually treated as a perturbation causing transitions between quantum states, but it has been neglected in the description of these states. The purpose of our presentation is to fill these gaps. The main idea behind our approach to non-confining electric fields is to consider finite sample dimensions, which are then taken to be very large. Our description is valid for ballistic electrons in solids as well as in vacuum [5].

We consider first an electron of the mass m in an external field F [described by a monotonic potential $V(y)$] and confined by two infinite barriers at $y = 0$ and $y = a$. We take $V(0) = 0$ and $V(a) = U$, cf. Fig. 1. The semiclassical (WKB) quantization condition for the energies $\varepsilon(n)$ is

$$\sqrt{2m^*}\int_0^{y_n}[\varepsilon(n) - V(y)]^{1/2}\mathrm{d}y = \hbar\pi(n+\gamma), \tag{1}$$

where $n = 0, 1, 2, \ldots$ The turning point y_n and the phase γ are given by $V(y_n) = \varepsilon(n)$ and $\gamma = 3/4$ for $\varepsilon(n) < U$, while $y_n = a$ and $\gamma = 1$ for $\varepsilon(n) \geq U$. In the following we will be interested in large values of a and $U =$ const. In this limit the energy $\varepsilon(n)$ becomes a quasicontinuous function of n and the semiclassical approximation (1) is known to give almost exact results.

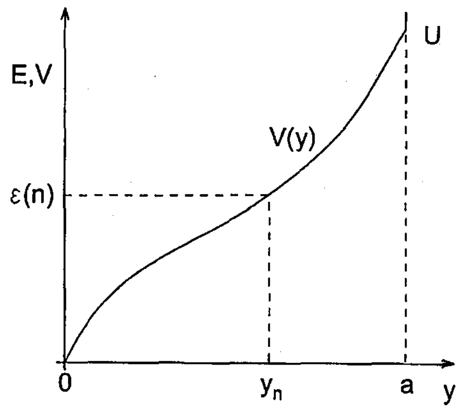

Fig. 1. Electric potential, two infinite barriers, and classical turning points, as used for the semiclassical energy quantization.

DOS in the energy space E is given, in general, as

$$\rho(E) = (2/Vol)\mathrm{Tr}\delta(E - \widehat{H}), \tag{2}$$

where the factor 2 accounts for the spin degeneracy, Vol is the volume of the system, $\widehat{H}$ is the Hamiltonian and δ is the Dirac delta function. For a one-dimensional (1D) system in the quasi-continuous limit of energies the formula (2) gives

$$\rho_{1\mathrm{D}}(E) = \frac{2}{a}\int_0^{\infty}\delta[E - \varepsilon(n)]\mathrm{d}n = \frac{2}{a}\frac{\mathrm{d}n}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon(n)=E}. \tag{3}$$

The derivative $\mathrm{d}n/\mathrm{d}\varepsilon$ can be calculated from Eq. (1). The final result is (cf. Appendix)

$$\rho_{1\mathrm{D}}(E) = \frac{\sqrt{2m^*}}{\pi\hbar a}\int_0^{y_0}[E - V(y)]^{-1/2}\mathrm{d}y. \tag{4}$$

For $E < U$ the value of y_0 is to be determined from the condition $V(y_0) = E$, while for $E \geq U$ there is $y_0 = a$, cf. Fig. 1. Formula (4) can be used to calculate DOS once the potential $V(y)$ is specified. For a constant electric field we take $V(y) = (U/a)y$ and Eq. (4) gives

$$\rho_{1\mathrm{D}}(E) = \frac{\sqrt{8m^*}}{\pi\hbar U}[E^{1/2} - (E-U)^{1/2}], \tag{5}$$

where the second term contributes only for $E \geq U$. For a vanishing electric field one has $U \to 0$. In this limit Eq. (6) leads to the derivative with respect to U and one gets the well known result for the free electron: $\rho_{1\mathrm{D}} \sim E^{-1/2}$.

In case of two dimensions the energy is $\varepsilon(n, k_x) = \varepsilon(n) + \hbar^2 k_x^2/2m^*$ and the trace in Eq. (2) involves an integration over k_x. After some manipulation we obtain for $E < U$

$$\rho_{2\mathrm{D}}(E) = \frac{m^*}{\pi\hbar^2}\frac{y_0(E)}{a}, \tag{6}$$

in which y_0 is to be determined from $V(y_0) = E$. For $E \geq U$ we calculate

$$\rho_{2\mathrm{D}}(E) = \frac{m^*}{\pi\hbar^2}, \tag{7}$$

independently of the form of $V(y)$. For a constant electric field Eq. (6) gives $\rho_{2\mathrm{D}} \sim E$. For a vanishing electric field $U \to 0$ and Eq. (7) gives the well known expression for a 2D subband.

