

Selfconsistent Calculations of 2D Electron Gases
Bachelorproject, 2000

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Abstract

This is the abstract.

Books [2], [3], [4] and [1].

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1 Outline of this writing

This writing is parted in the following sections.

Contents This section list the sections, subsections and subsubsections of this writing along with pagenumbers.

Section 1 This section.

Section 2 This sections gives a short introduction the project and describes the main phycical aspects.

Section 3 This section describes the phycical system in detail and explains the important phycial properties.

Section 4 This section we introduce som numnericalmethods that we will use.

Section 5 This section we describe how we did the self consistent calculations of 2DEG.

Section 7 In this section we use our numnerical method to do calculations on a known testsample.

Section 8 This section evaluates the chosen numnerical methods and give comments on posible improvements.

Section 9 This section gives conclusion on project, what have we learned and

2 Introduction

This project is concerned with a special setup of semiconductors, which have special properties regarding the distribution of electrons. A large percentage of the free electrons seems - in one of the dimensions - to be concentrated in a very narrow area (about $5 - 10nm$). This distribution is called a 2 Dimensional Electron Gass or 2DEG in short, because the electrons is bounded in one of the dimensions.

The special setup of semiconductors is depicted in figure 1. The system is parted in two main parts. One consisting pimarily of GaAlAs and one consisting primarialy of GaAs.

Figure 1: A scematic figure of the speical setup of semicondiuctors, which we are considering in this project.

The GaAlAs is dopped with Si-atoms to get free electrons in the system. There electrons will seek toward the GaAs because of its lower quantum mecanical energi levels.

The electron will find an equilibrium between the gain in lower energi levels and the increased electical potential between the electrons and the positive atom cores.

In this project we will do self consistent calculations of the two dimentional electron gass. Hence do numnerical calculations of the electron distribution in the bounded dimension.

3 The physical system

In this section comes all the physics which is not directly concerned with the calculations of the self-consistent solutions. This includes but is not restricted to the following.

- The crystal.
- The doping of Si-atoms.
- Equation of state and other, constrained to one dimension.
- Electrons in two dimensions.
- Donors and acceptors (pollution of the crystal)
- Electrical potential at the surface.
- Temperature problems/influence.
- Nearly free electrons
- Bands
- Other things from chapter 6,7,8.
- Free electron gas in two dimensions.
- Bloch's Theorem
- Effective mass
- Energy gap (fig p1)
- Fermi-Dirac distribution function / Maxwell distribution

3.1 The setup

Figure 2: The physical system

3.2 The physical properties of the semiconductor setup

The special setup of semiconductors which we consider in the project have some special physical properties.

The two solid GaAlAs and GaAs have almost the same lattice constants. This means that the two systems can be considered equal when it comes to

Quantum mechanically the two systems differ quite a lot. Figure 3 shows how there is a difference of 0.3eV between ε_f of the two systems.

Figure 3: This figure describes the difference in the quantum mechanical energy levels of the two different solids.

3.3 Free electron gas in two dimensions

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) \quad (1)$$

$$\psi_n(\mathbf{r}) = \mathbf{A} \sin(\pi \mathbf{n}_x \mathbf{x} / L) \sin(\pi \mathbf{n}_y \mathbf{y} / L) \quad (2)$$

$$\psi(x + L, y) = \psi(x, y) \quad (3)$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (4)$$

$$k_x, k_y = \pm \frac{2\pi n}{L}, \quad n \in N \quad (5)$$

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \exp(i\mathbf{k} \cdot \mathbf{r}) = \epsilon_k \exp(i\mathbf{k} \cdot \mathbf{r}) \Leftrightarrow \quad (6)$$

$$-\frac{\hbar^2}{2m} (-k_x^2 - k_y^2) \exp(ik_x x + ik_y y) = \epsilon_k \exp(i\mathbf{k} \cdot \mathbf{r}) \Leftrightarrow \quad (7)$$

$$\epsilon_k = \frac{\hbar^2}{2m} (k_x^2 + k_y^2) \quad (8)$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = -i\hbar \nabla \psi_{\mathbf{k}}(\mathbf{r}) = \hbar \mathbf{k} \psi_{\mathbf{k}}(\mathbf{r}) \quad (9)$$

