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Two-period magneto-oscillations in coherent double barrier-resonant tunnelling

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Abstract. Applying a magnetic field B to a double-barrier resonant-tunnelling diode, perpendicular to the layer structure, introduces oscillations in current density and capacitance that are periodic in $1/B$. A derivation of this periodicity is given, based on coherent wave propagation. Two magneto-periods are found, corresponding to the electron concentration in emitter and well, respectively. Numerical calculations are presented for a semiconductor model with self-consistently determined electron potential.

The application of a magnetic field in the study of resonant tunnelling may reveal relevant information, a fact long acknowledged by both experimentalists and theorists [1–4]. In the case of the double-barrier resonant-tunnelling (DBRT) structure, the $\boldsymbol{B} \| \boldsymbol{J}$ geometry enables a direct probing of the charge build up in the well [2, 3]. Since this phenomenon plays a key role in explaining the intrinsic bistability in the I–V curve of a DBRT structure, magneto-tunnelling experiments have been of importance in the discussion of the nature of the observed bistability [2–4]. Information about charge density and the Fermi level is contained in the magneto-oscillations in charge and current that result from the passing of the Landau levels through the Fermi level when varying the magnetic field at fixed applied bias voltage. These Shubnikov–de Haas-like oscillations are periodic in $1/B$ with a period $1/B_{\mathrm{fr}}$ which is inversely proportional to the space charge in the well; this periodicity has been reported by a number of authors [1–3].

The careful analysis of the magneto-oscillation spectrum reveals a second peak, corresponding to a period that is related to the space charge in the accumulation layer in front of the structure. This second peak has been reported by Payling *et al* [3, 4]. In their description of the magnetospectrum, they start from a sequential tunnelling picture [4, 5].

In this paper, we present a derivation of the magneto-spectrum based on the description of electron transport as coherent wave propagation. To a great extent, this derivation is independent of the specific model of the 1D-tunnelling or of the contact layers: for, both classically and quantum mechanically, the influence of a magnetic field perpendicular to the layers is on the lateral motion only. Thus, questions like whether the tunnelling is or is not sequential, or whether the Fermi level is or is not constant, do not affect the following presentation.

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In a DBRT-structure, there will be a build-up of charge in three layers (see figure 1). In the emitter layer, an accumulation of electrons will give rise to a negative charge density. Quantum mechanical tunnelling enables the formation of an electron gas, 2D in nature, within the well. Furthermore, the ionized doping in the depleted collector layer provides a positive space charge. Since the latter density is determinable via overall charge neutrality considerations, we concentrate on the electron densities in the emitter and the well.

Our starting point is a well-known formula for the 3D electron concentration $n(r)$ at position r:

$$n(r) = \sum_k f[(E_k - E_F)/kT]|\Psi_k(r)|^2. \tag{1}$$

Here, the $\Psi_k(r)$ are the envelope functions describing the electron states labeled by $k \equiv (k_x, k_y, k_z)$. The function $f(\varepsilon) = (1 + \exp(\varepsilon))^{-1}$ is the Fermi–Dirac distribution. We take $r = 0$ to be the middle of the well. Two remarks should be made about (1). First, the normalization of the functions $\Psi_k(r)$ is with respect to the reservoir formed by the doped layers that sandwich barriers and well, i.e. for large $|r|$ the electron concentration should equal the impurity density N_D to ensure charge neutral contacts. Secondly, the label k refers to the allowed states in the reservoir. If we let the volume of the reservoir tend to infinity, the Hamiltonian equation for the envelope function [6]:

$$(1/2m)[(\hbar/i)\nabla + eA(r)]^2\Psi_k(r) + E_{co}(r)\Psi_k(r) = E_k\Psi_k(r) \tag{2}$$

where $E_{co}(r)$ is the conduction band minimum and $A(r)$ is the vector potential, related to the magnetic field B via $B = \nabla \times A$, has a continuous spectrum of allowed electron energies E_k above the conduction band minimum $E_{co}(r)$ in the reservoir.

