Finite wire in a magnetic field with a Gauss potential

– Web Version –

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Contents

1 Introduction

Electrons moving in a infinitely long wire is a well known problem and rather easily solved. But what if the wire is finite in length and in a constant magnetic field, perpendicular to the wire? This system cannot be solved analytically. Therefore, one must search the toolbox of numerical methods. Our task is to find the eigenvalues and eigenvectors of the Hamiltonian of our system. We will turn it into a eigenvalue problem of an infinite matrix but solve it for a finite one (numerical part). To add a little extra fun to the system, we also place a Gauss potential in the wire and look for bound states.

2 Description of the system

2.1 The Basic System with Magnetic Field

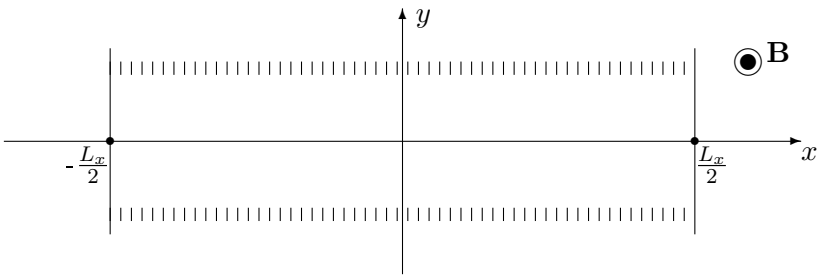

Figure 1. Diagram of the system – a finite length wire in a constant magnetic field and central Gauss potential (not depicted).

The system is depicted on figure 1. The length of the wire stub is L_x and we assume parabolic confinement in the y-direction of strength Ω_0. The basic Hamiltonian is thus

$$\hat{H}_{\text{basic}} = \tfrac{1}{2m}\hat{\mathbf{P}}^2 + \tfrac{1}{2}m\Omega_0^2\hat{Y}^2 \qquad -\tfrac{1}{2}L_x < \hat{X} < \tfrac{1}{2}L_x \tag{1}$$

where $\hat{\mathbf{P}}$ is the conjugate momentum operator, m the effective mass of the electron and $\hat{X}$ and $\hat{Y}$ are the x- and y-position operators.

Now we consider the potential due to a constant magnetic field in the z direction, $\mathbf{B}(\mathbf{r}) = B\boldsymbol{e}_z$. Because of the magnetic field, the operator denoting mechanical momentum ($\frac{1}{2m}\hat{\mathbf{P}}^2$) no longer depends on $\hat{\mathbf{P}}$ only. We need the substitution

$$\hat{\mathbf{P}} \mapsto \hat{\mathbf{P}} - e\hat{\mathbf{A}}(\hat{\mathbf{R}}) \tag{2}$$

where e is the charge of an electron and $\hat{\mathbf{A}}$ is a vector field dependent on position $\hat{\mathbf{R}} = (\hat{X}, \hat{Y}, \hat{Z})$, such that $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ [1, pp. 315-322]. We choose the Landau gauge, i.e.

$$\mathbf{A}(\mathbf{r}) = -By\boldsymbol{e}_x = (-By, 0, 0) \tag{3}$$

Our Hamiltonian is thus, putting eqs. (1), (2) and (3) together,

$$\begin{aligned}\hat{H}_0 &= \tfrac{1}{2m}(\hat{\mathbf{P}} + eB\hat{Y}\boldsymbol{e}_x)^2 + \tfrac{1}{2}m\Omega_0^2\hat{Y}^2 \\ &= \tfrac{1}{2m}\left[(\hat{P}_x + eB\hat{Y})^2 + \hat{P}_y^2 + \hat{P}_z^2\right] + \tfrac{1}{2}m\Omega_0^2\hat{Y}^2 \end{aligned} \tag{4}$$

We note that in the z direction we have the Hamiltonian of a free particle. We therefore ignore that part of the Hamiltonian and concentrate on the behaviour of the particle in the x and y direction. Thus we have

$$\begin{aligned}\hat{H}_0 &= \tfrac{1}{2m}\left[(\hat{P}_x + eB\hat{Y})^2 + \hat{P}_y^2\right] + \tfrac{1}{2}m\Omega_0^2\hat{Y}^2 \\ &= \tfrac{1}{2m}\hat{P}_x^2 + \left[\tfrac{1}{2m}\hat{P}_y^2 + \tfrac{1}{2}m\Big(\underbrace{\big(\tfrac{eB}{m}\big)^2}_{\equiv\omega_c^2} + \Omega_0^2\Big)\hat{Y}^2\right] + \tfrac{eB}{m}\hat{P}_x\hat{Y} \\ &= \tfrac{1}{2m}\hat{P}_x^2 + \left[\tfrac{1}{2m}\hat{P}_y^2 + \tfrac{1}{2}m\Omega_\omega^2\hat{Y}^2\right] + \tfrac{\hbar}{ml^2}\hat{P}_x\hat{Y}, \qquad -\tfrac{1}{2}L_x < \hat{X} < \tfrac{1}{2}L_x \end{aligned} \tag{5}$$

where we have set $\Omega_\omega^2 = \Omega_0^2 + \omega_c^2$ and $l^2 = \frac{\hbar}{eB} = \frac{\hbar}{m\omega_c}$; l is the characteristic length of the system. We see that the system consists of a infinite potential well in the x direction

$$\hat{H}_x = \tfrac{1}{2m}\hat{P}_x^2, \qquad -\tfrac{1}{2}L_x < \hat{X} < \tfrac{1}{2}L_x, \tag{6}$$

a harmonic oscillator with frequency Ω_ω in the y direction

$$\hat{H}_y = \frac{1}{2m}\hat{P}_y^2 + \frac{1}{2}m\Omega_\omega^2\hat{Y}^2 \tag{7}$$

and a coupled perturbation in the x and y direction

$$\hat{W} = \frac{\hbar}{ml^2}\hat{P}_x\hat{Y} = \omega_c\hat{P}_x\hat{Y}\,. \tag{8}$$

We will exploit this representation of the Hamiltonian,

$$\hat{H}_0 = \hat{H}_x + \hat{H}_y + \hat{W}, \tag{9}$$

in our numerical calculations (see section 3).

2.2 Gauss Potential

To play a little with the system previously described, we additionally place a Gauss potential at the centre of our wire. Then we must add the term

$$\hat{W}_G = -V_0\exp(-\beta_1^2\hat{X}^2 - \beta_2^2\hat{Y}^2) \tag{10}$$

to $\hat{H}_0$, where $V_0, \beta_1, \beta_2 \in \mathbb{R}$, thus obtaining the new Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{W}_G\,. \tag{11}$$

3 Numerical Method

3.1 The basic idea

Our approach (see [3]) is to write the eigenstates of the Hamiltonian $\hat{H}$, $|\alpha)$, as a linear combination of the vectors in the well known complete orthonormal basis $\{|\alpha\rangle\}$ consisting of the eigenstates of the Hamiltonian $\hat{H}_x+\hat{H}_y$, i.e. the (tensor) product of the eigenstates of $\hat{H}_x$ (infinite square well) and the eigenstates of $\hat{H}_y$ (harmonic oscillator), $|\alpha\rangle = |nk\rangle = |\varphi_n\rangle|\psi_k\rangle$ with some bijection $\alpha \leftrightarrow (n,k)$. Thus

$$|\alpha) = \sum_\beta |\beta\rangle\langle\beta|\alpha\rangle = \sum_\beta C_{\beta\alpha}|\beta\rangle \tag{12}$$

Let E_α and ε_α be the eigenvalues of $|\alpha\rangle$ and $|\alpha)$, respectively. Now,

$$\langle\beta|\hat{H}|\gamma\rangle = \langle\beta|\hat{H}_x + \hat{H}_y + \hat{W} + \hat{W}_G|\gamma\rangle = E_\gamma\delta_{\beta\gamma} + \langle\beta|\hat{W} + \hat{W}_G|\gamma\rangle \tag{13}$$

Multiplying each side by $C_{\gamma\alpha}$ and summing over γ gives

$$\langle\beta|\hat{H}\left[\sum_\gamma C_{\gamma\alpha}|\gamma\rangle\right] = \sum_\gamma C_{\gamma\alpha}\left[E_\gamma\delta_{\beta\gamma} + \langle\beta|\hat{W} + \hat{W}_G|\gamma\rangle\right] \tag{14}$$

that is, by eq. (12) and since $\hat{H}|\alpha) = \varepsilon_\alpha|\alpha)$,

$$\sum_\gamma \varepsilon_\alpha C_{\gamma\alpha}\langle\beta|\gamma\rangle = \sum_\gamma C_{\gamma\alpha}\left[E_\gamma\delta_{\beta\gamma} + \langle\beta|\hat{W} + \hat{W}_G|\gamma\rangle\right] \tag{15}$$

thus giving

$$\varepsilon_\alpha C_{\beta\alpha} = \sum_\gamma C_{\gamma\alpha}\left[E_\gamma\delta_{\beta\gamma} + \langle\beta|\hat{W} + \hat{W}_G|\gamma\rangle\right] \tag{16}$$

This is an eigenvalue problem for the infinite dimensional matrix with elements

$$A_{\beta\gamma} = E_\gamma\delta_{\beta\gamma} + \langle\beta|\hat{W} + \hat{W}_G|\gamma\rangle \tag{17}$$

where ε_α are the eigenvalues with corresponding eigenvectors $[C_{1\alpha}\ C_{2\alpha}\ \cdots]^T$. The numerical step is to truncate the basis $\{|\alpha\rangle\}$ and solve the (then finite) eigenvalue problem (16). The accuracy of the results can be checked by varying the size of the basis $\{|\alpha\rangle\}$.

3.2 The basis and its eigenvalues

As mentioned above, we will need a bijection between the parameter α and the pair (n,k) to determine the basis $|\alpha\rangle = |nk\rangle$ uniquely. Our choice is to decide how many of the vectors $|\varphi_n\rangle$ and $|\psi_k\rangle$ to use. Denote these numbers N_x and N_y, respectively, and set

$$\alpha = n + kN_x \tag{18}$$

where $n \in [\![1, N_x]\!]$ and $k \in [\![0, N_y - 1]\!]$, see figure 2.