$$\epsilon_F = \frac{\hbar^2}{2m} k_F^2 \quad (10)$$

$$2 \frac{2\pi k_F^2}{(2\pi/L)^2} = \frac{k_F^2 L^2}{\pi} = \frac{k_F^2 A}{\pi} = N \quad (11)$$

$$k_F = \sqrt{\frac{N\pi}{A}} \quad (12)$$

$$\epsilon_F = \frac{\hbar^2 \pi N}{2mA} \quad (13)$$

$$\frac{\hbar \mathbf{k}}{m} = \frac{\hbar}{m} \sqrt{\frac{N}{A}} \quad (14)$$

$$N = \frac{2\epsilon_F A m}{\hbar^2 \pi} \quad (15)$$

$$D(\epsilon) = \frac{\partial N}{\partial \epsilon} \left(\frac{2\epsilon_F A m}{\hbar^2 \pi} \right) \quad (16)$$

$$= \frac{a A m}{\hbar^2 \pi} \quad (17)$$

3.4 Acceptors and doners

The GaAlAs is doped with Si to make doners of electrons to form the 2DEG. However not all electrons will be used to form the 2DEG, this is the result of carbon (C) pollutions of the two simiconductors.

The carbon atoms works as acceptors for the electrons and certain amount of the electrons will therefore be bounded by the carbon atoms. Figure 4 show the the carbon atoms binds some of the electrons.

Figure 4: This figure shows how the carbonatom pollution will bind some of the electrons.

3.5 Electical potential at the surface

The surface of the semiconductor will cause a distrubance in the electical potential. This have to be accounted for if we want to calculate the number of electrons bounded in the 2DEG.

Figure 5 shows how the surface change the electical potential.

Figure 5: This figure shows have the surface of the semiconductor have influence on the electical potential through the semiconductor.

4 Numerical methods

5 Selvconsistent calculations

In this section we will show how we do the selfconsistent calculations of the 2DEG.

The section is split up into several smaller sections, which each explains our progress toward the selfconsistent solution.

5.1 The general idea

In order to do the selfconsistent calculations of the 2DEG, we need to consider the two main equations of the system. The Schrödinger equation and the Poisson equation.

$$\frac{-\hbar^2}{2m}\psi''(z) + (\varphi(z)ez - \epsilon)\psi(z) = 0 \quad (18)$$

$$\varphi''(z) = \frac{(-N_d(z) + N_a(z) + |\psi(z)|^2N) e}{\epsilon^*} \quad (19)$$

The two equations are dependent on each other. That is, to calculate ψ you have to know φ , and to calculate φ you have to know ψ .

The general idea behind the selfconsistent calculations is to make an initial guess of φ , calculate ψ from this, then do a calculating φ which uses the newly found ψ . It is now possible to iterate between calculating ψ and φ , until the solutions converges.

We introduce the following notation for the different solutions.

ψ^p denotes the p'th calculation of ψ .

E_n^p denotes the p'th calculation of the n'th energy.

φ^p denotes the p'th calculation of the electrical potential.

this will endorse understanding the discussions.

5.2 Initial guess of the electrical potential, φ^0

To make an initial guess of the electrical potential, φ^0 , we need to do some considerations about the physical system.

If a lot of the electrons is located in the area where the crystal have changed from GaAlAs to GaAs, the electrical potential will be higher here. The electrical potential will be lower where the crystal have change from GaAs to GaAlAs, because of the extra charge in the "free" Si-atoms.

The potential could look like in figure 6.

Size of variables (z-size and energy).

Gaussbox and sawtooth.

Figure 6: The figure shows how the electrical potential may look like, when alot of the electrons is located just inside the GaAs.

5.3 Calculation of ψ^0 , first estimate of the statefunction

From the electrical potential (the guess), the Schro" dinger equation and an numerical method it is now possible to calculate