For three dimensions the electron energy is $\varepsilon(n, k_x, k_z) = \varepsilon(n) + \hbar^2(k_x^2 + k_z^2)/2m^*$, and the formula (2) involves integrations over k_x and k_z. Performing the latter and using Eq. (1), we obtain

$$\rho_{3\mathrm{D}}(E) = \frac{1}{2\pi^2 a}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^{y_0}[E - V(y)]^{1/2}\mathrm{d}y, \tag{8}$$

where y_0 is to be determined from $V(y_0) = E$ for $E < U$, and $y_0 = a$ for $E \geq U$. Formula (8) describes DOS for the electron in 3D space accelerated by an electric field of almost arbitrary shape. For a constant electric field, i.e. $V(y) = (U/a)y$, one gets

$$\rho_{3\mathrm{D}}(E) = \left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{1}{3\pi^2 U}[E^{3/2} - (E - U)^{3/2}], \tag{9}$$

where the second term contributes for $E \geq U$. The DOS given by Eq. (9) for different electric field intensities is illustrated in Fig. 2. The main effect of the field is to transfer DOS from small to high energies as a result of electron acceleration. For vanishing electric field one has $U \to 0$. In this limit Eq. (11) leads to the well known result: $\rho_{3\mathrm{D}} \sim E^{1/2}$. As can be seen from Eqs. (5) and (9), DOS for constant electric field depends only on the total voltage drop across the sample: $U = eFa$. Formulas (5), (6), and (9) are only approximative for energies E very near zero since in this limit they neglect the discrete character of energies in the triangular potential well.

Now we want to compare the above semiclassical results for DOS with an exact quantum calculation for an electron in a constant electric field. The Schrödinger equation reads (1D case)

$$\left(\frac{p_y^2}{2m^*} + eFy\right)\Psi = E\Psi. \tag{10}$$

By changing the variable one reduces the problem to the Airy equation. The solutions are [6]: $\Psi = C\mathrm{Ai}[(eFy - E)/eFl]$, where the electric length is $l = (\hbar^2/2m^* eF)^{1/3}$. The spectrum is continuous, so that the solutions must be normalized to the Dirac delta function. This gives $C = (4m^{*2}/eF\hbar^4)^{1/6}$.

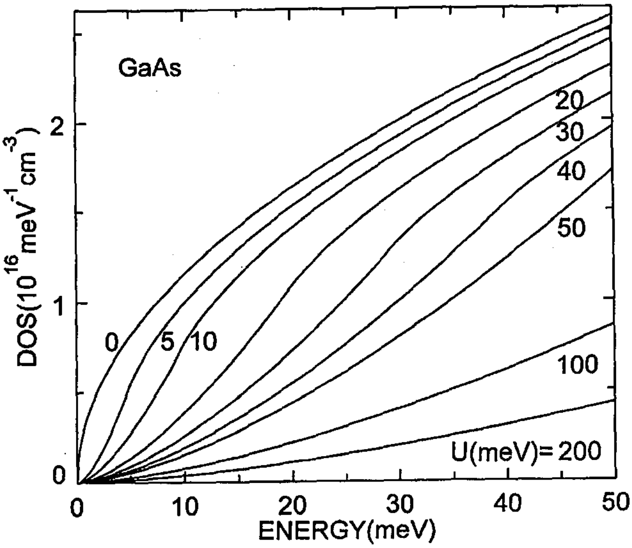

Fig. 2. Density of states for a 3D electron in a constant electric field F, calculated for various values of $U = eFa$ (the effective mass $m = 0.067m_0$ was used).