Our first step is to cast (1) into a quasi-1D form. Let z be the direction perpendicular to the barriers. A valid choice for the vector potential A is then $(-By, 0, 0)$, corresponding to $\nabla \cdot A = 0$ and $\nabla \times A = (0, 0, B)$. Because of the layered structure, the band edge E_{co} depends on z only. Separation of variables is possible:

$$\Psi_k(r) = G_{k_xk_y}(x, y)F_{k_z}(z) \qquad E_k = E_{k_xk_y} + E_{k_z} \tag{3}$$

replacing (2) by an equation for the lateral state $G_{k_xk_y}(x, y)$ containing all field dependence but no band edge:

$$\frac{1}{2m}\left[\left(\frac{\hbar\partial}{i\partial x} - eBy\right)^2 + \left(\frac{\hbar\partial}{i\partial y}\right)^2\right]G_{k_xk_y}(x, y) = E_{k_xk_y}G_{k_xk_y}(x, y) \tag{4a}$$

and an equation for the tunnelling state $F_{k_z}(z)$ containing the band edge but no field dependence:

$$\frac{1}{2m}\left(\frac{\hbar d}{i dz}\right)^2 F_{k_z}(z) + E_{co}(z)F_{k_z}(z) = E_{k_z}F_{k_z}(z). \tag{4b}$$

After substituting (3) in (1), we perform the summation over k_x and k_y to introduce a new weighing function g in which the density of the lateral states is incorporated:

$$g[x, y; (E_{k_z} - E_F)/kT] = \sum_{k_xk_y} f[(E_{k_xk_y} + E_{k_z} - E_F)/kT]|G_{k_xk_y}(x, y)|^2 \tag{5}$$

so (1) now reads:

$$n(r) = \sum_{k_z} g[x, y; (E_{k_z} - E_F)/kT]|F_{k_z}(z)|^2. \tag{6}$$

In the perfectly layered structures that we consider, $g(x, y; \varepsilon)$ will turn out to be

independent of the coordinates x and y, i.e. the electron concentration depends on z only. Anticipating this, we will write $g(\varepsilon)$ instead of $g(x, y; \varepsilon)$. The function $g(\varepsilon)$ has the same weighing role as the Fermi–Dirac distribution function $f(\varepsilon)$, but differs from the latter in having a dimension, the dimension of an areal density. In (6), the 1D tunnelling described by the functions $F_{k_z}(z)$ is separated from the effect of the lateral states, incorporated in g. A magnetic field in the z direction will introduce no direct changes to $F_{k_z}(z)$ but affect only the weighing function g.

Our next step is to ensure that in the well only one k_z (corresponding to the resonance energy E_r) is present. We indicate this wave number by k_{zr}, leave out for $z = 0$ all terms with $k_z \neq k_{zr}$, and write $n_{\text{well}} \equiv n(z = 0) = g[(E_r - E_F)/kT]|F_{k_{zr}}(0)|^2$. This result can be improved by averaging $n(z)$ over the z interval $(-w/2, +w/2)$, where w is the well width. Also, the finite width of the resonance level can be taken into account, changing the factor $|F_{k_{zr}}(0)|^2$. However, the essence of our result: the proportionality of n_{well} and $g[(E_r - E_F)/kT]$:

$$n_{\text{well}} \sim (1/w)g[(E_r - E_F)/kT] \tag{7a}$$

will survive these modifications.

Contrary to the well, the emitter may contain electrons with any positive energy E_{k_z} (upto E_F at zero temperature). If we neglect the dependence of $|F_{k_z}(z)|^2$ on k_z, i.e. if we take the reflection coefficient of the structure equal to unity, we find:

$$n_{\text{emitter}} \sim \int_0^\infty \mathrm{d}k_z\, g[(E_{k_z} - E_F)/kT] \tag{7b}$$

With (7), the basis for our discussion of magneto-oscillations is laid. The electron concentration in the well depends on $\eta_r \equiv E_r/kT$ via the function $g(\varepsilon)$, which is the Fermi–Dirac distribution dressed with the density of lateral states. The latter density depends on the magnetic field strength. The electron concentration in the emitter can be expressed as the integral of the same function, and depends on the reduced Fermi energy $\eta \equiv E_F/kT$.

