

Volume particle density in a 2D electron gas

Consider a free 2-dim electron gas confined to a quantum well of arbitrary shape and thickness. The eigenstates are labeled by the 2D wavenumber \mathbf{k} , the subband index n and the spin s :

$$\Psi_{n,s,\mathbf{k}}(\mathbf{R}) = \chi_s \phi_n(z) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (1.1)$$

where $\mathbf{R} = (z, \mathbf{r})$. The wave functions ϕ_n are determined by the actual shape of the potential well. These functions will be assumed normalized,

$$\int \phi_n^*(z) \phi_n(z) dz = 1. \quad (1.2)$$

The electron energy in the state $\Psi_{n,s,\mathbf{k}}$ is given by

$$E_{n,s,\mathbf{k}} = E_n + \frac{\hbar^2 \mathbf{k}^2}{2m} \equiv E_n + E_{\mathbf{k}}, \quad (1.3)$$

assuming no magnetic field, so that the spin degeneracy is not lifted.

At a finite temperature T , the electron density per unit volume is given by

$$\begin{aligned} \rho(\mathbf{R}) &= \sum_{n,s,\mathbf{k}}^{\text{occ. states}} \Psi_{n,s,\mathbf{k}}^*(\mathbf{R}) \Psi_{n,s,\mathbf{k}}(\mathbf{R}) \\ &= \sum_{s,n} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \Psi_{n,s,\mathbf{k}}^*(\mathbf{R}) \Psi_{n,s,\mathbf{k}}(\mathbf{R}) f(E_{n,s,\mathbf{k}} - E_F), \end{aligned} \quad (1.4)$$

where E_F is the Fermi level, and $f(E)$ is the Fermi function,

$$f(E) \equiv \frac{1}{1 + e^{E/kT}} = - \frac{d\Phi}{dE}, \quad \Phi \equiv kT \ln \left[1 + e^{-\frac{E}{kT}} \right]. \quad (1.5)$$

Performing the angular integration and the summation over s in Eq. (1.4), we have

$$\begin{aligned} \rho(\mathbf{R}) &= \sum_n |\phi_n(z)|^2 \frac{m}{\pi \hbar^2} \int_0^\infty dE_{\mathbf{k}} f(E_{\mathbf{k}} + E_n - E_F) \\ &= \sum_n |\phi_n(z)|^2 \frac{m}{\pi \hbar^2} \Phi(E_n - E_F). \end{aligned} \quad (1.6)$$

Let us specialize to the case of one subband only. This means that subbands corresponding to $n=1, 2, \dots$ are not occupied, $E_n - E_F \gg kT$. The electron density is given by:

$$\rho(\mathbf{R}) = \rho_0(z, \mathbf{r}) = |\phi_0(z)|^2 \frac{m}{\pi \hbar^2} \Phi(E_0 - E_F). \quad (1.7)$$

The z dependence in (1.7) is sharp, while the \mathbf{r} dependence is (strictly speaking) absent. However, we can assume that ρ depends "adiabatically" on the position within the plane of 2DEG – through the dependence on \mathbf{r} of the difference $E_F - E_0 \equiv \hbar^2 k_F^2 / 2m$, where k_F is the Fermi wavenumber of the lowest subband. The adiabatic assumption means that the characteristic length $(\nabla \ln k_F)^{-1}$ of in-plane variations in k_F is much larger than the localization length in the z direction.

In a variety of problems we are not really interested in an accurate determination of $\rho(z)$, only in the smooth variation of $\rho(\mathbf{r})$. In this case, we are free to assume a narrow quantum well of thickness d and unspecified shape, and take $|\phi(z)|^2 = 1/d$ inside the well and 0 outside.