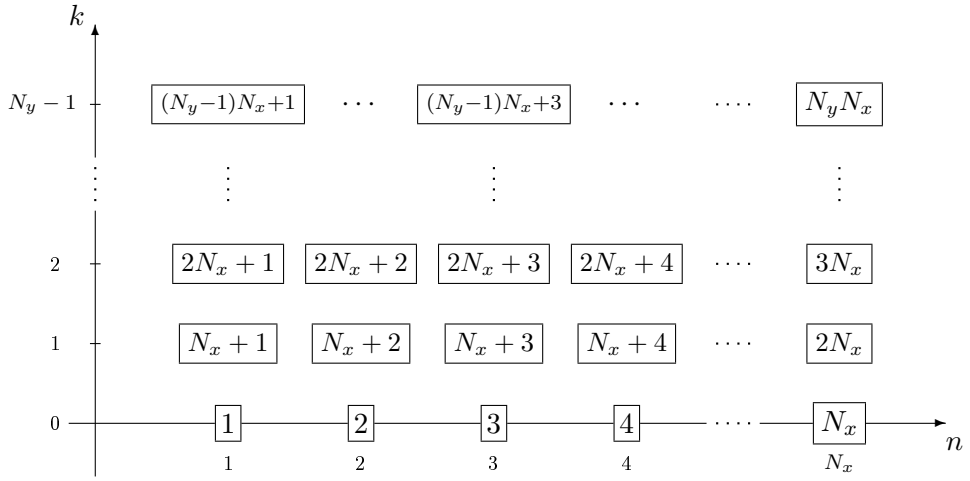

Figure 2. A graph of α as a function of (n, k).

Having decided upon the bijection, we will henceforth use $|nk\rangle$ and E_{nk} in our discussion, instead of $|\alpha\rangle$ and E_α.

We know that

$$E_{nk} = E_n^x + E_k^y \tag{19}$$

where E_n^x is the eigenvalue of $\hat{H}_x$ corresponding to $|\varphi_n\rangle$ and E_k^y is the eigenvalue of $\hat{H}_y$ corresponding to $|\psi_k\rangle$. Now, $\hat{H}_x$ is the Hamiltonian for an infinite square well between $x = -L_x/2$ and $x = L_x/2$, and thus

$$E_n^x = \frac{\hbar^2 n^2 \pi^2}{2mL_x^2} = \hbar\Omega_\omega \frac{a_\omega^2}{L_x^2}\frac{n^2\pi^2}{2} \tag{20}$$

where $a_\omega^2 = \frac{\hbar}{m\Omega_\omega} = \frac{\omega_c}{\Omega_\omega} l^2$. Also, $\hat{H}_y$ is the Hamiltonian for a harmonic oscillator with frequency Ω_ω, so

$$E_k^y = \hbar\Omega_\omega \left(k + \frac{1}{2}\right) . \tag{21}$$

Combining these, we have

$$E_{nk} = \hbar\Omega_\omega \left[k + \frac{1}{2} + \frac{a_\omega^2}{L_x^2}\frac{n^2\pi^2}{2}\right] . \tag{22}$$

3.3 Matrix elements

Each matrix element in eq. (17) is the sum of

$$E_{nk}\delta_{n'n}\delta_{k'k}, \qquad \langle n'k'|\hat{W}|nk\rangle \qquad \text{and} \qquad \langle n'k'|\hat{W}_G|nk\rangle .$$

The first term was found in eq. (22) but we need to find a formula for the other two.

We note that by eq. (8)

$$\langle n'k'|\hat{W}|nk\rangle = \omega_c \langle\varphi_{n'}|\hat{P}_x|\varphi_n\rangle\langle\psi_{k'}|\hat{Y}|\psi_k\rangle \tag{23}$$

Since

$$\varphi_n(x) = \begin{cases} \sqrt{\frac{2}{L_x}}\cos\left(\frac{n\pi x}{L_x}\right), & \text{if } n = 1,3,5,\ldots \\ \sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi x}{L_x}\right), & \text{if } n = 2,4,6,\ldots \end{cases} \tag{24}$$

it is easy to calculate

$$\langle\varphi_{n'}|\hat{P}_x|\varphi_n\rangle = \mathrm{i}\hbar\langle\varphi_{n'}|\hat{\partial}_x|\varphi_n\rangle = \begin{cases} 0 & , \quad \text{if } n+n' \equiv_2 0 \\ -\dfrac{4\mathrm{i}\hbar}{L_x}\dfrac{nn'}{n^2-n'^2} & , \quad \text{if } n+n' \equiv_4 1 \\ \dfrac{4\mathrm{i}\hbar}{L_x}\dfrac{nn'}{n^2-n'^2} & , \quad \text{if } n+n' \equiv_4 3 \end{cases} \tag{25}$$

$$= \left(1-(-1)^{n+n'}\right)(-1)^{(n+n'+1)/2}\,\frac{2\mathrm{i}\hbar}{L_x}\,\frac{nn'}{n^2-n'^2} \tag{26}$$

With the help of ladder operators we obtain

$$\langle\psi_{k'}|\hat{Y}|\psi_k\rangle = \sqrt{\frac{a_\omega^2}{2}}\left[\sqrt{k+1}\,\delta_{k',k+1} + \sqrt{k}\,\delta_{k',k-1}\right] \tag{27}$$

see [1, p. 499]. Putting eqs. (23), (26) and (27) together,

$$\begin{aligned}\langle n'k'|\hat{W}|nk\rangle = {} & \left(1-(-1)^{n+n'}\right)(-1)^{(n+n'+1)/2}\,\mathrm{i}\hbar\omega_c\sqrt{2\frac{a_\omega^2}{L_x^2}} \\ & \times\frac{nn'}{n^2-n'^2}\left[\sqrt{k+1}\,\delta_{k',k+1} + \sqrt{k}\,\delta_{k',k-1}\right]\end{aligned} \tag{28}$$

By eq. (10)

$$\langle n'k'|\hat{W}_G|nk\rangle = -V_0\langle\varphi_{n'}|\exp(-\beta_1^2\hat{X}^2)|\varphi_n\rangle\langle\psi_{k'}|\exp(-\beta_2^2\hat{Y}^2)|\psi_k\rangle \equiv -V_0 I^x_{n'n} I^y_{k'k} \tag{29}$$

Now, from eq. (24) we see that if $n+n' \equiv_2 1$, then $\varphi^*_{n'}(x)\varphi_n(x)\mathrm{e}^{-\beta_1^2x^2}$ is an odd function. Hence

$$I^x_{n'n} = \langle\varphi_{n'}|\exp(-\beta_1^2\hat{X}^2)|\varphi_n\rangle = 0 \qquad \text{if } n+n' \equiv_2 1 \tag{30}$$

since the integration interval is symmetric. On the other hand, if $n+n' \equiv_2 0$, then

$$\begin{aligned} I^x_{n'n} &= \frac{2}{L_x}\int_{-L_x/2}^{L_x/2}\sin\left(\frac{n'\pi x}{L_x}\right)\sin\left(\frac{n\pi x}{L_x}\right)\mathrm{e}^{-\beta_1^2x^2}\,\mathrm{d}x \\ &= \frac{2}{\pi}\int_0^{\pi/2}\left(\cos(n-n')x - \cos(n+n')x\right)\mathrm{e}^{-\alpha_1^2x^2}\,\mathrm{d}x \qquad (n+n' \equiv_4 0) \end{aligned} \tag{31}$$

or

$$I^x_{n'n} = \frac{2}{L_x}\int_{-L_x/2}^{L_x/2} \cos\left(\frac{n'\pi x}{L_x}\right)\cos\left(\frac{n\pi x}{L_x}\right)\mathrm{e}^{-\beta_1^2x^2}\,\mathrm{d}x$$
$$= \frac{2}{\pi}\int_0^{\pi/2}\left(\cos(n-n')x - \cos(n+n')x\right)\mathrm{e}^{-\alpha_1^2x^2}\,\mathrm{d}x \qquad (n+n' \equiv_4 2) \tag{32}$$

where $\alpha_1 = \dfrac{\beta_1 L_x}{\pi}$. We have for some $N \in \mathbb{Z}$,

$$\begin{aligned}
\int_0^{\pi/2}\cos(Nx)\mathrm{e}^{-\alpha_1^2x^2}\,\mathrm{d}x &= \frac{1}{2}\int_0^{\pi/2}\left(\mathrm{e}^{\mathrm{i}Nx}+\mathrm{e}^{-\mathrm{i}Nx}\right)\mathrm{e}^{-\alpha_1^2x^2}\,\mathrm{d}x\\
&= \frac{1}{2}\int_0^{\pi/2}\mathrm{e}^{-N^2/4\alpha_1^2}\left[\mathrm{e}^{-(\alpha_1 x-\mathrm{i}\frac{N}{2\alpha_1})^2}+\mathrm{e}^{-(\alpha_1 x+\mathrm{i}\frac{N}{2\alpha_1})^2}\right]\mathrm{d}x\\
&= \frac{1}{2}\mathrm{e}^{-N^2/4\alpha_1^2}\left[\int_{-\mathrm{i}\frac{N}{2\alpha_1}}^{\frac{\alpha_1\pi}{2}-\mathrm{i}\frac{N}{2\alpha_1}}\mathrm{e}^{-x^2}\frac{\mathrm{d}x}{\alpha_1}+\int_{\mathrm{i}\frac{N}{2\alpha_1}}^{\frac{\alpha_1\pi}{2}+\mathrm{i}\frac{N}{2\alpha_1}}\mathrm{e}^{-x^2}\frac{\mathrm{d}x}{\alpha_1}\right]\\
&= \frac{\mathrm{e}^{-N^2/4\alpha_1^2}}{2\alpha_1}\,\frac{\sqrt{\pi}}{2}\Bigg[\operatorname{erf}\left(\tfrac{\alpha_1\pi}{2}-\mathrm{i}\tfrac{N}{2\alpha_1}\right)-\operatorname{erf}\left(-\mathrm{i}\tfrac{N}{2\alpha_1}\right)\\
&\qquad\qquad +\operatorname{erf}\left(\tfrac{\alpha_1\pi}{2}+\mathrm{i}\tfrac{N}{2\alpha_1}\right)-\operatorname{erf}\left(\mathrm{i}\tfrac{N}{2\alpha_1}\right)\Bigg]\\
&= \frac{\sqrt{\pi}}{4\alpha_1}\mathrm{e}^{-N^2/4\alpha_1^2}\left[\operatorname{erf}\left(\tfrac{\alpha_1\pi}{2}-\mathrm{i}\tfrac{N}{2\alpha_1}\right)+\operatorname{erf}\left(\tfrac{\alpha_1\pi}{2}+\mathrm{i}\tfrac{N}{2\alpha_1}\right)\right]\\
&= \frac{\sqrt{\pi}}{2\alpha_1}\mathrm{e}^{-N^2/4\alpha_1^2}\operatorname{Re}\left[\operatorname{erf}\left(\tfrac{\alpha_1\pi}{2}+\mathrm{i}\tfrac{N}{2\alpha_1}\right)\right]
\end{aligned} \tag{33}$$