Let us have a closer look at the function $g(\varepsilon)$, and work out (5) in the case of zero magnetic field. The function $G_{k_xk_y}(x, y)$ is then a plane wave (see (4*a*)), and the energy $E_{k_xk_y} = (\hbar^2/2m)(k_x^2 + k_y^2)$. Substitution of this in (5) yields:

$$g(\varepsilon) = N_c^{2/3}\mathcal{F}_0(-\varepsilon) \tag{8}$$

where $N_c \equiv (mkT/2\pi\hbar^2)^{3/2}$ is the effective number of states in the conduction band per unit volume (no spin degeneracy), and $\mathcal{F}_j(\varepsilon)$ is the Fermi–Dirac integral of order j [7]. Substitution of (8) in (7) yields:

$$n_{\text{well}} \sim (1/w)N_c^{2/3}\mathcal{F}_0(\eta - \eta_r) \tag{9a}$$

$$n_{\text{emitter}} \sim N_c\mathcal{F}_{1/2}(\eta). \tag{9b}$$

The difference between (9*a*) and (9*b*) is the difference between a 2DEG and a 3DEG.

In the case of $B \neq 0$, we proceed in the same way. Now, the envelope function in (4*a*) is essentially a Hermite polynomial $H_l(u)$, and the energy is quantized into equidistant levels:

$$G_{k_xl}(x, y) \sim \mathrm{e}^{\mathrm{i}k_xx}\mathrm{e}^{-1/2u^2}H_l(u) \qquad u = \sqrt{(eB/\hbar)}[y - \hbar k_x/eB]$$

$$E_{k_xl} = E_l = (l + \tfrac{1}{2})(\hbar eB/m)$$

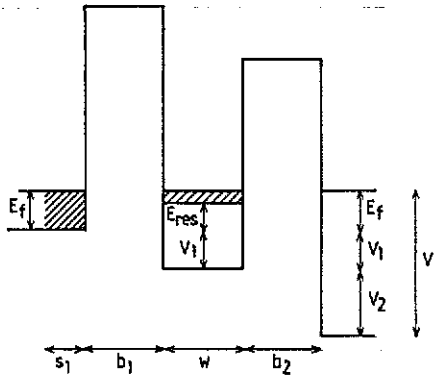

Figure 1. Conduction-band minimum in the DBRT structure as a function of position z.

where the quasi-continuous label k_y is replaced by the non-negative integer l, expressing the quantizing effect of the magnetic field. In fact, l labels the so-called Landau levels of the energy associated with the lateral motion. Substitution in (5) yields:

$$g(\varepsilon, \theta) = N_c^{2/3}\,\theta \sum_l f[\varepsilon + (l + \tfrac{1}{2})\theta] \tag{10}$$

where $\theta = \hbar eB/mkT$ is the 'reduced' magnetic field. Since now g depends also on B or θ, an extra slot to g is added. Using (10) in (7), the electron concentrations in emitter and well are found to be:

$$n_{well} \sim (1/w)N_c^{2/3}\,\theta \sum_l f[\eta_r - \eta + (l + \tfrac{1}{2})\theta] \tag{11a}$$

$$n_{emitter} \sim N_c\,\theta \sum_l \mathcal{F}_{-1/2}[\eta - (l + \tfrac{1}{2})\theta]. \tag{11b}$$

In figure 2 the expressions (11) are drawn for three values of the temperature. Two limits of (11) can easily be evaluated. If $\theta \ll 1$, i.e. if the spacing between the Landau levels is much smaller than kT, then the summation in (11) can be replaced by an integration, so that the results of (9) are retrieved, as expected; the effect of the magnetic field is effaced by the temperature. If, on the other hand, $\theta \gg 1$, we find:

$$n_{well} \sim (1/w)N_c^{2/3}\,\theta\,\mathrm{Int}[(\eta - \eta_r)/\theta + \tfrac{1}{2}] \tag{12a}$$

$$n_{emitter} \sim N_c\,\theta^{3/2} \sum_{l=0}^{l_{max}} \sqrt{\eta/\theta - (l + \tfrac{1}{2})}. \tag{12b}$$

The upper limit in the summation of (12b), l_{max}, is equal to $\mathrm{Int}[\eta/\theta - \frac{1}{2}]$. $\mathrm{Int}[x]$ denotes the integral part of x. The expressions in (12) are independent of temperature. It is in this limit, $\theta \gg 1$, that the magneto-oscillations are easily recognised: n_{well} is a decreasing function of $1/\theta$ on every interval $(l - \frac{1}{2})/(\eta - \eta_r) < 1/\theta < (l + \frac{1}{2})/(\eta - \eta_r)$, $l \geqslant 0$; at $1/\theta = (l + \frac{1}{2})/(\eta - \eta_r)$, however, n_{well} increases abruptly by $N_c^{2/3}.(\eta - \eta_r)/(l + \frac{1}{2})$. Hence, the resulting oscillations in n_{well} will have a period $1/(\eta - \eta_r)$† as a function of $1/\theta$, corresponding to a period $\hbar e/m(E_F - E_r)$ as a function of reciprocal field $1/B$. Because the reciprocal period has the dimension of a magnetic field, we call it a 'fundamental field' where the notation and terminology are adopted from [4], and denote it by B_{fr}:

$$B_{fr} = m(E_F - E_r)/\hbar e \tag{13a}$$

† Here, the use of the work 'periodic' does not imply invariance under translation, but the presence of a peak in the Fourier spectrum.