Einstein relation

Equation (1.6) can be viewed as describing several 2D electron gases ρ_n in parallel. Regarding these gases as independent (i.e., neglecting the intersubband scattering), we can endow each of the subbands n with its own mobility μ_n and diffusivity D_n . The drift-diffusion flux in each subband is of the form:

$$e \rho_n \mu_n \mathbf{F}_n + e D_n \nabla \rho_n \quad (2.1)$$

where $\nabla = \partial/\partial \mathbf{r}$ is the 2D gradient and \mathbf{F}_n is the effective in-plane field,

$$e \mathbf{F}_n \equiv \nabla E_n \quad (2.2)$$

acting in the subband n (these fields do not have to be the same for each subband, in general).

The coefficients μ_n and D_n must be connected by an Einstein relation in order for the flux (2.1) to vanish in equilibrium. Let us write down this relation explicitly, dropping the subband indices for brevity.

$$e D = \mu E_D, \quad E_D^{-1} \equiv \frac{d \ln \rho}{d E_F}. \quad (2.3)$$

Proof: In equilibrium $\nabla E_F = 0$, and the variation of ρ is due to that of E_0 only. Therefore,

$$\nabla \rho = \frac{\partial \Phi(E_0 - E_F)}{\partial E_0} \nabla E_0 = - \frac{\partial \Phi(E_0 - E_F)}{\partial E_F} \nabla E_0. \quad (2.4)$$

Letting (2.1) to be zero and using Eqs. (2.2) and (2.4), we obtain (2.3). Substituting the explicit expression (1.5) for Φ , we have:

$$E_D = \frac{\Phi(E_0 - E_F)}{f(E_0 - E_F)} = kT \left[1 + e^{-(E_F - E_0)/kT} \right] \ln \left[1 + e^{(E_F - E_0)/kT} \right]. \quad (2.5)$$

In the truly degenerate case $E_F - E_0 \gg kT$, the "diffusion energy" $E_D \approx E_F - E_0$. In the nondegenerate case, $E_F - E_0 \ll kT$, one has $E_D \approx kT$.

3D from 2D

Using Eq. (1.6) and any complete set of states ϕ_n , we can derive the familiar formulae for 3D statistics. Take, for example, plane waves – corresponding to free motion in z direction and therefore uniform $\rho \equiv n$. Then equation (1.6) reads

$$n = \frac{m kT}{\pi \hbar^2} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \ln \left[1 + e^{\frac{1}{kT} \left[E_F - \frac{\hbar^2 k^2}{2m} \right]} \right] = N_C F_{1/2}(\eta), \quad (2.6)$$

where

$$\eta \equiv \frac{E_F}{kT}, \quad \xi \equiv e^\eta, \quad N_C = \frac{1}{4} \left[\frac{2m kT}{\pi \hbar^2} \right]^{3/2}, \quad (2.7)$$

and the Fermi integral $F_{1/2}(\eta)$ is of the form

$$F_{1/2} = \frac{2}{\sqrt{\pi}} \int_0^\infty \ln \left[1 + e^{\eta - x^2} \right] dx = \frac{2}{\sqrt{\pi}} \int_0^\infty \ln \left[1 + \xi e^{-x^2} \right] dx. \quad (2.8)$$

Equation (2.8) is equivalent (check integrating by parts) to the more familiar

$$F_{1/2}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2} dx}{1 + e^{x - \eta}}. \quad (2.9)$$

Fermi integrals

In general, the Fermi integrals are defined by:

$$F_s(\eta) = \frac{1}{\Gamma(s+1)} \int_0^\infty \frac{x^s dx}{1 + e^{x-\eta}} = \frac{1}{\Gamma(1+1/k)} \int_0^\infty \ln \left[1 + \xi e^{-x^k} \right] dx, \quad (3.1)$$

$$\Gamma(n) = (n-1)! \quad \Gamma\left[n + \frac{1}{2}\right] = \frac{\sqrt{\pi}}{2^n} (2n-1)!! \quad \Gamma\left[\frac{1}{2} - n\right] = (-1)^n \frac{2^n \sqrt{\pi}}{(2n-1)!!}$$