We now define the local DOS (cf. Davies [7])

$$n(E,y) = \sum_{\alpha} |\Psi_\alpha(r)|^2 \delta(E - E_\alpha), \tag{11}$$

where the summation is over all quantum numbers. For 1D case the integration over E' gives

$$n(E,y) = \frac{2}{\hbar}\left(\frac{2m^*}{E_0}\right)^{1/2} \mathrm{Ai}^2\left(\frac{eFy - E}{E_0}\right), \tag{12}$$

where $E_0 = eFl$. For 2D case the energy contains the term $\hbar^2 k_x^2/2m^*$ and the formula (11) involves also the integration over k_x. The result is

$$n(E,y) = \left(\frac{2m^*}{\pi\hbar^2}\right) \int_0^\infty t^{-1/2} \mathrm{Ai}^2(t + c)\mathrm{d}t, \tag{13}$$

where $c = (eFy - E)/E_0$. The above integral is given in the Appendix. For 3D case one has to integrate over k_x, k_z, and E'. This gives

$$n(E,y) = \frac{\sqrt{2m^{*3}E_0}}{\pi\hbar^3}[\mathrm{Ai}'^2(c) - c\mathrm{Ai}^2(c)], \tag{14}$$

where Ai$'$ is the derivative of the Airy function [8, 9].

The local DOS for 3D case is illustrated in Fig. 3. It is compared to the DOS for the free electrons: $\rho(E) \sim E^{1/2}$. The exponential tail of DOS for $E < 0$ (in the classically forbidden region) is responsible for the Franz–Keldysh effect, i.e. the optical interband absorption for photon energies below the direct gap due to the presence of an electric field. This effect is also known as the photon-assisted tunneling.

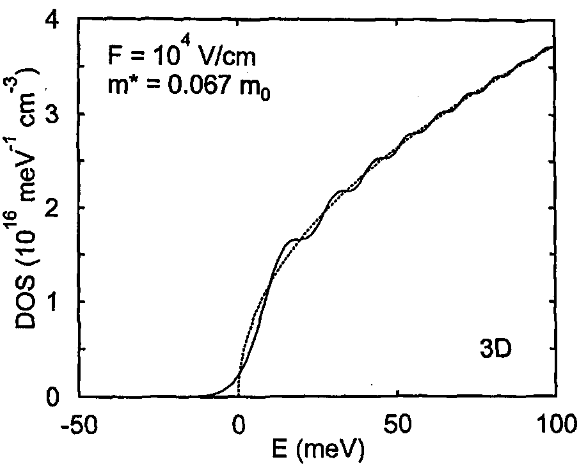

Fig. 3. The local 3D density of states for electrons in a constant electric field as a function of local kinetic energy $E-eFy$. The dotted line indicates DOS for free electrons.

The total DOS is calculated taking an average over the sample having the macroscopic length a,

$$\rho(E) = \frac{1}{a}\int_0^a n(E,y)\mathrm{d}y. \tag{15}$$

For 1D one calculates from Eq. (12)

$$\rho_{1\mathrm{D}}(E) = \frac{2\sqrt{2m^*E_0}}{\hbar U}\left[F_1\left(\frac{U-E}{E_0}\right) - F_1\left(\frac{-E}{E_0}\right)\right], \tag{16}$$

where $U = eFa$, and

$$F_1(t) = t\mathrm{Ai}^2(t) - \mathrm{Ai}'^2(t). \tag{17}$$

For 2D one obtains from Eq. (13) after some manipulations

$$\rho_{2\mathrm{D}}(E) = \frac{4m^*E_0}{\pi\hbar^2 U}\int_0^\infty t^{1/2}\left[\mathrm{Ai}^2\left(t-\frac{E}{E_0}\right) - \mathrm{Ai}^2\left(t+\frac{U-E}{E_0}\right)\right]\mathrm{d}t. \tag{18}$$

The integral appearing in the above formula is given in Appendix.

For 3D one calculates from Eq. (14)

$$\rho_{3\mathrm{D}}(E) = \frac{2m^{*3}E_0^3}{\pi\hbar^3 U}\left[F_3\left(\frac{U-E}{E_0}\right) - F_3\left(\frac{-E}{E_0}\right)\right], \tag{19}$$

where

$$F_3(t) = \frac{1}{3}[\mathrm{Ai}(t)\mathrm{Ai}'(t) + 2t\mathrm{Ai}'^2(t) - 2t^2\mathrm{Ai}^2(t)]. \tag{20}$$

In Fig. 4 we show $\rho_{3\mathrm{D}}(E)$ calculated using the complete quantum procedure from Eqs. (19) and (20). It is practically the same as DOS calculated semiclassically and shown in Fig. 2. Very small differences between the two calculations (most notably the small exponential tail for $E < 0$, which does not appear in the semiclassical procedure) are indicated in the inset (note the large difference of scales). Thus, the analytical semiclassical results provide excellent approximation to the calculations of DOS. In addition, they are valid for an electric field of almost any shape, while the full quantum treatment is tractable only for rather special potentials (for which solutions of the Schrödinger equation are known). It should be mentioned that the semiclassical results can be obtained from the exact results by using asymptotic expansions for the Airy functions [8, 9] for large (positive and negative) values of the argument.