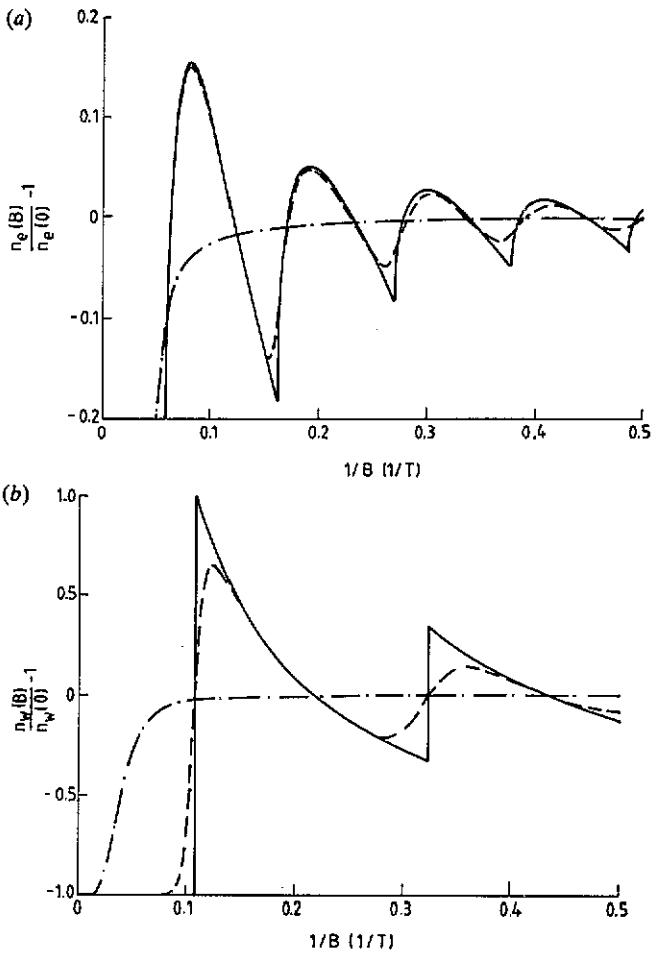

Figure 2. (*a*) The electron density n_{emitter} as function of $1/B$, relative to its value at zero magnetic field (see (11) and (9)), at three temperatures $T = 0.01$ K, 4.2 K and 77 K. (*b*) The same for n_{well}. E_f is taken to be 10 meV and $E_{\text{res}} = \frac{1}{2}E_F$. m is 0.067 times the electron mass.

(12*b*) can be analyzed in the same way: $l_{\max}$ is constant for $(l - \frac{1}{2})/\eta < 1/\theta < (l + \frac{1}{2})/\eta$, $l \geqslant 0$. Now, n_{emitter} is continuous and not monotonous on this interval. However, its first derivative is discontinuous at $1/\theta = (l + \frac{1}{2})/\eta$, $l \geqslant 0$, and this results in oscillations with period $1/\eta$, corresponding to a period $\hbar e/mE_F$ in $1/B$. The fundamental field, B_f, is in this case:

$$B_f = mE_F/\hbar e. \tag{13b}$$

Thus, the two quantities B_f and B_{fr} of (13) are a brief characterization of the magneto-oscillations in n_{emitter} and n_{well}, respectively. Because the electron concentration in the collector is related to those in emitter and well via the demand of charge neutrality, it will contain both periods. In the same way, the capacitance of the DBRT structure, measured as a function of inverse magnetic field, will peak in its magneto-spectrum at both B_f and B_{fr}.