5.3.1 Asymtotic behavior, deformation of equation of state

Find the characteristic length

$$\left[\frac{\hbar^2}{2m} \right] = \text{Jm}^2 \quad (20)$$

$$[F_2] = \text{Jm}^{-1} \quad (21)$$

$$\left[\frac{\hbar^2}{2mF} \right] = \text{m}^3 \quad (22)$$

The eqation of state is (right side)

$$-\frac{\hbar^2}{2m}\psi''(z) + F_2z\psi(z) = \varepsilon\psi(z) \quad (23)$$

if we change coordinates like this

$$l = \left(\frac{\hbar^2}{2mF_2} \right)^{1/3} \quad \xi = z/l \quad (24)$$

$$\psi(z) = f(\xi/l) \Rightarrow \psi''(z) = \frac{1}{l^2}f''(\xi) \quad (25)$$

from this we get

$$-\frac{\hbar^2}{2ml^2}f''(\xi) + F_2l\xi f(\xi) - \varepsilon f(\xi) = 0 \quad (26)$$

$$-\frac{\hbar^2}{2mF_2l^3}f''(\xi) + \xi f(\xi) - \frac{\varepsilon}{F_2l}f(\xi) = 0 \quad (27)$$

$$-f''(\xi) + \left(\xi - \frac{\varepsilon}{F_2l} \right) f(\xi) = 0 \quad (28)$$

an change again

$$x = \xi - \frac{\varepsilon}{F_2 l} \quad (29)$$

$$g(x) = f\left(\xi - \frac{\varepsilon}{F_2 l}\right) \Rightarrow f''(\xi) = g''(x) \quad (30)$$

which gives

$$-g''(x) + xg(x) = 0 \quad (31)$$

The eqation of state is (left side)

$$-\frac{\hbar^2}{2m}\psi''(z) + F_1(z + \delta)\psi(z) = \varepsilon\psi(z) \quad (32)$$

if we change coordinates like this

$$l = \left(\frac{\hbar^2}{2mF_1}\right)^{1/3} \quad \xi = z/l \quad (33)$$

$$\psi(z) = f(\xi/l) \Rightarrow \psi''(z) = \frac{1}{l^2}f''(\xi) \quad (34)$$

from this we get

$$-\frac{\hbar^2}{2ml^2}f''(\xi) + F_1(l\xi + \delta)f(\xi) - \varepsilon f(\xi) = 0 \quad (35)$$

$$-\frac{\hbar^2}{2mF_1 l^3}f''(\xi) + \xi f(\xi)\left(\frac{\delta}{l} - \frac{\varepsilon}{F_1 l}\right) = 0 \quad (36)$$

$$-f''(\xi) + \left(\xi + \frac{\delta}{l} - \frac{\varepsilon}{F_1 l}\right) f(\xi) = 0 \quad (37)$$

and change again

$$x = \xi + \frac{\delta}{l} - \frac{\varepsilon}{F_1 l} \quad (38)$$

$$g(x) = f\left(\xi + \frac{\delta}{l} - \frac{\varepsilon}{F_1 l}\right) \Rightarrow f''(\xi) = g''(x) \quad (39)$$

which gives

$$-g''(x) + xg(x) = 0 \quad (40)$$

5.3.2 Asymtotic behavior

If the equation of state has the form

$$-g''(x) + xg(x) = 0 \quad (41)$$

it can be aproximated for $x \rightarrow \pm\infty$ as

$$A(x) = x^{-1/4} e^{\pm 2/3 x^{3/2}} \quad (42)$$

$$A'(x) = \left(\frac{-x^{-5/4}}{4} \pm x^{1/4} \right) e^{\pm 2/3 x^{3/2}} \quad (43)$$

$$(44)$$

This comes from the following

$$A(x) = x^\gamma e^{-\alpha x^\beta} \quad (45)$$

$$A'(x) = (\gamma x^{\gamma-1} - \alpha \beta x^{\beta+\gamma-1}) e^{-\alpha x^\beta} \quad (46)$$

$$A''(x) = (\gamma(\gamma-1)x^{\gamma-2} - (\alpha\beta\gamma + (\beta + \gamma - 1))x^{\beta+\gamma-2} + \alpha^2\beta^2 x^{2\beta+\gamma-2}) e^{-\alpha x^\beta} \quad (47)$$

Equation of state looks like this

$$0 = (\gamma(\gamma-1)x^{\gamma-2} + (\alpha\beta\gamma + (\beta + \gamma - 1))x^{\beta+\gamma-2} - \alpha^2\beta^2 x^{2\beta+\gamma-2}) e^{-\alpha x^\beta} + x x^\gamma e^{-\alpha x^\beta} \quad (48)$$

$$0 = \gamma(\gamma-1)x^{\gamma-2} - (\alpha\beta\gamma + (\beta + \gamma - 1))x^{\beta+\gamma-2} + \alpha^2\beta^2 x^{2\beta+\gamma-2} + x^{\gamma+1} \quad (49)$$