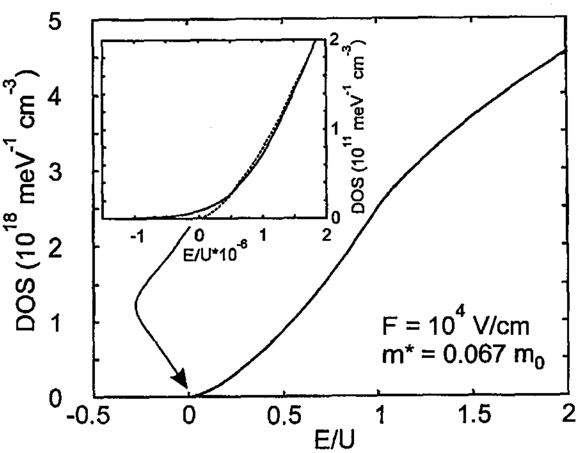

Fig. 4. The total 3D density of states for electrons in a constant electric field as a function of normalized energy, calculated semiclassically (dotted line) and exactly (solid line). The difference between the two methods is seen only in the inset (note the vastly different scale).

Now we consider the electron in crossed electric and magnetic fields. This configuration is of importance for various phenomena, most notably for the classical and quantum Hall effects [10], but also for a tunable laser in the infrared [11]. Taking a constant electric field $\boldsymbol{F} \parallel y$ and a magnetic field $\boldsymbol{B} \parallel z$, described by the vector potential $\boldsymbol{A} = [-By, 0, 0]$, one can separate variables x and z in the Schrödinger equation and reduce the latter to the equation for harmonic oscillator. For the conduction electron the energies are (spin is omitted)

$$\varepsilon(n, k_x, k_z) = \hbar\omega_c \left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m^*} + \frac{1}{2}m^* c2 \frac{F^2}{B^2} + eFY_0, \tag{21}$$

where $\omega_c = eB/m^*c$ is the cyclotron frequency, $n = 0, 1, 2, \ldots$ is the Landau quantum number, $Y_0 = k_x L^2 - m^* c^2 F/eB^2$ represents the y coordinate of the center of oscillations, and $L = (\hbar c/eB)^{1/2}$ is the magnetic radius. In the form (21) all terms in the energy have clear physical meaning: the cyclotron motion in the x–y plane, the free motion in the z direction, the drift in the x direction (with the velocity $v_{dr} = cF/B$), and the electric potential of the oscillation center.

To calculate DOS for the energies of Eq. (21) one has to integrate over k_x and k_z and sum over n. The integration over k_z is elementary and leads to an expression of the form: $(E - \varepsilon_n + eFY_0)^{-1/2}$, where $\varepsilon_n = \hbar\omega_c(n + 1/2) + m^* c^2 F^2/2B^2$. As to the integration over k_x, we consider again a finite sample in the y direction. It is instructive to change the variable from k_x to Y_0, as defined above. The resulting situation is similar to that shown in Fig. 1, with y replaced by Y_0 and $V(y)$ by eFY_0, so that $U = eFa$. The oscillation center Y_0 should be contained between 0 and a. For $\varepsilon_n < E < U$ the upper limit of integration over Y_0 is to be determined from $\varepsilon_n + eFY_0^0 = E$, while for $E \geq \varepsilon_n + U$ the upper limit is $Y_0^0 = a$. The integration gives

$$\rho_{3D}(E) = \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \frac{1}{\pi^2 L^2 U} \sum_n [(E-\varepsilon_n)^{1/2} - (E-\varepsilon_n - U)^{1/2}], \tag{22}$$

where the second term contributes for $E \geq \varepsilon_n + U$. If the spin degeneracy is lifted by magnetic field, one should divide ρ_{3D} by the factor 2 and perform the summation also over the spin levels. The limit of vanishing electric field is equivalent to $U \to 0$, which leads to the well known Landau singularities: $\rho_{3D} \sim (E-\varepsilon_n)^{-1/2}$, with $\varepsilon_n = \hbar\omega_c(n+1/2)$.

