A Computational Introduction To Quantum Physics

Soutions to the Additional Exercises

SØLVE SELSTØ

19 Solutions to Additional Exercises

19.1 Exercises for Chapter 1

19.1.1 Design the right expectation values

a) Our starting point is a wave function of form

$$\Psi(x) = \psi(x) \cdot e^{\mathrm{i}kx} \quad ,$$

where $\psi(x)$ is real. We have already learned that real wave functions have no mean momentum, so

$$\langle\psi|\hat{p}|\psi\rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \hat{p}\psi(x)\,\mathrm{d}x = 0 \quad .$$

For the wave function with the complex factor $\exp(\mathrm{i}kx)$, the product rule for differentiation gives

$$\hat{p}\Psi(x) = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\left(\psi(x)\cdot e^{\mathrm{i}kx}\right) = -\mathrm{i}\hbar\left(\psi'(x)\cdot e^{\mathrm{i}kx} + \psi(x)(\mathrm{i}k)e^{\mathrm{i}kx}\right) \quad ,$$

so that

$$\begin{aligned}
&\langle p\rangle = \langle\Psi|\hat{p}|\Psi\rangle = \int_{-\infty}^{\infty} [\Psi(x)]^* \hat{p}\,\Psi(x)\,\mathrm{d}x = \\
&\int_{-\infty}^{\infty} [\psi(x)\cdot e^{\mathrm{i}kx}]^* \left(-\mathrm{i}\hbar\right)\left(\psi'(x)\cdot e^{\mathrm{i}kx} + \psi(x)(\mathrm{i}k)e^{\mathrm{i}kx}\right)\,\mathrm{d}x = \\
&\int_{-\infty}^{\infty} [\psi(x)]^* \left(-\mathrm{i}\hbar\right)\psi'(x)\,\mathrm{d}x + (-\mathrm{i}\hbar)\,\mathrm{i}k\int_{-\infty}^{\infty} [\psi(x)]^*\psi(x)\,\mathrm{d}x = \\
&\langle\psi|\hat{p}|\psi\rangle + k\hbar\langle\psi|\psi\rangle = 0 + k\hbar\cdot 1 = k\hbar \quad .
\end{aligned}$$

b) We write out the wave function, without normalization factor, in terms of real parameters:

$$\begin{aligned}
&\Psi(x) \sim e^{-(x-z)^2} = e^{-(x-z_r-\mathrm{i}z_i)^2} = \\
&\exp(-(x^2 - 2xz_r + z_r^2 + 2\mathrm{i}z_r z_i - z_i^2 - 2\mathrm{i}xz_i)) = \\
&\exp(-2\mathrm{i}z_r z_i + z_i^2)\cdot\exp(-(x-z_r)^2)\cdot\exp(2\mathrm{i}z_i x) \sim e^{-(x-z_r)^2}\cdot e^{2\mathrm{i}z_i x} \quad .
\end{aligned}$$

Apart from an over all normalization factor we need not worry about, this expression is of the form of Eq. (18.1) with $\psi(x) \sim \exp(-(x-z_r)^2)$ and $k = 2z_i$.

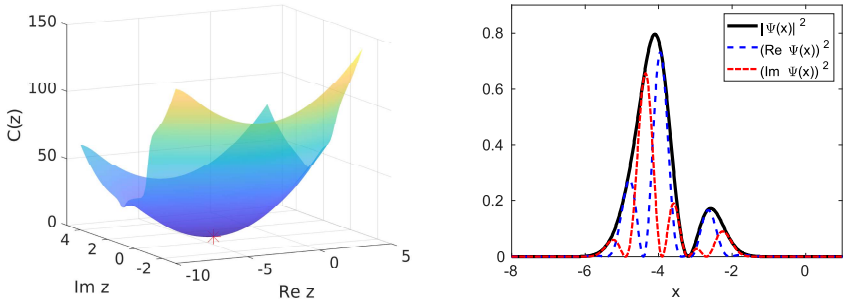

Fig. 19.1 The left panel shows the cost landscape according to the function in Eq. (18.5) for the wave function in Eq. (18.4). The star marks the minimum found by using the method of gradient descent. The right panel shows the normalized wave function with the parameters z_r and z_i which ensures mean values as dictated by Eqs. (18.3).

So $\psi(x)$ is a Gaussian centred around $x = z_r$ and, according to what we found in a), $\langle p \rangle = 2z_i\,\hbar$. Consequently, we must insist that

$$z_r = -4 \quad \text{and} \quad z_i = \frac{3}{2} \quad .$$

c) For this exercise, we may write code which, for a given numerical grid and a given wave function, calculates expectation values for position and momentum – along the lines of what was done in Exercises 1.4.2 and 1.5.1. Within this implementation we define an function variable for $\Psi(x)$ which takes z_r and z_i as inputs in addition to the variable x. If we do so and plot the cost function in Eq. (18.5) for a range of z-values in the complex plane, the result will look something like the left panel of Fig. 19.1. If we try to read off the z_r and z_i values which minimizes the cost function, we would see that $z_r \approx -4$ and $z_i \approx 1$.