If this should be correct for $x \rightarrow \pm\infty$ the following should apply.

$$\gamma + 2\beta - 2 = 1 + \gamma \quad \wedge \quad -\alpha^2\beta^2 + 1 = 0 \Rightarrow \quad (50)$$

$$\alpha = \pm \frac{2}{3} \quad \wedge \quad \beta = \frac{3}{2} \quad (51)$$

Now follows

$$\frac{1}{2} x^{\gamma-2} (-2\gamma^2 + x^{\frac{3}{2}} + \gamma(2 + 4x^{\frac{3}{2}})) = 0 \quad (52)$$

This implies

$$4\gamma + 1 = 0 \Rightarrow \quad (53)$$

$$\gamma = \frac{-1}{4} \quad (54)$$

5.3.3 Asymtotic expantions (NOTES)

Shooting method. Border conditions.

Functionvalue and direvative should be the same at the fitting point.

We fix the functionvalue at one of the starting points, the functionvalue at the other and the energi are free variables. The direvative at both starting points are set according to a asymtotic expansion.

The asymtotic expansion are done by asuming a certain form of the solution. E.g. like this.

$$\psi(z) = z^\gamma e^{-\alpha z^\beta} \quad (55)$$

where γ, α, β are real numbers.

Putting this into the Shrödinger equation and doing a asymtotic behavior analysis will yill values for γ, α, β that fit with the physics in the Shrödinger equation.

5.3.4 Linear potential with wall (NOTES)

If we simplify our problem it is posible to do a analytical calculation of the wavefunction. If we assume the potential has to following restrictions

- The potential is infinity in GaAlAs
- The potential grows linear in the GaAs

Figure 5.3.4 shows the simplification.

Figure 7: Potential with linear wall

With there restrictions it is posible to do analytic calculations of the wavefunction. The Schrödinger equation now looks like this

$$-\frac{\hbar^2}{2m}\psi'' + Fz\psi = \mathcal{E}\psi \quad (56)$$

where F is the slope of the potential.

This is ψ''

$$\left[\gamma(\gamma - 1)z^{\gamma-2} - \alpha\beta(\beta + \gamma - 1)z^{\beta+\gamma-2} - \alpha\beta\gamma z^{\gamma+\beta-2} + \alpha^2\beta^2 z^{2\beta+\gamma-2} \right] e^{-\alpha z^\beta} \quad (57)$$

This is the asymtotic calculation

$$-\psi'' + z\psi = \mathcal{E}\psi \quad (58)$$

$$-\left(\gamma(\gamma-1)z^{\gamma-2} - \alpha\beta(\beta+\gamma-1)z^{\beta+\gamma-2} - \alpha\beta\gamma z^{\gamma+\beta-2} + \alpha^2\beta^2 z^{2\beta+\gamma-2}\right) + z^{\gamma+1} = \epsilon z^\gamma \quad (59)$$

$$-\gamma(\gamma-1)z^{\gamma-2} + (\alpha\beta(\beta+\gamma-1) + \alpha\beta\gamma) z^{\beta+\gamma-2} - \alpha^2\beta^2 z^{2\beta+\gamma-2} = -z^{\gamma+1} + \epsilon z^\gamma \quad (60)$$

$$2\beta + \gamma - 2 = \gamma + 1 \quad (61)$$

$$2\beta = 3 \quad (62)$$

$$\beta = \frac{3}{2} \quad (63)$$

$$-\alpha^2\beta^2 = -1 \quad (64)$$

$$\alpha\beta = \pm 1 \quad (65)$$

$$\alpha \frac{3}{2} = \pm 1 \quad (66)$$

$$\alpha = \pm \frac{2}{3} \quad (67)$$

5.4 Calculation of φ^1 , second estimate of the potential

Known potentials (bands, and other).