Note that this is also true for $N = 0$. By combining eqs. (31), (32) and (33) the result is

$$\begin{aligned}
I^x_{n'n} = \frac{1}{\alpha_1\sqrt{\pi}}\Bigg[&\mathrm{e}^{-(n-n')^2/4\alpha_1^2}\cdot\operatorname{Re}\left[\operatorname{erf}\left(\tfrac{(n-n')\mathrm{i}+\pi\alpha_1^2}{2\alpha_1}\right)\right]\\
&+(-1)^{n+1}\mathrm{e}^{-(n+n')^2/4\alpha_1^2}\cdot\operatorname{Re}\left[\operatorname{erf}\left(\tfrac{(n+n')\mathrm{i}+\pi\alpha_1^2}{2\alpha_1}\right)\right]\Bigg]
\end{aligned} \tag{34}$$

Next we consider

$$I^y_{k'k} = \begin{cases} \dfrac{2}{\sqrt{2^{k+k'}\pi k!k'!}}\displaystyle\int_0^{+\infty} H_k(\xi)H_{k'}(\xi)\mathrm{e}^{-\alpha_2\xi^2}\,\mathrm{d}\xi\,, & \text{if } k+k' \equiv_2 0\\ 0 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad , & \text{if } k+k' \equiv_2 1 \end{cases} \tag{35}$$

where $H_k(\xi)$ is the k^{th} Hermite polynomial and $\alpha_2 = \frac{1}{2} + \beta_2^2 a_\omega^2$. By [2, 3.461:2 and 3], we have for all $\alpha_2 > 0$ and $n \in \mathbb{N}_0$ that

$$\int_0^{+\infty}\xi^{2n}\mathrm{e}^{-\alpha_2\xi^2}\,\mathrm{d}\xi = \frac{(2n-1)!!}{2(2\alpha_2)^n}\sqrt{\frac{\pi}{\alpha_2}} \tag{36}$$

and

$$\int_0^{+\infty}\xi^{2n+1}\mathrm{e}^{-\alpha_2\xi^2} = \frac{n!}{2\alpha_2 n+1}\,. \tag{37}$$

Also, by [2, 8.952:2], we have the recursion formula

$$H_{k+1}(\xi) = 2\xi H_k(\xi) - 2kH_{k-1}(\xi) \tag{38}$$

By using the recursion formula above to find the coefficients of each Hermite polynomial, we can compute the integral in eq. (35) exactly by using eqs. (36) and (37). We have obtained

$$\begin{aligned}\langle n'k'|\hat{W}_G|nk\rangle = \frac{-V_0}{\alpha_1\sqrt{\pi}}\Bigg[&\mathrm{e}^{-(n-n')^2/4\alpha_1^2}\cdot\mathrm{Re}\left[\mathrm{erf}\left(\tfrac{(n-n')\mathrm{i}+\pi\alpha_1^2}{2\alpha_1}\right)\right]\\ &+(-1)^{n+1}\mathrm{e}^{-(n+n')^2/4\alpha_1^2}\cdot\mathrm{Re}\left[\mathrm{erf}\left(\tfrac{(n+n')\mathrm{i}+\pi\alpha_1^2}{2\alpha_1}\right)\right]\Bigg]\\ &\times\tfrac{1}{2}(1+(-1)^{k+k'})\,\frac{2}{\sqrt{2^{k+k'}\pi k!k'!}}\int_0^{+\infty}H_k(\xi)H_{k'}(\xi)\mathrm{e}^{-\alpha_2\xi^2}\,\mathrm{d}\xi\end{aligned} \tag{39}$$

if $n+n' \equiv_2 0$ and $k+k' \equiv_2 0$, but otherwise $\langle n'k'|\hat{W}_G|nk\rangle = 0$.

Each of our matrix elements can now be calculated by summing the results of eqs. (22), (28) and (39). By choosing an appropriate Fortran subroutine from e.g. the MKL Library we can then obtain an approximation to the eigenvalues of $\hat{H}$ and its eigenvectors as a linear combination of the truncated basis $\{|\alpha\rangle\}_{\alpha=1}^{N_xN_y}$.

3.4 Procedure

An overview of the program codes used for the numerical calculations along with their connections is shown in figures 3 and 4. The header of each code can be found in appendix A, but the interested reader may contact the author for a full version of the project, which includes all program codes.

A brief summary of the functionality of each program follows:

`Mod_Precision`: Defines global variables for single (4), double (8) and working (8) precision.

`Mod_Param`: Defines various global variables regarding the Hamiltonian $\hat{H}$ (N_x, N_y, B, Ω_0, V_0, etc.), some physical constants, numbers often used (inverse integers, factorials, etc.), and some constants, variables and arrays needed by the `ZHEEVD` subroutine.

`mainEnergy`: Runs the `eigen` subroutine (see below) and prints the possible energy values to the file `eigenval??????.dat` where the first 3 question marks are to be replaced by N_x and the latter 3 question marks by N_y.

`mainProbDens`: Runs the `eigen` subroutine (see below) and calculates the probability density of some eigenstates of $\hat{H}$ on some grid. Prints the density values to the file `density????????.dat` where the first 3 question marks are to be replaced by N_x, the next 3 question marks by N_y and the last 2 by the number of the eigenstate.

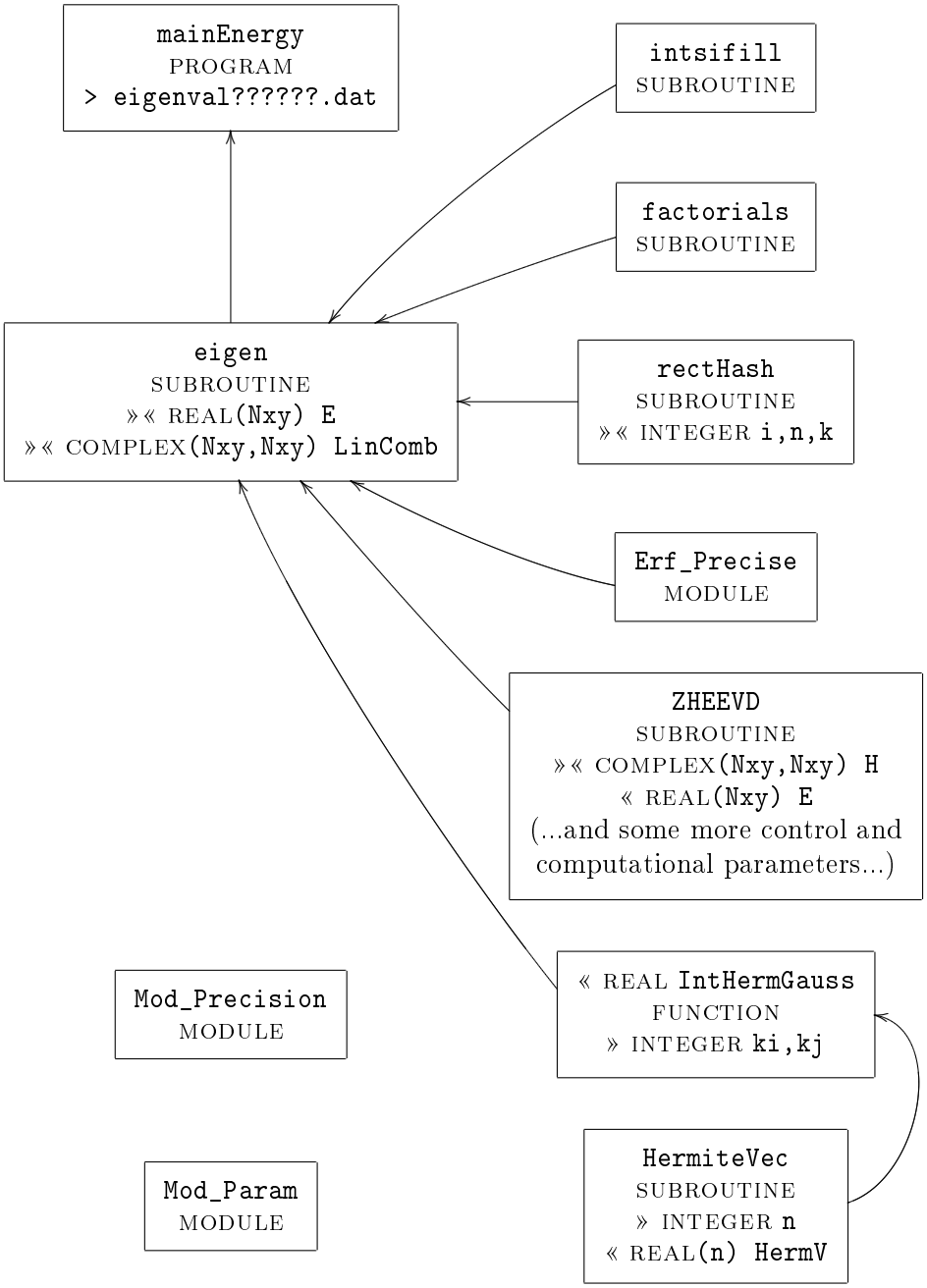

Figure 3. An overview of the program codes used to solve the eigenvalue problem. An arrow from A to B means that A is used by B. The two freestanding modules are however used in all the other codes. Notation: variable in » ; variable out « ; write to file > ; $N_xN_y =$ Nxy .