The following recurrence relation is valid for arbitrary s :

$$\frac{dF_s}{d\eta} = F_{s-1}. \quad (3.2)$$

The zeroth order Fermi integral is evaluated explicitly (as in Eq. 2.5)

$$F_0 = \ln \left[e^\eta + 1 \right], \quad (3.3)$$

and hence F_s can be expressed through elementary functions for all integer $s < 0$; for example, $F_{-1} = [\exp(-\eta) + 1]^{-1}$. For large ($|\eta| \gg 1$) negative η , all Fermi integrals equal $\exp(\eta)$, independent of the index s . For large positive η , the asymptotic form is

$$F_s(\eta) = \frac{\eta^{s+1}}{\Gamma(s+2)} \left[1 + \frac{\pi^2 \Gamma(s+2)}{6 \Gamma(s) \eta^2} + \dots \right]. \quad (3.4)$$

Sometimes, the logarithmic form may be more convenient. For example, expanding the logarithm (for $\xi < 1$) in Eq. (2.8) and integrating, we find

$$\frac{n}{N_C} = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\xi^k}{k^{3/2}} = \xi - 2^{-3/2} \xi^2 + 3^{-3/2} \xi^3 - \dots \quad (3.5)$$

The series (3.5) converges for $\xi \leq 1$, i.e., for $\eta < 0$; on the other hand, the concentration, of course, is well defined by Eq. (2.8) for any Fermi level value. The integral (2.8) is easy to evaluate by the Gauss' procedure. The simplest way of doing this is to change the variables $x = by$ with $b^2 \gg 1$, say $b = 5$. Then

$$\frac{n}{N_C} = \frac{2b}{\sqrt{\pi}} \int_0^1 \ln \left[1 + \xi e^{-b^2 y^2} \right] dy \quad (3.6)$$

Evaluating (3.6) by a 25-point gaussian quadrature we obtain essentially exact result: the error in the range $0.1 < \xi < 25$ is less than $10^{-4}\%$. Even a 5pt gaussian quadrature gives less than 2% error in this range. This is much better than the Joyce-Dixon procedure,

$$\eta = \ln F + \sum_{k=1} A_k F^k, \quad \text{where } F \equiv F_{1/2} = n/N_C, \quad (3.7)$$

and $A_1 = 3.53553 \times 10^{-1}$ $A_2 = -4.95009 \times 10^{-3}$ $A_3 = 1.48386 \times 10^{-4}$ $A_4 = 4.42563 \times 10^{-6}$,

which gives about 16% error at $\beta E_F \approx 10$ (where $F_{1/2} \approx 24$).

Joyce-Dixon is better than Gauss only at $F_{1/2} \ll 1$ where the result is known with a good accuracy anyway: $n/N_C = \exp(\eta)$. The usefulness of Joyce-Dixon asymptotic series (which actually diverges for $\xi > 1$ but with a few terms is reasonably accurate for $\eta \leq 10$) is only near $\xi = 1$, say $|\eta| \leq 1$. Its convenience seems to be only in the fact that it gives $\eta(F)$ rather than $F(\eta)$.

Statistics at low temperatures

Joyce-Dixon may be convenient for the evaluation of band concentration at low temperatures, where this evaluation reduces to an expression of F in terms of $\eta(F)$. Consider the case $N_D > N_A = K N_D$. Compensation $K < 1$.

We have $n + n_D = N_D - N_A$, where n_D is the electron concentration on donors,

$$n_D = \frac{N_D}{\frac{1}{2} e^{\beta(E_D - E_F)} + 1}. \quad (4.1)$$

Here $E_D < 0$ is the donor energy, relative to the conduction band edge. Determination of F reduces to the following nonlinear equation:

$$F = \frac{N_D}{N_C} \left[1 - K - \frac{1}{1 + \frac{1}{2} e^{\beta E_D - \eta(F)}} \right]. \quad (4.2)$$

Taking $\eta(F)$ in the form (3.7), we can obtain the solution to (4.2) in a few iterations.