5.4.1 The electrical potential, $\phi(z)$

We know the electrical potential, $\phi(z)$, at z_a :

$$\phi(z_a) = 1.35eV \quad (68)$$

$$\phi'(z_a) = 0 \quad (69)$$

$$\phi''(z_a) = N_a \quad (70)$$

Because $\phi''(z)$ is constant in $[z_e, z_a]$ we can calculate $\phi(z_e)$ and $\phi'(z_e)$.

$$\phi(z_e) = \frac{-eN_a}{2\epsilon_a}(z - z_a)^2 + 1.35eV \quad (71)$$

$$\phi'(z_e) = \frac{-eN_a}{\epsilon_a}(z - z_a) \quad (72)$$

5.4.2 NOTES

ϵ_f is calculated from

$$\epsilon_f = \frac{\hbar^2 \pi N^{2d}}{2m} \quad (73)$$

μ_0 from

$$\mu_0 = \phi(0)^{run} \epsilon_f - \epsilon_0^{run} \quad (74)$$

$\Delta = 0.3eV$, gab at surface is $0.8eV$.

At z_a we have the following

$$\phi(z_a) = 1.35eV(1.4eV) \quad (75)$$

$$\phi'(z_a) = 0 \text{ no more acceptors} \quad (76)$$

$$z_a \text{ is unknown} \quad (77)$$

At z_e we have the following

$$\phi(z_e) = -1/2N_a(z - z_a)^2 + \quad (78)$$

$$\phi'(z_a) = 0 \text{ no more acceptors} \quad (79)$$

$$z_a \text{ is unknown} \quad (80)$$

$$\varphi(z) = Az^2 + Bz + C \quad (81)$$

$$\varphi'(z) = 2Az + B \quad (82)$$

$$\varphi''(z) = 2A \quad (83)$$

$$\varphi(z_a) = k \quad (84)$$

$$\varphi'(z_a) = 0 \quad (85)$$

$$\varphi''(z) = -\frac{eN_a}{\epsilon_a} \Rightarrow \quad (86)$$

$$A = -\frac{eN_a}{2\epsilon_0} \quad (87)$$

$$-2\frac{eN_a}{2\epsilon_0}(z_a) + B = 0 \quad (88)$$

$$-\frac{eN_a}{2\epsilon_0}z_a^2 + Bz_a + C = k \quad (89)$$

$$-2\frac{eN_a}{2\epsilon_0}(z_a)^2 + Bz_a = 0 \quad (90)$$

$$+\frac{eN_a}{2\epsilon_0}(z_a)^2 + C = k \quad (91)$$

$$-\frac{eN_a}{2\epsilon_0}(z_a)^2 + k = C \quad (92)$$

$$\varphi(z) = -\frac{eN_a}{2\epsilon_0}z^2 + 2\frac{eN_a}{2\epsilon_0}(z_a)z - \frac{eN_a}{2\epsilon_0}(z_a)^2 + k \quad (93)$$

$$\varphi(z) = -\frac{eN_a}{2\epsilon_0}(z - z_a)^2 + k \quad (94)$$

$$(95)$$

$$\varphi(z) = Az^2 + Bz + C \quad (96)$$

$$\varphi'(z) = 2Az + B \quad (97)$$

$$\varphi''(z) = 2A \quad (98)$$

$$\varphi(z_s) = k_1 \quad (99)$$

$$\varphi'(z_s) = k_2 \quad (100)$$

$$\varphi'(z_s) = \varphi'(z_c) \quad (101)$$

$$\varphi(z_t) = k_3 \quad (102)$$

$$\phi(z_c) = \varphi(z_t) + \varphi'(z_c)(z_c - z_t) \quad (103)$$

$$\phi(z_c) = k_3 + \varphi'(z_c)(z_c - z_t) \quad (104)$$

$$\varphi''(z) = \frac{-eN_d}{\epsilon_d} = k_4 \Rightarrow A = k_4/2 \quad (105)$$

$$2A = \frac{-eN_d}{\epsilon_d} = k_4 \quad (106)$$

$$k_4 z_s + B = k_2 \Rightarrow B = k_2 - k_4 z_s \quad (107)$$

$$Az_s^2 + Bz_s + C = k_1 \Rightarrow \frac{k_4}{2} z_s^2 + (k_2 - k_4 z_s) z_s + C = k_1 \quad (108)$$

$$C = k_1 - \frac{k_4}{2} z_s^2 - (k_2 - k_4 z_s) z_s \quad (109)$$

$$\varphi(z) = \frac{k_4}{2} z^2 + (k_2 - k_4 z_s) z + k_1 - \frac{k_4}{2} z_s^2 - (k_2 - k_4 z_s) z_s \quad (110)$$