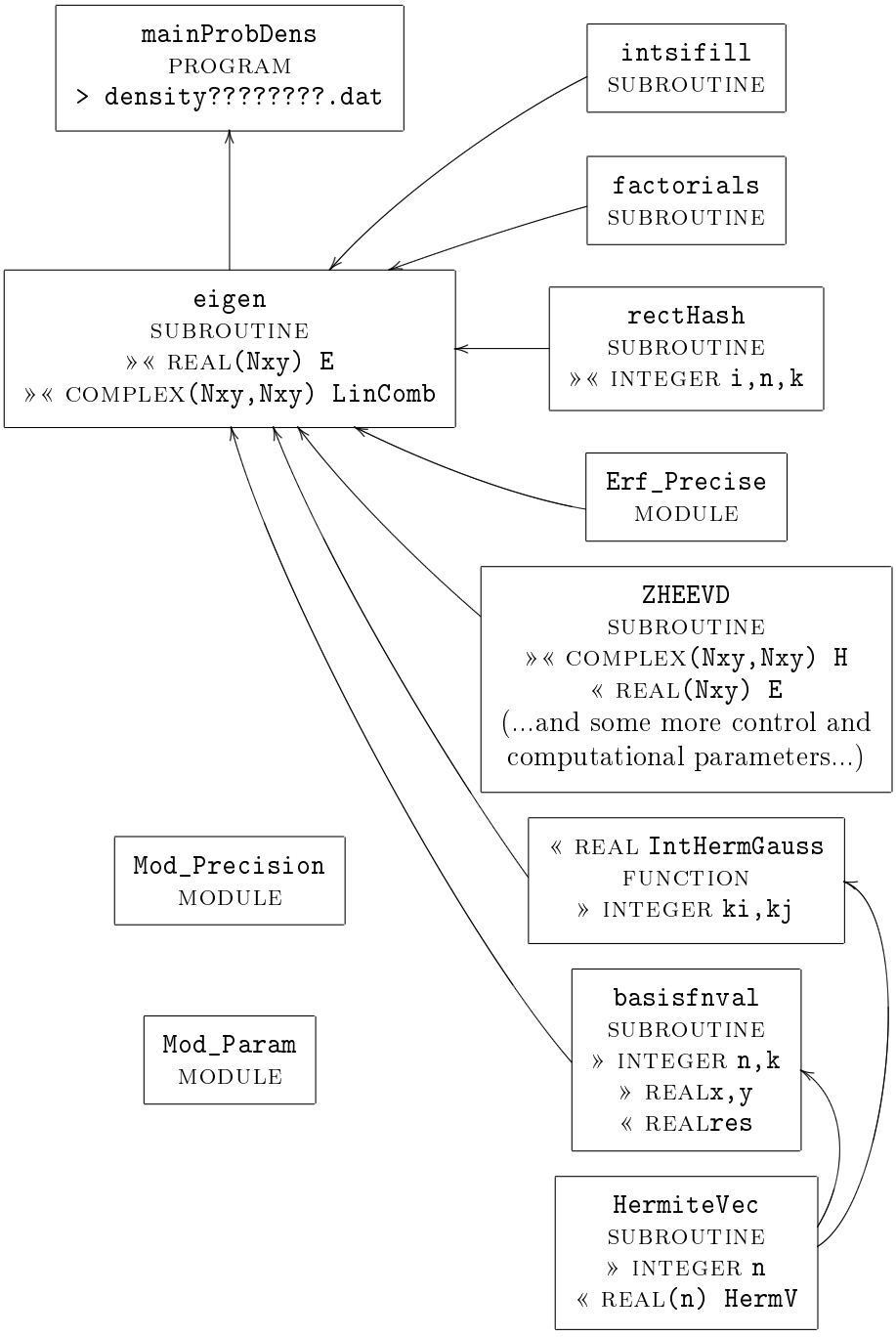

Figure 4. An overview of the program codes used to calculate the proability density of the eigenstates. An arrow from A to B means that A is used by B. The two freestanding modules are however used in all the other codes. Notation: variable in » ; variable out « ; write to file > ; $N_xN_y =$ Nxy .

`eigen`: Calculates the matrix elements in eq. (17) (see also eqs. (22), (28), (39)) with the help of `intsifill`, `factorials`, `deltafn`, `rectHash` and `IntHermGauss`. Uses the MKL Library subroutine `ZHEEVD` to calculate the eigenvalues of $\hat{H}$ and its eigenvectors' linear combination of $\{|\alpha\rangle\}_{\alpha=1}^{N_x N_y}$ (i.e. the coefficients of each linear combination).

`intsifill`: Fills inverse integers into the global array `intsi`.

`factorials`: Fills factorials into the global array `factorial` and the square root of inverse factorials into the global array `factorialqi`.

`rectHash`: The bijection described by eq. (18). This subroutine takes in three integers, i, and k (here i stands for α in eq. (18)). If $i = -1$, then the subroutine calculates the value of i from (n, k). Otherwise, it calculates the value of (n, k) from i.

`Erf_Precise`: Provides the function `ErfPrecise` which calculates precise values of the complex error function, $\mathrm{erf}(z)$.

`ZHEEVD`: This subroutine comes from the MKL Library. It calculates the eigenvalues and eigenvectors of a complex Hermitian matrix using a divide and conquer algorithm.

`IntHermGauss`: Computes the value of the integral in eq. (39).

`HermiteVec`: Computes the coefficients of the $\mathtt{n}^{\mathrm{th}}$ Hermite polynomial and stores them in the array `HermV`.

4 Results

4.1 Varying magnetic field and no Gauss potential

We set $V_0 = 0\,meV$ and

$$\begin{aligned} &m = 0.067 m_e = 6.103 \times 10^{-32}\,\mathrm{kg} \qquad \text{(we assume the wire is made of GaAs)} \\ &L_x = 300\,nm \\ &\hbar\Omega_0 = 1\,meV \\ &N_x = 128 \\ &N_y = 12 \end{aligned} \tag{40}$$

We consider the three cases $B = 0\,\mathrm{T}$, $B = 0.5\,\mathrm{T}$ and $B = 1\,\mathrm{T}$.

4.1.1 Eigenvalues - the energies ε_α

The eigenvalues (possible energy values) of the system are shown in figure 5. We note that when $B = 0\,\mathrm{T}$ the energy curve is pretty smooth for $\alpha \in [\![1, 4]\!]$ but then makes a bend for $\alpha = 5$, i.e. the difference between ε_3 and ε_4 is much more than between ε_4 and ε_5. By comparison to energy bands of a wire in a magnetic field that is for example periodic in x and with "hard walls" in y, one would expect the probability density of the 4^{th} excited state (corresponding to $\alpha = 5$) to be fairly localised in the bulk of the wire. This is indeed the case, see the graph in the bottom left corner of figure 6. Similarly for $B = 0.5\,\mathrm{T}$, we expect some kind of bulk localisation for the 6^{th} excited state ($\alpha = 7$). Again our assumption is good, see middle graph, second from top, in figure 7.

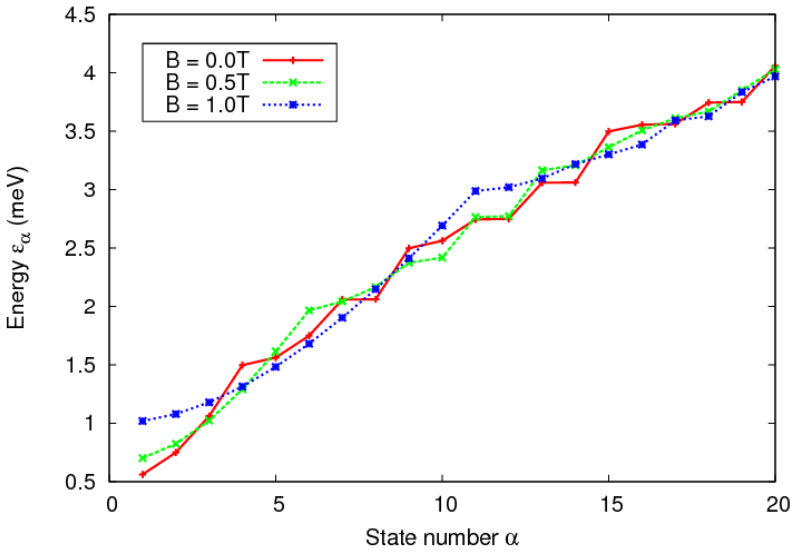

Figure 5. The eigenvalue (energy) ε_α as a function of the state number α for three strengths of the magnetic field: $B = 0\,\mathrm{T}$, $B = 0.5\,\mathrm{T}$ and $B = 1\,\mathrm{T}$.

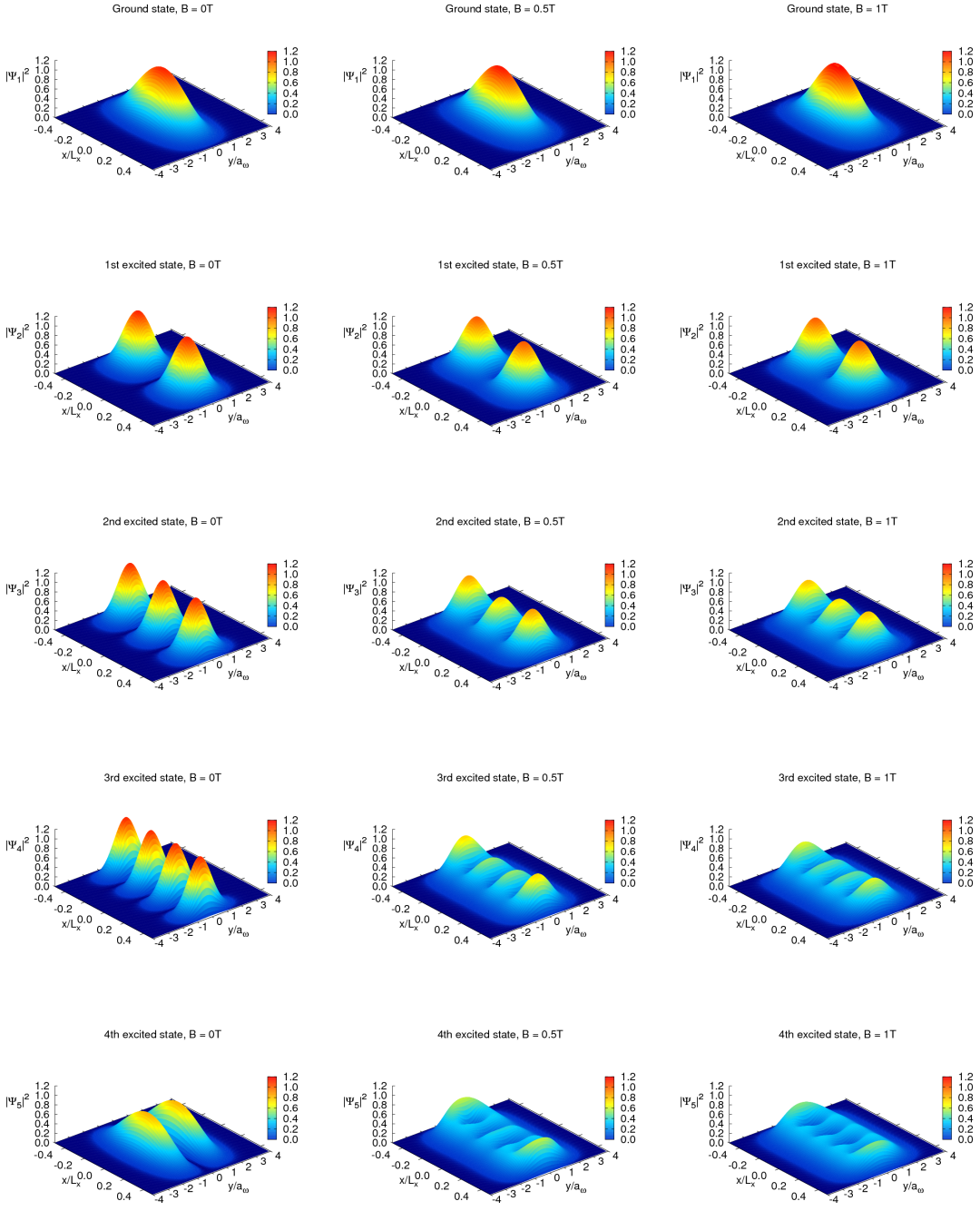

Figure 6. The probability density of the ground state (topmost line) and the first four excited states (2^{nd} line to 5^{th} line) for magnetic field strength $B = 0\,\text{T}$, $B = 0.5\,\text{T}$ and $B = 1\,\text{T}$ (along each line).