Degenerate Grading

In Shockley's drift diode (and later Moll's drift transistor) a nondegenerate base is inhomogeneously doped with an exponentially varying concentration of impurities. This results in a linear slope of the bands, i.e. constant field. The constant field is achieved if η varies linearly with distance. Consider a degenerately doped base as in modern HBT's. In the limit of large $\eta \gg 1$ we have from Eq. (3.4) $F_{1/2} \approx 4\eta^{3/2} 3\sqrt{\pi}$ and the condition of constant field F requires the carrier (hole) concentration to vary as

$$p(x) = p_{\max} (1 - x/a)^{3/2}, \quad \frac{1}{a} \equiv \frac{E_{F\max} - E_{F\min}}{L E_{F\max}}, \quad (4.3)$$

where $E_{F\max}$, $E_{F\min}$ are the Fermi levels at the position of highest doping ($x = 0$, $p = p_{\max}$) and lowest doping ($x = L$, $p = p_{\min}$). The electric field in the graded section of thickness L of the base is $F \equiv (E_{F\max} - E_{F\min})/eL$. The table below compares the approximation (4.3) against exact values. Assumed $N_V = 7 \cdot 10^{18}$.

$\eta \equiv \beta E_F$	$F_{1/2}$	$N_V \cdot F_{1/2}$	Eq. (4.3)
0.5	1.11733	7.82132E+18	1.88492E+18
1.0	1.57564	1.10295E+19	5.33137E+18
1.5	2.14486	1.50140E+19	9.79435E+18
2.0	2.82372	1.97660E+19	1.50794E+19
2.5	3.60698	2.52488E+19	2.10741E+19
3.0	4.48755	3.14128E+19	2.77026E+19
3.5	5.45804	3.82063E+19	3.49093E+19
4.0	6.51157	4.55810E+19	4.26509E+19
4.5	7.64203	5.34942E+19	5.08929E+19
5.0	8.84421	6.19095E+19	5.96065E+19
5.5	10.1137	7.07956E+19	6.87674E+19
6.0	11.4466	8.01262E+19	7.83548E+19
6.5	12.8398	8.98787E+19	8.83504E+19
7.0	14.2905	1.00034E+20	9.87383E+19
7.5	15.7963	1.10574E+20	1.09504E+20
8.0	17.3550	1.21485E+20	1.20635E+20
8.5	18.9648	1.32754E+20	1.32119E+20
9.0	20.6240	1.44368E+20	1.43947E+20
9.5	22.3311	1.56318E+20	1.56108E+20

10.0

24.0847

1.68593E+20

1.68593E+20

Confinement in polySi grains

Zero temperature: Let k_T and k_L be the semi-axes of the Si conduction-band Fermi surface (which is an ellipsoid of revolution). Since $E_F = \hbar^2 k_T^2 / 2m_T = \hbar^2 k_L^2 / 2m_L$, the relation between the carrier concentration and the Fermi level at $T = 0$ in the bulk is determined by

$$\frac{2 N_C}{(2\pi)^3} \frac{4\pi}{3} k_L k_T^2 = n, \quad \Leftrightarrow \quad E_F = \frac{\hbar^2}{2 \langle m \rangle} \left[\frac{3\pi^2 n}{N_C} \right]^{2/3}, \quad (5.1)$$

where $\langle m \rangle \equiv (m_L m_T^2)^{1/3}$ and $N_C = 6$ is the number of equivalent valleys in the Si conduction band.

On the other hand, in a confining grain (assumed a cube of side a) the Fermi level is the highest filled energy in the sequence of levels

$$E_{n_1, n_2, n_3} = \frac{\pi^2 \hbar^2}{2 m_L a^2} [(m_L/m_T)(n_1^2 + n_2^2) + n_3^2] \approx 3.76 [\text{meV}] \times [5(n_1^2 + n_2^2) + n_3^2], \quad (5.2)$$

where we have assumed $m_L = m_0 = 5 m_T$ and $a = 100 \text{ \AA}$.