$$\varphi(z_c) = \frac{k_4}{2} z_c^2 + (k_2 - k_4 z_s) z_c + k_1 - \frac{k_4}{2} z_s^2 - (k_2 - k_4 z_s) z_s = \phi(z_c) \quad (111)$$

$$k_3 + (2Az_c + B)(z_c - z_t) = \frac{k_4}{2} z_c^2 + (k_2 - k_4 z_s) z_c + k_1 - \frac{k_4}{2} z_s^2 - (k_2 - k_4 z_s) z_s \quad (112)$$

$$k_3 + (k_4 z_c + k_2 - k_4 z_s)(z_c - z_t) = \frac{k_4}{2} z_c^2 + (k_2 - k_4 z_s) z_c + k_1 - \frac{k_4}{2} z_s^2 - (k_2 - k_4 z_s) z_s \quad (113)$$

5.5 The iterations

5.6 The solutions, N_d , ψ and φ

6 Program description

Listing of program and description of it.

6.1 psitest.c

```

#include <stdio.h>
#include <math.h>
#define NRANSI
#include "nrutil.h"
#define N1 1
#define N2 2

#define LAMMAX 10000 /* Max number of points in lambda function */
#define iprange 8 /* number of points used to interpolate functional values */
#define EPS 1e-8 /* used in normfiles. */

#define meV_J (1000.0/echargeSI) /* meV per J */
#define nm_m (1.0e9) /* nm per m */
#define ddeltaEV 300 /* meV */
#define emass 0.067*9.109389e-31 /* kg */
#define hbarSI 1.05457266e-34 /* Js */
#define hbarEV (hbarSI*meV_J)
#define echargeSI 1.60217733e-19 /* C */
#define echargeEV echargeSI
#define vacpermSI 8.854187817e-12 /* F/m */
#define vacpermEV (vacpermSI/meV_J/nm_m)
#define NSI 1e15 /* elec/m^2 */
#define NEV (NSI/nm_m/nm_m)
#define pi 3.14159
#define N NEV
#define hbar hbarEV
#define ddelta ddeltaEV
#define vacperm vacpermEV
#define echarge echargeEV
#define hbarhbar (hbar*hbar)
#define K (echarge*1e15)
#define Zs -10 /* nm */
#define Ze 50 /* nm */
#define phiza 1350 /* meV */
#define NaSI 5e20 /* acceptor density 1/m^3 */
#define NaEV (NaSI/nm_m/nm_m/nm_m)
#define Na NaEV
#define epsilon_F hbarhbar*pi*N/2/emass
int m,n,mm,ll,no;
double m0,m1,e0,x0,dx,kappa;
int nn2,nvar,kmax,kount,kp,kq, NTOT;
double x1,x2,xf,*xp,**yp,*xq,**yq,dxsav,dxp,dxq,lambda,dlambda,**xx,*lam;
double mo,m1,e0;
double delta, delta2, ddelta2;
double F1, F2;
double E;
int calpsi; /* if we are calculating psi or phi */
double **psidata;
unsigned long psidatalength;
double potential(double);
double psimarkmark(double psi, double x, double e);
void fileprint(char *);
double psipsi(double);
double myEPS;

/* functions from Numerical Recipies */
void polint(double xa[],double ya[], int n, double x, double *y, double *dy);
void locate(double xx[], unsigned long n, double x, unsigned long *j);
double qromb(double (*func)(double), double, double);