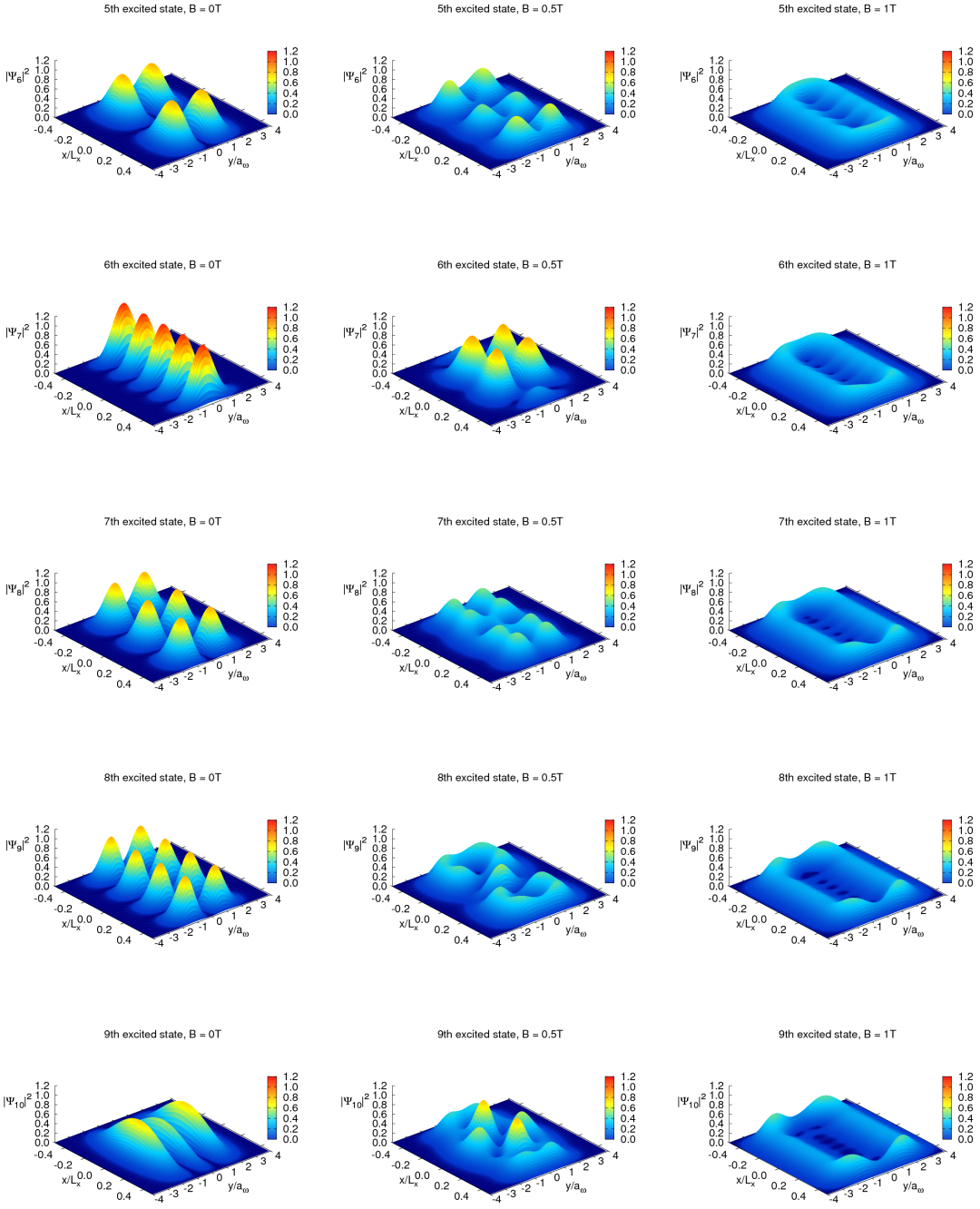

Figure 7. The probability density of the fifth to ninth excited states (from top to bottom) for magnetic field strength $B = 0\,\mathrm{T}$, $B = 0.5\,\mathrm{T}$ and $B = 1\,\mathrm{T}$ (along each line).

4.1.2 Probability distribution of the eigenstates

The probability density (squared norm of the wave function $\Psi_n(x, y)$) of the ground state and the first nine excited states is shown in figures 6 and 7 for $B = 0\,\mathrm{T}$, $B = 0.5\,\mathrm{T}$ and $B = 1\,\mathrm{T}$. The graphs in the figures are ordered such that state number increases from top to bottom and the magnetic field increases from left to right.

Considering figures 6 and 7 we notice how the magnetic field has very little effect on the ground state but increasingly affects the possible position of the electron as its excitation increases, gradually pushing it to the sides of the wire stub and forming a loop. This is as one would expect, since as the electron's energy increases, its velocity increases and thus the magnetic field has more effect on it - pushing it perpendicular off its route in the x-y plane.

4.2 Constant magnetic field and Gauss potential

We use the same parameters as in (40) but also

$$\begin{aligned} B &= 1\,\mathrm{T} \\ \beta_1 &= 15/L_x \\ \beta_2 &= 1/a_w \end{aligned} \tag{41}$$

and consider $V_0 = \pm 3\,m\mathrm{eV}$ and $V_0 = 0\,m\mathrm{eV}$. The Gauss potential for $V_0 = 3\,m\mathrm{eV}$ is depicted in figure 8.

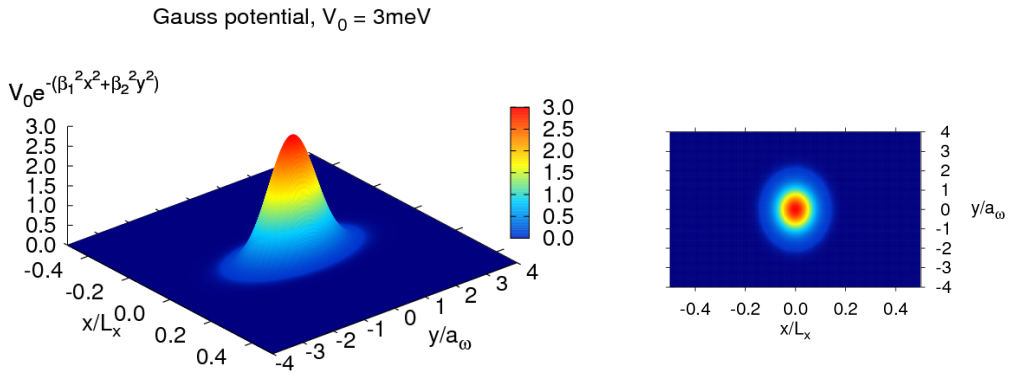

Figure 8. The Gauss potential for $V_0 = 3\,m\mathrm{eV}$ seen from aside and from above.

4.2.1 Eigenvalues - the energies ε_α

The possible energy values of the system are shown in figure 9. As one would expect, the negative Gauss potential reduces the energy values ε_α whereas the positive Gauss potential raises the energy values. Note that the energy of the ground state is negative for $V_0 = -3\,m\text{eV}$.

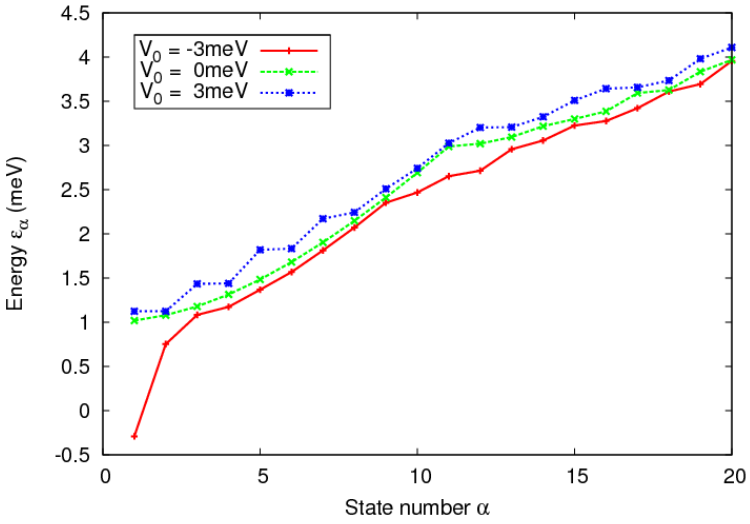

Figure 9. The eigenvalue (energy) ε_α as a function of the state number α with $B = 1\,\text{T}$ and for three strengths of the Gauss potential: $V_0 = -3\,m\text{eV}$, $V_0 = 0\,m\text{eV}$ and $V_0 = 3\,m\text{eV}$.

4.2.2 Probability distribution of the eigenstates

The probability density of the ground state and the first nine excited states is shown in figures 10 and 11 for $V_0 = \pm 3\,m\text{eV}$ and $V_0 = 0\,m\text{eV}$. First of all we notice how the gound state (top row in figure 10) either concentrates tighter to the centre of the wire as the negative Gauss potential ($V_0 = -3\,m\text{eV}$) traps the electron, or splits in two off-centre tops as the positive Gauss potential ($V_0 = 3\,m\text{eV}$) repulses the electron from the centre. In the second row of figure 10 we see how the first excited state is affected by the positive Gauss potential just as one would expect: the two tops are pushed further apart. The effect of the negative Gauss potential is a little peculiar, as the electron is drawn to the centre but stays however away from it such that the probability density forms a hollow cone (see figure 12 for a view from above).

Moving down the rows of figures 10 and 11 we see how the magnetic field gradually extinguishes the effect of the Gauss potential since the magnetic field pushes the electron to the sides of the wire, out of the Gauss potential's reach. An exception is the 9^{th} excited state in the case of negative Gauss potential (lower left corner of figure 11). There we have once more a bulk localisation, as discussed in section 4.1.1, seeing that $(10, \varepsilon_{10})$ is the first point that deflects from the smooth curve that corresponds to $V_0 = -3\,m\text{eV}$ in figure 9.