Figure 5 shows DOS for electrons in crossed fields, as described by Eq. (22), in which the shift of ε_n due to electric field was omitted. It can be seen that the presence of electric field destroys the singularities in DOS. This is due to the k_x dependence of the energies (21). The decisive parameter is the ratio of electric and magnetic energies: $\gamma = eFa/\hbar\omega_c$. For $\gamma < 1$ DOS has pronounced maxima in the form of spikes, which characterizes the magnetic regime. For $\gamma > 1$ the spikes progressively disappear and DOS acquires the electric character, cf. Fig. 2. It should be emphasized that this transition occurs for electrons in a parabolic band, so it is not related to band's nonparabolicity, which can produce similar transition [12].

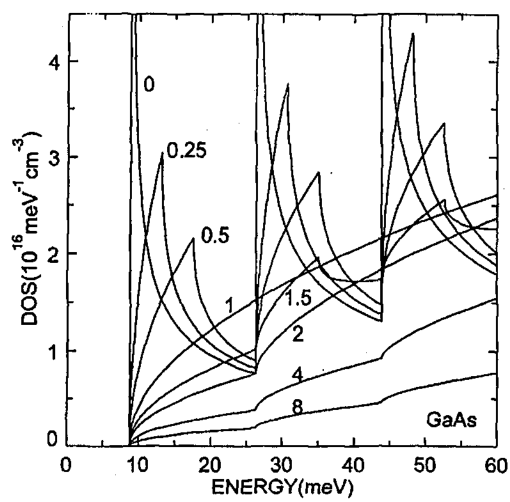

Fig. 5. Density of states for a 3D electron in crossed electric and magnetic fields, calculated for various values of $\gamma = eFa/\hbar\omega_c$. (The values $m = 0.067m_0$ and $B = 10$ T were used.) The shifts of onsets due to the electric field were disregarded (see text). A transition from the magnetic-type to the electric-type of DOS around $\gamma = 1$ can be seen.

As follows from Eq. (21), the onsets of DOS occur at $\varepsilon_n = \hbar\omega_c(n+1/2) + m^*c^2F^2/2B^2$, which means that the conduction subbands in crossed fields shift *upwards* as E/B increases. This result is unexpected. The last two terms in the energy (21) can be written equivalently as: $-mc^2F^2/2B^2 + eFk_xL^2$. In direct optical transitions the value of k_x is conserved, the last term cancels out, and the remaining conduction subband shifts *downwards* when E/B increases, while the valence subbands shift upwards (due to the opposite sign of the mass). This has been in fact observed experimentally [13]. Thus, depending on whether the k_x dependence of the conduction subbands (21) is included or not, they shift upwards or downwards at the rate $m^*c^2F^2/2B^2$, respectively.

However, one should keep in mind that in real samples the broadening of DOS peaks due to the k_x dependence of the energies is several orders of magnitude larger than their shift, so the latter can be disregarded (contrary to the situation in direct optical transitions with no k_x dependence, cf. Ref. [11]).

Finally, we consider an electron in two dimensions in the presence of crossed fields. The energy in this case is $\varepsilon(n,k_x) = \varepsilon_n + eFY_0$, cf. Eq. (21). Thus the energy for a given subband is smeared uniformly as Y_0 varies and the contribution to DOS vanishes outside the smearing interval. We require again that Y_0 in a finite sample varies from 0 to a. The result of integration over Y_0 is

$$\rho_{2\mathrm{D}}(E) = \frac{1}{\pi L^2 U}\sum_n \Theta(E-\varepsilon_n) - \Theta(E-\varepsilon_n-U), \tag{23}$$

where $U = eFa$, and $\Theta(x)$ is the theta step function. Each subband gives the same constant contribution to DOS for energies $\varepsilon_n < E < \varepsilon_n + U$, where $\varepsilon_n = \hbar\omega_c(n+1/2) + m^*c^2F^2/2B^2$. In the limit of vanishing electric field there is $U \to 0$, the formula (23) leads to the derivative with respect to U and one obtains the well known result for the Landau levels in 2D system: $\rho_n(E) \sim \delta(E-\varepsilon_n)$. In Fig. 6 we show DOS described by Eq. (23), omitting the shift of levels due to electric field.