```

```

double ident(double x)
{
    printf( "x: %e\n", x);
    return(x*x);
};

int main(void) /* Program osc.c - 1D harmonic oscillator */
{
    void newt(double x[], int n, int *check,
              void (*vecfunc)(int, double [], double []));
    void shootf(int n, double v[], double f[]);

    int check, i;
    double *v1,*v2,*v;
    double a;

    myEPS = EPS;
    NTOT=3; /* SKAL PUDSES AF!!! */
    v = dvector(1,NTOT);
    v1 = v;
    nvar = NTOT;
    nm2 = N2;
    kmax = 10000; /* Max number of points in solution */
    xp = dvector(1,kmax);
    xq = dvector(1,kmax);
    yp = dmatrix(1,nvar,1,kmax);
    yq = dmatrix(1,nvar,1,kmax);
    psidata = dmatrix(1, 2, 1, 2*kmax);
    /*F=eN/2epsilon */
    F2= (echarge/vacperm)*N*echarge/2; /* Calculated from the Gauss-box. */
    F1=F2;
    ddelta2 = 0+epsilon_F; /* \varepsilon_0+\epsilon_F */
    delta = ddelta/F1;
    delta2 = ddelta2/F2;
    printf("echarge: %e, vacperm: %e, N: %e, F2: %e, delta: %e\n", echarge, vacperm, N, F2, delta);

    printf("\nInput E: ");
    if (scanf("%lf",&v1[2]) == EOF) exit(0);

    /* calculate psi */
    NTOT=3;
    v2 = &v[N2];
    v2[1]=v1[2];
    calpsi = 1;
    x1 = Zs; /*left startpoint for shooting nm*/
    x2 = Ze; /*right startpoint for shooting nm*/
    xf = 0; /*fitting point nm*/
    dxq = (xf-x1)/500.0;
    dxp = (x2-xf)/500.0;
    newt(v,NTOT,&check,shootf);
    if (check) {
        printf("shootf failed; bad initial guess\n");
    } else {
        E=v1[2];
        psidatalength = kq+kp-1;
        for(i=1;i<=kq; i++){
            psidata[1][i]= xq[i];
            psidata[2][i]= yq[1][i];
        }
        for(i=1;i<kp; i++){
            psidata[1][kq+i]= xp[kp-i];
            psidata[2][kq+i]= yp[1][kp-i];
        }
        a=qromb(psipsi, x1, 26);

        a=1/sqrt(a);
    }
}

```

```

    for(i=1; i<=psidatalength; i++)
    {
psidata[2][i] *= a;
    };

    ddelta2=E+epsilon_F;
    /* 2519 */
    /* Calculate phi */
    NTOT=2;
    nvar=NTOT;
    calpsi = 0;
    v2 = &v[1];
    v1[1]=F2;
    v2[1]=2000;
    x1=0;
    x2=Ze;
    xf = (x1+x2)/2.; /*fitting point nm*/
    newt(v,NTOT,&check,shootf);

    fileprint("osc.");
}
free_dvector(v,1,NTOT);
free_dvector(xp,1,kmax);
free_dvector(xq,1,kmax);
free_dmatrix(yp,1,nvar,1,kmax);
free_dmatrix(yq,1,nvar,1,kmax);
free_dmatrix(psidata, 1, 2, 1, 2*kmax);
return 0;
};

void load1(double x1, double v1[], double y[])
{
    double x;
    double l;

    if(calpsi)
    {
        y[3]= v1[2];
        l=pow(hbarhbar/(2*emass*F1),1./3.);
        x=(x1+delta-y[3]/F1)/l;
        y[1] = v1[1] ; /* psi(x1) */
        y[2]=(-1./(4.*x)-sqrt(x))*y[1];

        printf ("Load 1: y1: %e, y2: %e, y3: %e x: %e\n",y[1], y[2],y[3], x);
    }
    else
    {
        y[1]=-ddelta2;
        y[2]=v1[1];
        printf("Load 1 (phi): y1: %e, y2: %e\n",y[1], y[2]);
    }
}

void load2(double x2, double v2[], double y[])
{
    double x, l;

    if (calpsi)
    {
        y[3] = v2[1];
        l=pow(hbarhbar/(2*emass*F2),1./3.);
        x=(x2+delta2-y[3]/F2)/l;
        y[1] = 1e-8;
        y[2]=(-1./(4.*x)+sqrt(x))*y[1];
        printf ("Load 2: y1: %e, y2: %e, y3: %e x: %e\n",y[1], y[2],y[3], x);
    }
    else
    {
        y[1]=Na*(echarge*echarge)/vacperm*(-1./2.*x2+2*x2*v2[1]-1./2.*v2[1]*v2[1]);
    }
}