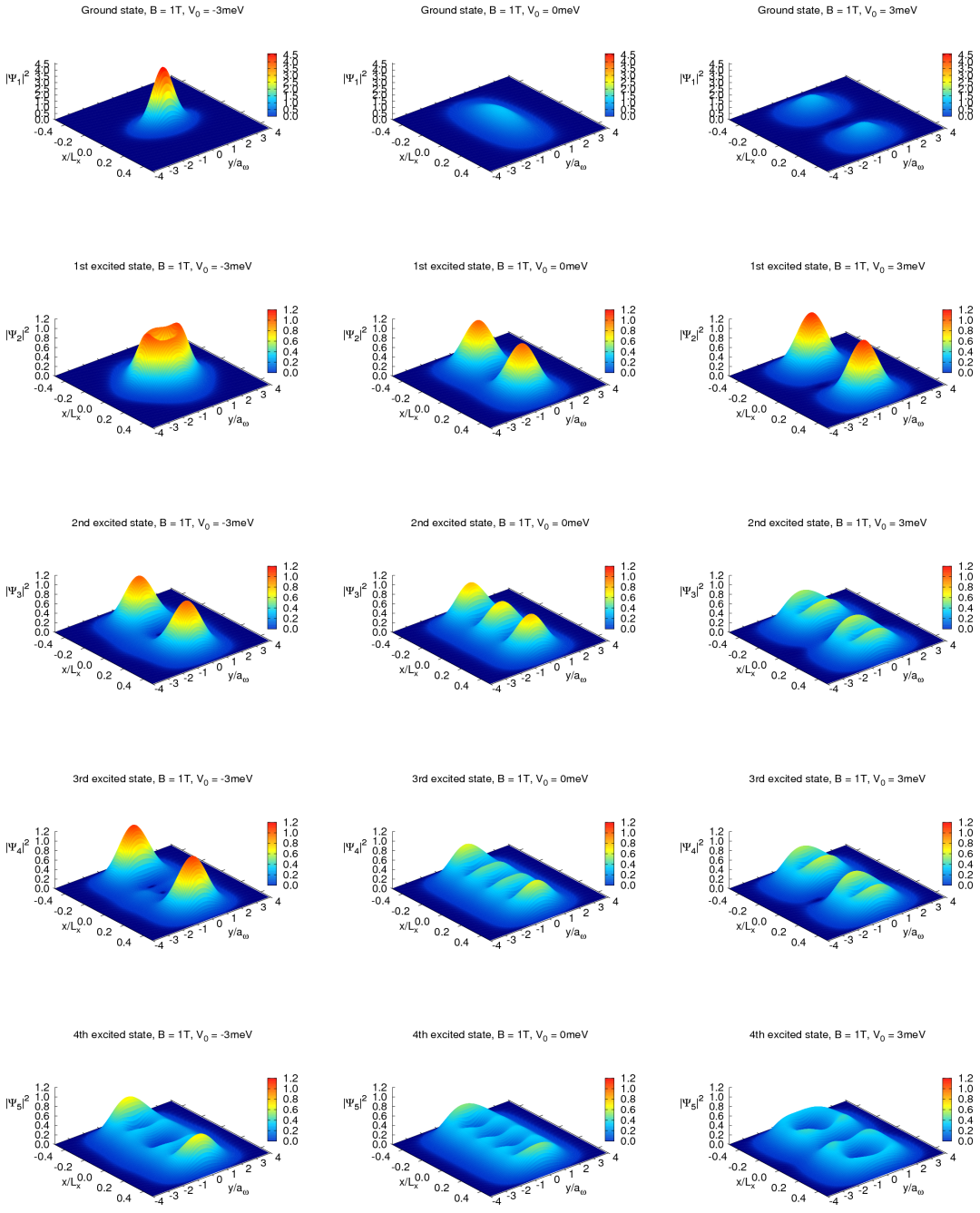

Figure 10. The probability density of the ground state (topmost line) and the first four excited states (2^{nd} line to 5^{th} line) for magnetic field $B = 1\,\text{T}$ and Gauss potential of strength $V_0 = -3\,m\text{eV}$, $V_0 = 0\,m\text{eV}$ and $V_0 = 3\,m\text{eV}$ (along each line). Note that for the ground state, the z-axis and colouring scale is other than in the other cases (0-4.5 vs. 0-1.2).

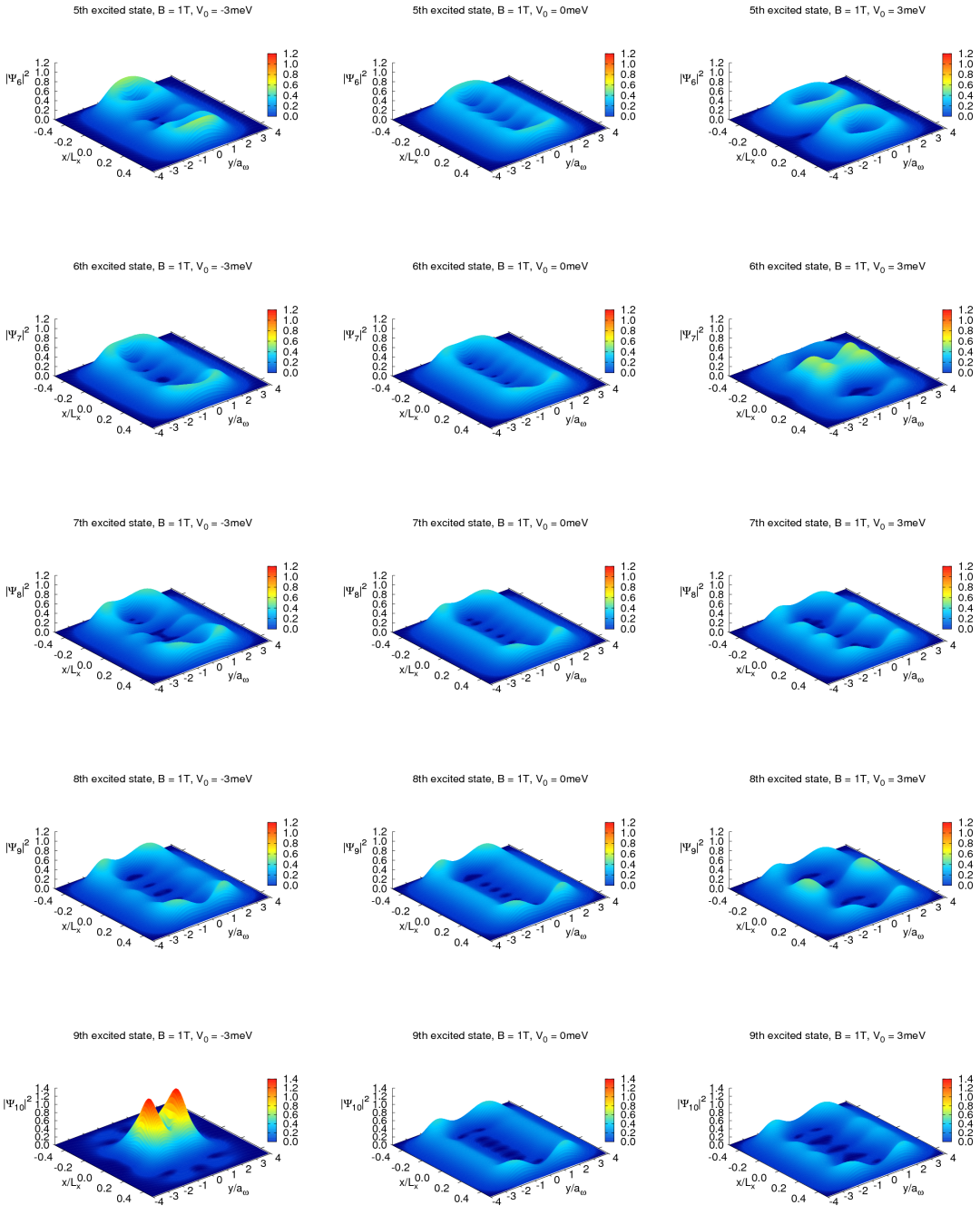

Figure 11. The probability density of the fifth to ninth excited states (from top to bottom) for magnetic field $B = 1\,\mathrm{T}$ and Gauss potential of strength $V_0 = -3\,m\mathrm{eV}$, $V_0 = 0\,m\mathrm{eV}$ and $V_0 = 3\,m\mathrm{eV}$ (along each line). Note that for the 9^{th} excited state, the z-axis and colouring scale is other than in the other cases (0-1.4 vs. 0-1.2).

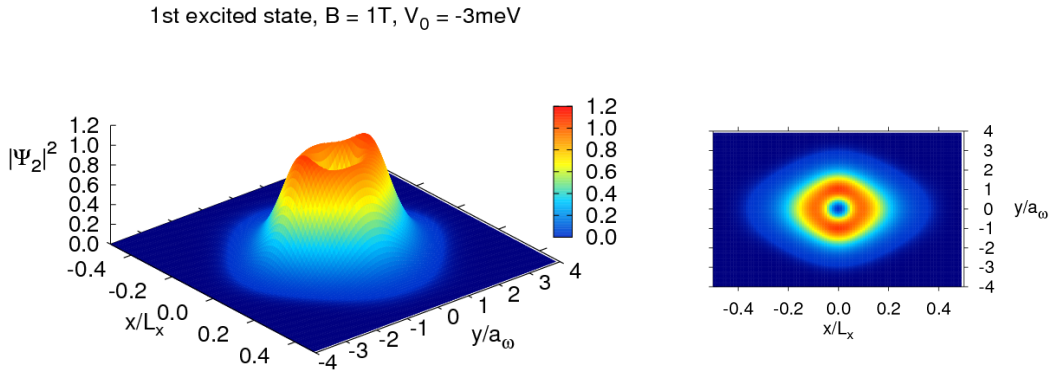

Figure 12. The probability density of the first excited state for $B = 1\,\mathrm{T}$ and $V_0 = -3\,m\mathrm{eV}$, seen from aside and from above. The probability density forms a hollow cone.

4.2.3 Bound states

The ground state is most probably a bound state when $V_0 = -3\,m\mathrm{eV}$, since the electron seems to be trapped down in the Gauss potential, having negative energy.

4.3 Gauss potential and no magnetic field

We use the same parameters as in (40) and (41), except $B = 0\,\mathrm{T}$, and consider the Gauss potential strengths $V_0 = \pm 3\,m\mathrm{eV}$ and $V_0 = 0\,m\mathrm{eV}$.

4.3.1 Eigenvalues - the energies ε_α

The possible energy values of the system are shown in figure 13. The ground state has negative energy for $V_0 = -3\,m\mathrm{eV}$ as in the case of magnetic field and is now even lower.