Expressions for the fundamental fields were arrived at by considering only the lateral motion and assuming that E_r and E_F do not change with magnetic field. We could

avoid considering the motion in the z-direction, i.e. from specifying the factors of proportionality in (7). However, in order to couple the fundamental fields to the external handle, the bias voltage V applied to the DBRT structure, we need to specify the model for tunnelling and reservoirs. Let us first look at what we might term a 'metal picture' of the structure: the Fermi level is determined by the impurity density in the doped contact layers, and independent of V. The resonance level with respect to the band edge in the well is a constant, E_0, determined by the structure parameters; with respect to the band edge in the emitter, however, this level E_r decreases with increasing V, and if the effect of the charge in the well on the band bending is neglected, this dependence is linear. Thus, in a metal picture, the function $B_f(V)$ is a constant function, whereas $B_{fr}(V)$ is a linear function of V. Since, at zero temperature, there is resonant charge build-up in the well only if $0 < E_r < E_F$, the function $B_{fr}(V)$ is only defined for the corresponding voltage interval, in which the field increases from 0 to the constant B_f.

A remark about the condition that E_F be independent of B is in order: in a metal picture of the contact layers, the electron concentration should equal the ionized-impurity density and if the latter does not depend on the magnetic field then neither will the former. Hence, magneto-oscillations will now not be found in $n_{emitter}$ but in E_F instead†, and in such a way that (12b) is still valid. Since the oscillations in E_F correspond to the same fundamental field B_f‡, and since quantities like the capacitance or the current depend on E_F, we will still find the two periods derived above.

Characterizing the contrasting 'semiconductor picture' by a voltage-dependent Fermi level $E_F(V)$, we now find an increasing function $B_f(V)$. Also in this picture, B_{fr} is defined on a small voltage interval only, the beginning of which corresponds to $E_r = E_F$ (i.e. $B_{fr} = 0$) and the end of which corresponds to $E_r = 0$ (i.e. $B_{fr} = B_f$). It is within this semi-conductor picture that our numerical calculations for a symmetric GaAs/$Al_{0.4}Ga_{0.6}As$ structure are performed [8]. By assuming $E_F(V = 0) = 0$, we neglect all doping effect on the Fermi level. Values of $E_F(V)$ for $V \neq 0$ are determined via the self-consistency demand that V be equal to the charge-induced potential drop plus E_F, neglecting, however, the potential drops in emitter and collector. These simplifications yield, in general, over-large values of E_F and hence of B_f and B_{fr} (see figure 3). The 1D tunnelling through the barriers is calculated in the transfer matrix approach; the sharp peak in the transmission probability is approximated by a Dirac-delta function with the correct weight. In this way, the factor of proportionality in (7a), (9a), (11a) or (12a) is found to be $\frac{1}{2}(1 - R_e)(1 + R_c)/(1 - R_eR_c)$, where R_e and R_c are the reflection coefficients of the emitter and collector barrier for a wave of energy E_r. This 'storage factor' expresses the ability of the well to hold the charge: if $R_c \approx 1$ (at low bias), it is unity, but if $R_c \to 0$ (at higher biases), it approaches $\frac{1}{2}(1 - R_e) \ll 1$. In particular, when $R_e \to 1$ (i.e. when $E_r \to 0$ and B_{fr} reaches its maximum), the storage factor, and hence n_{well}, approaches zero. This is in contrast with a true 2DEG characterized by a storage factor of unity. There, the zero-field–zero-temperature concentration is proportional to B_{fr} (cf. (9a) and (13a)). Here, it is the decreasing storage factor, i.e. the leaky nature of the well, that frustrates such a linear relation between B_{fr} and the amount of space charge in the well§.

A similar remark to that for the metal picture must be made for the semiconductor

† Even when $n_{emitter}$ is constant, the areal charge density in the emitter will still fluctuate with changing B, due to a fluctuating screening length for that layer.

‡ With a field-dependent Fermi level $E_F(B)$, (13) is to be read as: $B_f = mE_F(0)/\hbar e$.

§ Surprisingly, this 'coherent' storage factor coincides with the 'sequential' one as given by Sheard and Toombs (see (5) and (8) in [5]), at least for R_c and R_e close to unity. However, since they regard this factor as independent of the bias voltage, in their theory a proportionality between B_{fr} and n_{well} still holds.