```

```

        y[2]=Na*(echarge*echarge)/vacperm*(v2[1]-x2);
        printf ("Load 2 (phi): y1: %e, y2: %e, za: %e\n",y[1], y[2], v2[1]);
    }
}

void score(double xf, double y[], double f[])
{
    int i;

    for (i=1;i<=NTOT;i++) f[i]=y[i];
}

void derivs(double x, double y[], double dydx[])
{
    if(calpsi)
    {
        dydx[1] = y[2];
        dydx[2] = psimarkmark(y[1],x,y[3]);
        dydx[3] = 0;
        /* printf("x: %f, dydx[1]: %e, dydx[2]: %e, (potential(x), y[3]): %f,%f\n", x, dydx[1], dydx[2], potential(x),y[3]); */
    }
    else
    {
        dydx[1] = y[2];
        dydx[2] = -(psipsi(x)*N+Na)*(-echarge)*(-echarge)/vacperm;
        /* printf("x: %f, dydx[1]: %e, dydx[2]: %e\n", x, dydx[1], dydx[2]);*/
    }
}

double psimarkmark(double psi, double x, double e)
{
    return((potential(x)-e)*psi)*2*emass/hbarhbar/K;
}

double potential(double z)
{
    if (z<=0)
    {
        return(z*F1+ddelta-ddelta2);
    }
    else
    {
        return(z*F2-ddelta2);
    }
}

double psi(double x)
{
    unsigned long j, intmin;
    double psival, error;

    /* printf("psi(%e) =", x);*/
    locate(psidata[1],psidatalength,x,&j);
    intmin = IMIN(IMAX(j- (iprange-1)/2,1),psidatalength+1-iprange);
    polint(&psidata[1][intmin], &psidata[2][intmin], iprange, x, &psival, &error);
    /* printf("%f, %d, %d, %e\n", psival,intmin, j, psidata[1][intmin]); */
    return(psival);
};

double psipsi(double x)
{
    double val;
    val = psi(x);
    val *=val;
    /* printf("psipsi(%f) =%f\n", x, val); */
    return(val); /* Im(psi(x))=0 => |psi|^2 = psi^2 */
};

void fileprint(char *name)
/*

```

```

print the solution to file
*/
{
FILE *fout;
char filename[80];
int i, j;
double x;
for (j=1;j<=nvar;j++)
{
sprintf(filename, "%s%.2d",name,j);
fout = fopen(filename,"w");
if (fout==0) {printf("Error: Can't open %s\n",name); exit(0);}

for (i=1;i<=kq;i++)
{
fprintf(fout,"%e %e\n",xq[i], yq[j][i]);
}
for (i=kp-1;i>=1;i--)
{
fprintf(fout,"%e %e\n",xp[i],yp[j][i]);
}
fclose(fout);

};
/*
print psipsi
*/
sprintf(filename, "%spsipsi",name);
fout = fopen(filename,"w");
if (fout==0) {printf("Error: Can't open %s\n",name); exit(0);}

for (x=x1;x<=26; x+=1)
{
fprintf(fout,"%e %e\n", x, psipsi(x)*1000);
}

/* for (i=1;i<=psidatalength;i++) */
/* { */
/* fprintf(fout,"%e %e\n", psidata[1][i], psidata[2][i]); */
/* } */

fclose(fout);

/*
print the potential
*/
sprintf(filename, "%spot",name);
fout = fopen(filename,"w");
if (fout==0) {printf("Error: Can't open %s\n",name); exit(0);}

for (i=1;i<=kq;i++)
{
fprintf(fout,"%e %e\n",xq[i], potential(xq[i]));
}
for (i=kp-1;i>=1;i--)
{
fprintf(fout,"%e %e\n",xp[i],potential(xp[i]));
}
fclose(fout);

/*
print psi''
*/

sprintf(filename, "%smarkmark",name);
fout = fopen(filename,"w");
if (fout==0) {printf("Error: Can't open %s\n",name); exit(0);}

for (i=1;i<=kq;i++)
{
fprintf(fout,"%e %e\n",xq[i], psimarkmark(yq[1][i],xq[i], E));
}

```

```
    }  
    for (i=kp-1;i>=1;i--)  
    {  
        fprintf(fout,"%e %e\n",xp[i],psimarkmark(yp[1][i],xp[i], E));  
    }  
    fclose(fout);  
};
```

7 Test sample

8 Evaluation of the nummerical method

9 Conclusion

10 Notes

Characteristic length.

$$V(z) = -e\phi(z)\theta(z)\Delta \quad (114)$$

$$\phi_0 = -(\varepsilon_F + \varepsilon_0) \quad (115)$$

$$\varepsilon_F = \frac{\pi\hbar^2}{m}n^{2d} \quad (116)$$

$$E_{n,k} = E_n + \frac{\hbar^2 k^2}{2m} \quad (117)$$

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