4.3.2 Probability distribution of the eigenstates

The probability density of the ground state and the first nine excited states is shown in figures 14 and 15 for $V_0 = \pm 3\,m\mathrm{eV}$ and $V_0 = 0\,m\mathrm{eV}$. The changes of the ground state are very much as in the case of magnetic field: The negative Gauss potential traps the electron tightly in the middle of the wire whereas the positive Gauss potential pushes it away from the centre. In general, the effect of the Gauss potential is as one would have expected; the negative potential draws the electron towards itself and the positive one pushes the electron away. How great the effect is, is in accordance with if the energy ε_α

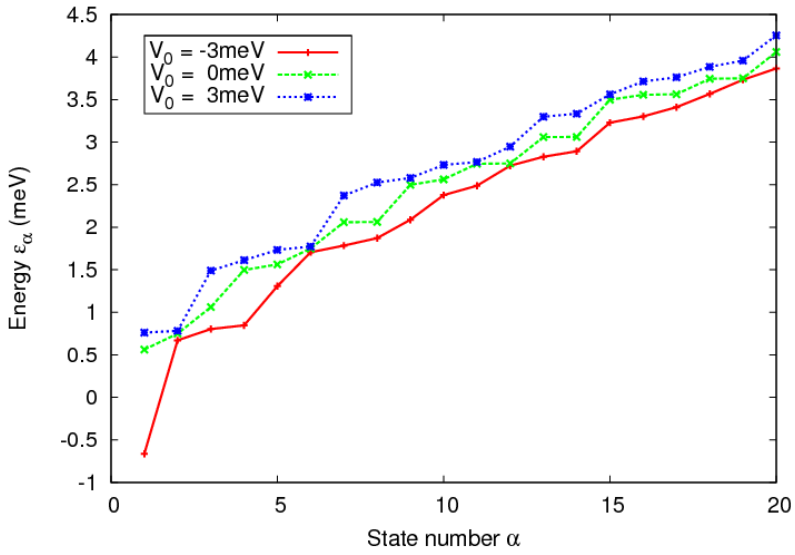

Figure 13. The eigenvalue (energy) ε_α as a function of the state number α with $B = 0\,\mathrm{T}$ and for three strengths of the Gauss potential: $V_0 = -3\,m\mathrm{eV}$, $V_0 = 0\,m\mathrm{eV}$ and $V_0 = 3\,m\mathrm{eV}$.

changes much or not for each α. For example, the probability denstity of the 1^{st} and 5^{th} excited states barely changes for the different values of V_0 in keeping with the very little change in ε_2 and ε_6, see figure 13.

4.4 Bound states

The ground state is a bound state when $V_0 = -3\,m\mathrm{eV}$ since it has negative energy and no potential in the system, except the normalizable Gauss potential, is negative. In other words, the electron is completely stuck in the Gauss potential.

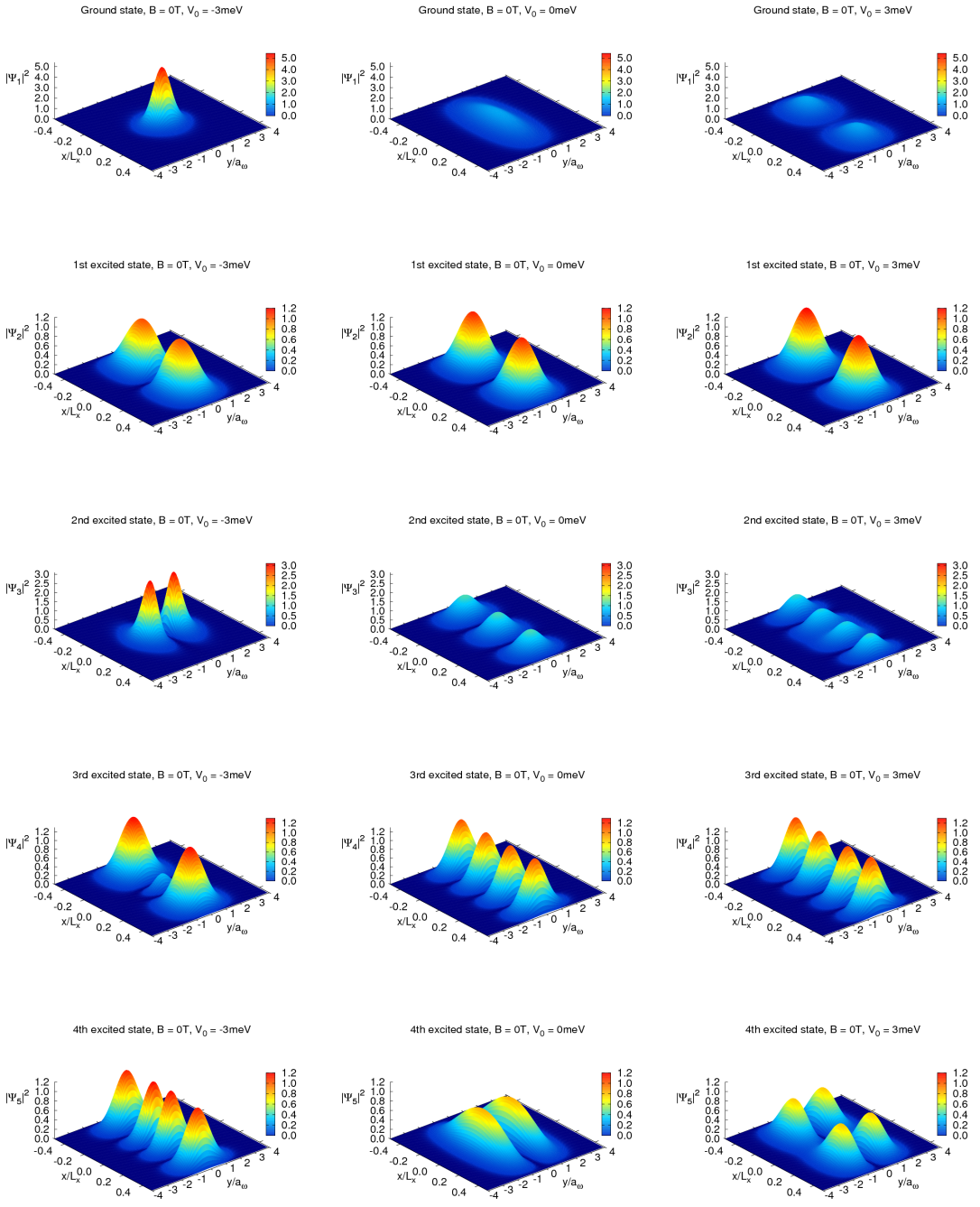

Figure 14. The probability density of the ground state (topmost line) and the first four excited states (2^{nd} line to 5^{th} line) for no magnetic field ($B = 0\,\text{T}$) and Gauss potential of strength $V_0 = -3\,m\text{eV}$, $V_0 = 0\,m\text{eV}$ and $V_0 = 3\,m\text{eV}$ (along each line). Note that for the ground state and the 2^{nd} excited state, the z-axis and colouring scale is other than in the other cases (0-5.4 and 0-3.1 vs. 0-1.2).

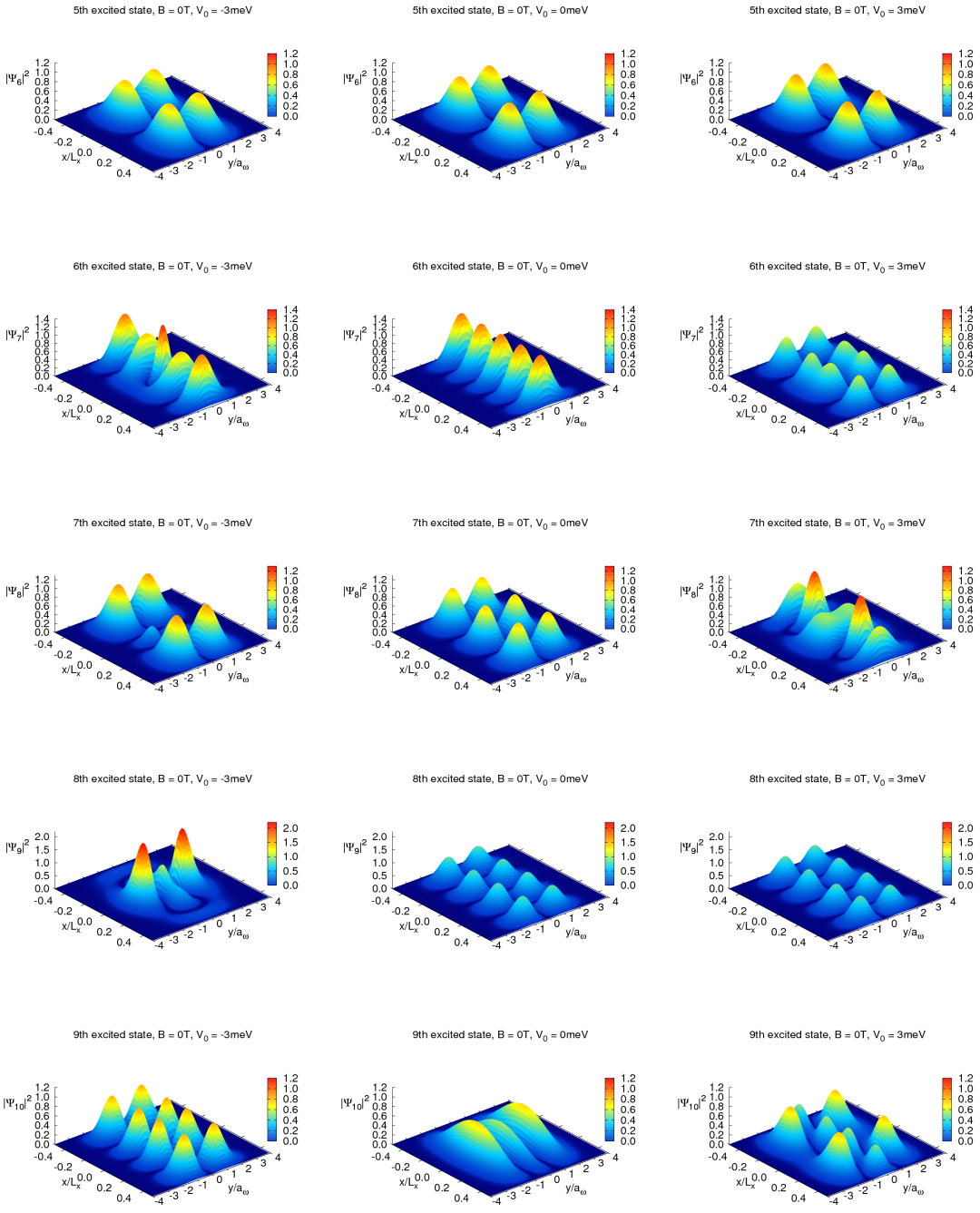

Figure 15. The probability density of the fifth to ninth excited states (from top to bottom) for no magnetic field ($B = 0\,\mathrm{T}$) and Gauss potential of strength $V_0 = -3\,m\mathrm{eV}$, $V_0 = 0\,m\mathrm{eV}$ and $V_0 = 3\,m\mathrm{eV}$ (along each line). Note that for the 6^{th} and 8^{th} excited state, the z-axis and colouring scale is not the same as in the other cases (0-1.4 and 0-2.2 vs. 0-1.2).