The first few levels and their degeneracies (including the spin and the valley degeneracy, $N_S \times N_C = 2 \times 6$) are:

Energy (meV)	$5(n_1^2 + n_2^2) + n_3^2$	Degeneracy
41.36	11	$1 \times 12 = 12$
52.65	14	$1 \times 12 = 12$
71.45	19	$1 \times 12 = 12$
97.77	26	$3 \times 12 = 36$
109.1	29	$2 \times 12 = 24$
127.9	34	$2 \times 12 = 24$
131.6	35	$1 \times 12 = 12$
154.2	41	$3 \times 12 = 36$
165.5	44	$1 \times 12 = 12$
173.0	46	$1 \times 12 = 12$
184.3	49	$1 \times 12 = 12$
188.0	50	$2 \times 12 = 24$
191.8	51	$2 \times 12 = 24$
203.1	54	$2 \times 12 = 24$
210.6	56	$1 \times 12 = 12$
221.9	59	$3 \times 12 = 36$
229.4	61	$2 \times 12 = 24$
244.4	65	$1 \times 12 = 12$
248.2	66	$4 \times 12 = 48$
259.5	69	$2 \times 12 = 24$
278.3	74	$5 \times 12 = 60$

At a finite temperature $T \neq 0$ the relation between n and E_F in a confined geometry can be calculated according to the basic relation:

$$n = \sum_{n_1, n_2, n_3} N_S N_C f(E_{n_1, n_2, n_3} - E_F), \quad \text{where} \quad f(E) = \frac{1}{1 + \exp(E/kT)}. \quad (5.3)$$

For the quasi-continuum, on the other hand we have

$$n = N_C F_{1/2} \left[\frac{E_F}{kT} \right], \quad \text{where} \quad N_C \equiv \frac{N_C \cdot N_S}{8} \left[\frac{2m kT}{\pi \hbar^2} \right]^{3/2}. \quad (5.4)$$

The calculated Fermi levels as functions of the carrier concentration for confined and unconfined geometries and zero and finite temperatures are plotted on the next page.

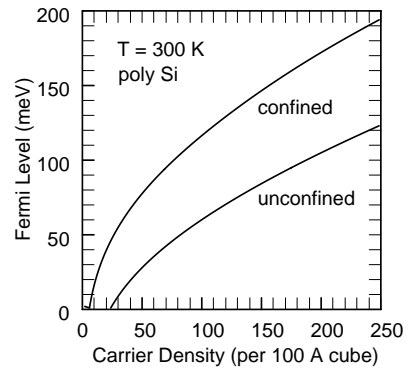
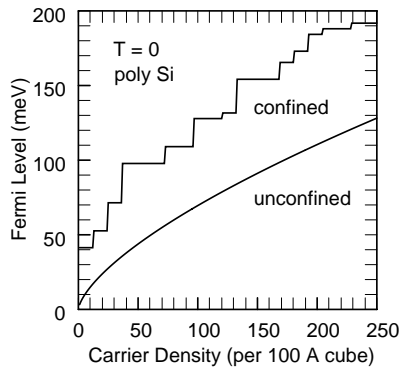


Fig. 1. Fermi levels as functions of the carrier concentration (number of carriers in a 100 Å cube) for carriers confined or unconfined to the cube volume.

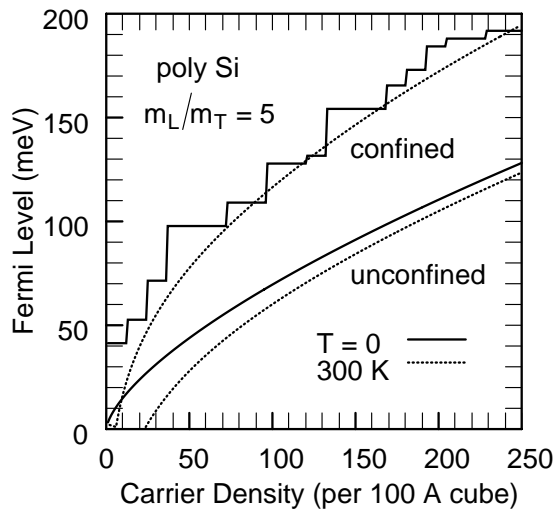


Fig. 2. Superimposed graphs 1a and 1b