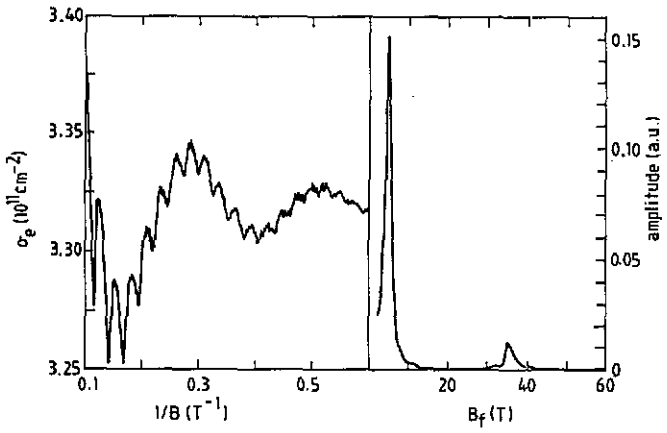

Figure 3. (*a*) Sheet density σ_a of the charge in the left spacer as a function of $1/B$ at fixed bias voltage $V_b = 0.156$ V, determined numerically with self-consistent electrostatic feedback. Structure parameters: s_1–b_1–w–b_2 = 2.5–5.6–5.0–5.6 nm; barrier height is taken to be 0.44 eV; m is 0.067 times the electron mass; $\epsilon_r = 13.4$ (GaAs–$Al_{0.4}Ga_{0.6}As$ values). (b) Its Fourier spectrum.

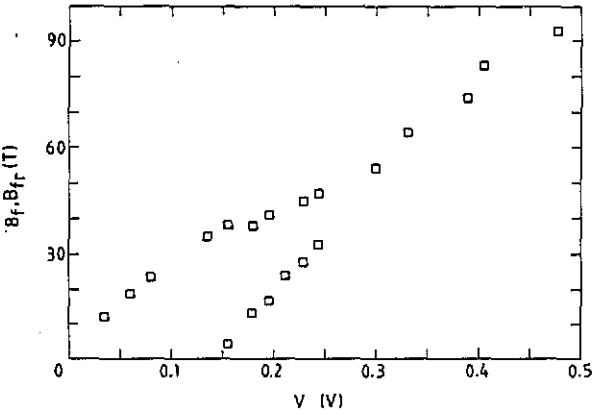

Figure 4. Inverse periods B_f and B_{fr} as functions of V. Structure parameters as in figure 3.

picture: since both E_F and $n_{emitter}$ appear in the self-consistency requirement, we are not free to choose one of the two independent of B. Consequently, both E_F and $n_{emitter}$ exhibit magneto-oscillations, that are restricted by (12*b*) only. Since also n_{well} appears in the self-consistency requirement, the resulting oscillations in all three quantities will contain both periods $1/B_f$ and $1/B_{fr}$ (see figure 4). In other words, it is the self-consistency requirement in the semiconductor model, that effectuates the concurrence of the two fundamental fields in the spectra of all quantities.

If we apply the above discussion to the experimental results of [3, 4], we find that, for the examined structures, the metal picture is most appropriate: the slope of $B_f(V)$ is found to be smaller than $10^{-2}\,\mathrm{T\,mV^{-1}}$, corresponding to a change in E_F with V of $10^{-2}\,\mathrm{eV\,V^{-1}}$, too small for a pure semi-conductor model. For a different type of structures, including spacers or moderately doped contact layers, a semiconductor picture may be more favourable.

Since we started our discussion from coherent wave propagation, we cannot compare our theory to the experiments of Leadbeater *et al* [9], where thermalization plays an

essential role. There, the tunnelling is not coherent, via a resonant state (i.e. a state with energy that is positive with respect to the band edge in both emitter and collector contact), but non-coherent or 'sequential', via a 'quasi-bound' state (i.e. a state with energy that is negative with respect to the band edge in one of the contacts). In the lightly doped emitter, a 2DEG builds up by thermionic processes, whereas in our coherent picture a 3DEG results (cf. (9)). This indicates once more that our analysis is restricted to the low bias region.

Summarizing, we have demonstrated that coherent tunnelling in a DBRT structure will lead to biperiodicity in the magneto-spectrum of charge and current densities. In the low bias region, the 3D contact and the 2DEG in the well each provides its own period. The self-consistent electrostatic feedback effectuates the appearance of both periods in all relevant quantities.

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[7] In this paper, $\mathcal{F}_j(\eta)$ is encountered for $j = -\frac{1}{2}, 0, +\frac{1}{2}$. For definitions and approximations of the integrals, see:
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