5 Conclusions

We have used a numerical method to find the energy values and probability distribution of an electron in a finite length GaAs-wire, to which there is either applied a constant magnetic field or a central Gauss potential or both.

In section 4.1 (no Gauss potential) we saw how the magnetic field had little influence on the ground state but increasingly affected the electron with its greater excitation, whereby the electron's probability density was gradually pushed to the sides of the wire stub and formed a loop. Section 4.2 (magnetic field and Gauss potential) showed us how the negative Gauss potential caught the electron in the ground state whereas the positive Gauss potential kept the ground state away from the centre of the wire stub, splitting it into two tops. There we also realised that as the electron's excitation grew, the magnetic field gradually takes over the effect of the Gauss potential. In section 4.3 (no magnetic field) we observed the same effect of the Gauss potential on the ground state, where the negative potential turned the ground state into a bound state and the positive potential split it in two. We also noticed that the extent of the change in the probability distribution due to the Gauss potential, came up to if the change in energy of the corresponding state was great or not.

References

[1] Cohen-Tannoudji, C., B. Diu og F. Laloë. 2005. *Quantum Mechanics, Vol. 1.* 2nd Ed. Wiley-VCH, Singapore.

[2] Gradshteyn, I.S., and I.M. Rhyzik. 1994. *Table of Integrals, Series, and Products.* 5th Ed. Edited by Alan Jeffrey. Academic Press.

[3] Viðar Guðmundsson. 2002. „Mean field approach – Technical details". Lecture notes in Computational Physics. On the Internet: http://hartree.raunvis.hi.is/~vidar/Nam/TE/MF_2.pdf

A Program Codes' Heads

A.1 Mod_Precision

```
! Mod_Precision.f90
! Defines single, double and working precision.
MODULE Mod_Precision
   PUBLIC
   INTEGER, PARAMETER :: sp=KIND(0.0E0), dp=KIND(0.0D0)
   INTEGER, PARAMETER :: wp=dp  ! Use double precision as default
END MODULE Mod_Precision
```

A.2 Mod_Param

```
! Mod_Param.f90
! Defines all global variables and constants.
MODULE Mod_Param
    USE Mod_Precision
    IMPLICIT NONE

! --------------- SIZE OF BASIS ------------------------------------------------
    INTEGER,            PARAMETER   :: Nx=128       ! Size of basis in x
    INTEGER,            PARAMETER   :: Ny=20        ! Size of basis in y
    INTEGER,            PARAMETER   :: Nxy=Nx*Ny    ! Total size of basis

! --------------- VARIOUS CONSTANTS --------------------------------------------
    REAL(KIND=wp),      PARAMETER   :: PI=atan(1._wp)*4._wp
    REAL(KIND=wp),      PARAMETER   :: PIqi=1._wp/SQRT(PI)
    REAL(KIND=wp),      PARAMETER   :: int2qi=1._wp/SQRT(2._wp)
    REAL(KIND=wp),      PARAMETER   :: meV2J=1.60217648740E-22_wp   ! [J/meV]
    REAL(KIND=wp),      PARAMETER   :: J2meV=1._wp/meV2J            ! [meV/J]
    REAL(KIND=wp),      PARAMETER   :: qe=1.60217648740D-19         ! [C]
    REAL(KIND=wp),      PARAMETER   :: hbar=6.5821189916E-13_wp     ! [meV.s]
    REAL(KIND=wp),      PARAMETER   :: hbarJ=1.05457162853D-34      ! [J.s]
    REAL(KIND=wp),      PARAMETER   :: me=9.1093821545D-31          ! [kg]
    REAL(KIND=wp),      PARAMETER   :: effm=0.067_wp*me             ! [kg]
    REAL(KIND=wp),DIMENSION(-Nx:2*Nx)  :: intsi         ! inverse integers
    REAL(KIND=wp),DIMENSION(0:2*Ny) :: factorial
    REAL(KIND=wp),DIMENSION(0:2*Ny) :: factorialqi
    COMPLEX(KIND=wp),   PARAMETER   :: II=(0.0_wp,1.0_wp)

! --------------- BASIC SYSTEM PARAMETERS --------------------------------------
    REAL(KIND=wp), PARAMETER    :: Lx=300.0D-09             ! [m]
    REAL(KIND=wp), PARAMETER    :: B=1._wp                  ! [Tesla]
    REAL(KIND=wp), PARAMETER    :: hbarOmega0=1._wp         ! [meV]

! --------------- DERIVED BASIC SYSTEM PARAMETERS ------------------------------
    REAL(KIND=wp), PARAMETER    :: hbaroc=hbar*qe*B/effm
    REAL(KIND=wp), PARAMETER    :: hbarOw=SQRT(hbarOmega0**2+hbaroc**2)
    REAL(KIND=wp), PARAMETER    :: Lxi=1._wp/Lx
    REAL(KIND=wp), PARAMETER    :: awi=SQRT((effm*(hbarOw/hbar))/hbarJ)
    REAL(KIND=wp), PARAMETER    :: aw=1._wp/awi
    REAL(KIND=wp), PARAMETER    :: aw2Lx2=hbarJ/(effm*(hbarOw/hbar)) * Lxi**2

! --------------- GAUSS POTENTIAL PARAMETERS -----------------------------------
    REAL(KIND=wp), PARAMETER    :: V0=3._wp                 ! [meV]
    REAL(KIND=wp), PARAMETER    :: beta1=15._wp*Lxi         ! [1/m]
    REAL(KIND=wp), PARAMETER    :: beta2=1._wp*awi          ! [1/m]

! --------------- DERIVED GAUSS POTENTIAL PARAMETERS ---------------------------
    REAL(KIND=wp), PARAMETER    :: alpha1=beta1*Lx/PI
```

```
    REAL(KIND=wp), PARAMETER    :: alpha2=0.5_wp+(beta2*aw)**2
    REAL(KIND=wp), PARAMETER    :: alpha1i=1._wp/alpha1
    REAL(KIND=wp), PARAMETER    :: alpha2i=1._wp/alpha2

! --------------- ZHEEVD PARAMETERS -------------------------------------------
    INTEGER, PARAMETER      :: lwork=Nxy**2+2*Nxy       ! dimension of array work
    INTEGER, PARAMETER      :: lrwork=2*Nxy**2+5*Nxy+1  ! dimension of array rwork
    INTEGER, PARAMETER      :: liwork=5*Nxy+3           ! dimension of array iwork
    COMPLEX(KIND=wp),DIMENSION(Nxy,Nxy) :: H    ! The matrix of the Hamiltonian
                                                ! in the basis used, H-matrix
    COMPLEX(KIND=wp), DIMENSION(lwork)  :: work     ! Working array for ZHEEVD
    REAL(KIND=wp),    DIMENSION(lrwork) :: rwork    ! --''--
    INTEGER,          DIMENSION(liwork) :: iwork    ! --''--
    !   jobz:   compute eigenvalues only ('N') or eigenvectors also ('V')
    !   uplo:   H is a upper ('U') or lower ('L') triangular matrix
    CHARACTER(LEN=1), PARAMETER         :: uplo='U'
    CHARACTER(LEN=1)                    :: jobz='V'
    INTEGER                             :: info     ! information on success or
                                                    ! failure of ZHEEVD
END MODULE Mod_Param
```

A.3 mainEnergy

```
! mainEnergy.f90
! Runs the calculation of the energy/eigenvalues of our system.
! All system parameters are defined in Mod_Param.
!
! Uses the subroutine:
!   eigen   from    current directory
```

A.4 mainProbDens

```
! mainProbDens.f90
! Runs the calculation of the energy/eigenvalues and probability density
! of our system and prints the data to files. All system parameters are
! defined in Mod_Param.
!
! Uses subroutines:
!   eigen       from    current directory
!   rectHash    from    current directory
!   basisfnval  from    current directory
```

A.5 eigen

```
! eigen.f90
! Calculates the eigenvalues (energy) of a 2D wire of length Lx with
! parabolic confinement in the y-direction, placed in a magnetic field
! B in the y-direction and a Gauss potential in x and y.
!
! Using energy in meV and the Landau gauge, A(r)=(-B,0).
!
! Parameters characteristic of the system, defined in Mod_Param:
!   Lx          REAL, DOUBLE    Length of wire
!   B           REAL, DOUBLE    Magnetic field strength
!   hbarOmega0  REAL, DOUBLE    hbar * strength of parabolic confinement
!                               (1/2*m * Omega0^2 * y^2)
!   V0          REAL, DOUBLE    strength of Gauss potential
```

```
!   beta1       REAL, DOUBLE    Gauss decay in x
!   beta2       REAL, DOUBLE    Gauss decay in y
!
! Output:
!   E           REAL, DOUBLE    Array of length Nxy; Energy spectrum of system
!   LinComb     COMPLEX, DOUBLE Array of dimension (Nxy,Nxy); Each column gives
!                               an eigenvector of the Hamiltonian as constants
!                               in the linear combinaton of the Nxy basis vectors
! Uses subroutines:
!   factorials  from    current directory
!   intsifill   from    current directory
!   rectHash    from    current directory
!   ZHEEVD      from    MKL (LAPACK)
```

A.6 intsifill

```
! intsifill.f90
! Calculates the value of inverse integers and stores them in intsi for
! future use.
```

A.7 factorials

```
! factorials.f90
! Calculates the factorial and the inverse square root of the factorial
! of 0 to 2*Ny and stores in factorial and factorialqi (see Mod_Param).
SUBROUTINE factorials()
```

A.8 rectHash

```
! rectHash.f90
! hash function i<->(n,k) for a rectangular shaped grid, counting 1=(1,0),
! 2=(2,0), ... i.e. first along x and then along y with min(x)=1, max(x)=Nx,
! and min(y)=0, max(y)=Ny-1. For Nx and Ny, see Mod_Param.
!
! If i==-1, then rectHash is (n,k)->i.
! If i/=-1, then rectHash is i->(n,k).
```

A.9 Erf_Precise

```
!------------------------------------------------------------------------------
! Double precision complex error function
! Adapted from the Naval Surface Warfare Center Mathematics Library
! by Alan.Miller @ vic.cmis.csiro.au
! http://www.ozemail.com.au/~milleraj
! Adaptation made by Aleksandar Donev
! Latest revision - 18 September 2000
!------------------------------------------------------------------------------
```

A.10 IntHermGauss

```
! IntHermGauss.f90
! Finds the integral of the function  H_ki(x)*H_kj(x)*exp(-alpha2*x^2)
! from 0 to infinity, where alpha2>0 is defined in Mod_Param.
!
! Uses the subroutine:
!   HermiteVec  from    current directory
```

A.11 HermiteVec

```
! HermiteVec.f90
! Finds the coefficients of the n-th Hermite polynomial and stores them in
! the array HermV.
```