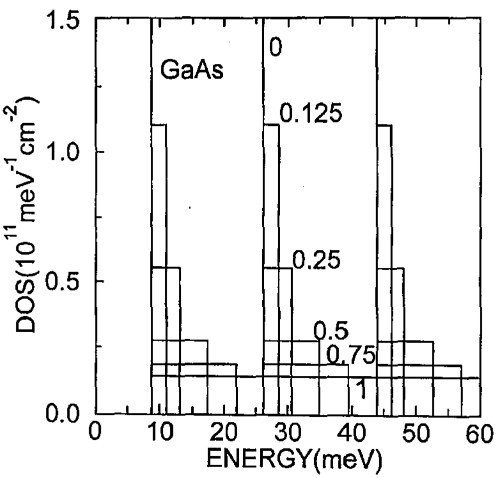

Fig. 6. The same as in Fig. 3, but for a 2D electron in crossed fields.

As in 3D case the decisive quantity is $\gamma = eFa/\hbar\omega_c$. For $\gamma \ll 1$ one deals with well pronounced peaks in the density of states (magnetic regime), for $\gamma \approx 1$ the peaks disappear, and for $\gamma > 1$ the contributions from different subbands overlap (electric regime).

The last result is directly related to the quantum Hall effect (QHE). In principle, there should be no QHE in the electric regime. However, it is still not clear whether QHE should be attributed to the volume or the edge currents in a 2D sample. Our considerations clearly apply to the volume picture, which seems to regain popularity lately (cf. Refs. [14, 15]). Kirtley et al. [16] measured the critical fields corresponding exactly to our result: $eF_{\rm cr}a = \hbar\omega_c$, but other experiments on critical (Hall) fields $E_{\rm cr}$, at which the breakdown occurs, give a confused picture (cf. the discussion in Ref. [14]). In a more realistic theoretical description one would have to include inhomogeneity of electric field, which is known to occur in the QHE regime.

Acknowledgments

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Appendix

We give here some mathematical information omitted in the text.

In order to calculate $\mathrm{d}n/\mathrm{d}\varepsilon$ appearing in DOS, cf. Eq. (3), one uses Eq. (1). This gives

$$\hbar\pi\frac{\mathrm{d}n}{\mathrm{d}\varepsilon} = \sqrt{2m^*}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_0^{y_n}[\varepsilon(n) - V(y)]^{1/2}\mathrm{d}y.$$

The right-hand side is calculated using the step function Θ and the Dirac delta function δ,

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_0^{y_n}(\varepsilon - V)^{1/2}\mathrm{d}y = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_0^{\infty}(\varepsilon - V)^{1/2}\Theta(y_n - y)\mathrm{d}y$$

$$= \int_0^{\infty}\frac{1}{2(\varepsilon - V)^{1/2}}\Theta(y_n - y)\mathrm{d}y + \int_0^{\infty}(\varepsilon - V)^{1/2}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Theta(y_n - y)\mathrm{d}y.$$

The second term vanishes since $\mathrm{d}\Theta(y_n - y)/\mathrm{d}\varepsilon = (\mathrm{d}y_n/d\varepsilon)\mathrm{d}\Theta(y_n - y)/\mathrm{d}y_n = (\mathrm{d}y_n/\mathrm{d}\varepsilon)\delta(y_n - y)$ and for $y = y_n$ there is $\varepsilon(n) - V(y_n) = 0$. The first term leads to Eq. (4) in the text.

The integral in Eq. (13) is (cf. Ref. [9])

$$\int_0^{\infty} t^{-1/2}\mathrm{Ai}^2(t + c)\mathrm{d}t = \frac{1}{2}\mathrm{Ai}_1(2^{2/3}c),$$

where $\mathrm{Ai}_1(y) = \int_y^{\infty}\mathrm{Ai}(x)\mathrm{d}x$.

The integral in Eq. (18) is

$$\int_0^{\infty} t^{1/2}\mathrm{Ai}^2(t + c)\mathrm{d}t = -\frac{1}{4}[2^{-2/3}\mathrm{Ai}'(2^{2/3}c) + c\mathrm{Ai}_1(2^{2/3}c)].$$

These integrals can be also expressed by the so-called inhomogeneous Airy functions (cf. Ref. [9]).

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