Of course, higher precision is achieved by plotting the cost function over a smaller region containing the minimum. We could also achieve higher accuracy by implementing the method of gradient descent, Eq. (3.33), and find that the optimal parameters are

$$z_r = -3.693 \quad \text{and} \quad z_i = 0.890 \quad .$$

In testing the implementation, it is reassuring that the method rediscovers the exact solutions found analytically in the b)-part.

19.1.2 The virial theorem

It is worth repeating that by treating the hydrogen atom as a one-dimensional system in this way, we have swept a few details under the rug.

a) Our "kinetic energy operator" reads $\hat{T} = -\hbar^2/(2m)\,\mathrm{d}^2/\mathrm{d}r^2$ and the potential energy is $V = -e^2/(4\pi\epsilon_0)\cdot 1/r$. With atomic units it simplifies: $\hat{T} = -1/2\cdot \mathrm{d}^2/\mathrm{d}r^2$ and $V = -1/r$. For the ground state,

$$\psi_1(r) = 2re^{-r} \quad ,$$

the respective expectation values are

$$\langle T\rangle = \int_0^\infty [2re^{-r}]^* \left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\right) 2re^{-r}\,\mathrm{d}r = -2\int_0^\infty re^{-r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}re^{-r}\,\mathrm{d}r \qquad (19.1)$$

and

$$\langle V\rangle = \int_0^\infty [2re^{-r}]^* \left(-\frac{1}{r}\right) 2re^{-r}\,\mathrm{d}r = -4\int_0^\infty re^{-2r}\,\mathrm{d}r \quad . \qquad (19.2)$$

In case you miss the Bohr radius a_0 in the above expressions, let us remind you that it is 1 in atomic units.

With

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}(re^{-r}) = \frac{\mathrm{d}}{\mathrm{d}r}(e^{-r} - re^{-r}) = -e^{-r} - (e^{-r} - re^{-r}) = -e^{-r}$$

inserted into Eq. (19.1) we may find that

$$\langle T\rangle = -2\int_0^\infty re^{-r}\dot{(}-e^{-r})\,\mathrm{d}r = 2\int_0^\infty re^{-2r}\,\mathrm{d}r \quad .$$

If we compare this with Eq. (19.2) we will see that this is half the negative of $\langle V\rangle$; Eq. (18.6) *is* satisfied.

Numerically, these quantities are estimated by rather simple adjustments of the script from Exercise 1.6.4 c).

b) By updating this script with the corresponding expressions for ψ_1 and ψ_2, we should be able to estimate the corresponding energy expectation values and gauge whether Eq. (18.6) still holds. Although this would not be any formal proof, the converged numerical calculation should still provide strong support for the validity. Note that a larger grid is needed for ψ_2 and ψ_3 than was the case for the ground state.

With four decimals, the energy expectation values are

$$\langle\psi_2|\hat{H}|\psi_2\rangle = -0.1250 \quad \text{and} \quad \langle\psi_3|\hat{H}|\psi_3\rangle = -0.0556 \quad .$$

As addressed in Exercise 3.1.3, the exact values are

$$\varepsilon_n = -\frac{1}{2n^2} \quad ,$$

with $n = 1, 2$ and 3 in our case.

19.2 Exercises for Chapter 2

19.2.1 Split equally

By repeatedly running the implementation from Exercise 2.4.1 we may, eventually, determine V_0 such that the transmission and reflection probabilities are equal. With three desimals, we should arrive at

$$V_0 = 0.542$$

for the parameters given in that exercise – that is, $s = 5$, $w = 2$ for the barrier and $p_0 = 1$, $\sigma_p = 0.2$ and $\tau = 0$ for the initial Gaussian wave packet.

The bisection method provides a more systematic approach: Suppose we happen to know that a continuous function $f(x)$ is negative for $x = a$ and positive for $x = b$ – or the opposite. Then we can estimate a solution to the equation $f(x) = 0$ iteratively by checking the sign of the function at the midpoint $c = (a + b)/2$: If $f(a)$ and $f(c)$ have the same sign, we shift a to c. Otherwise, we take c to be our new b. This way the interval $[a, b]$ becomes increasingly narrow while containing a solution. When the difference $b - a$ becomes smaller than the desired precision, we set $x = (a + b)/2$ and we are done.

In our case, our variable is V_0 and we would take our function to be $f(V_0) = T(V_0) - 1/2$. It should be rather easy to fix some choice of a, a V_0-value which is such that $T > 1/2$ and another, larger value which ensures that $T < 1/2$ – one that we can use as our initial b.

If we increase the width w, it would seem reasonable to assume that this must be accompanied by a decrease in the height V_0 in order to ensure equal transmission probability. Indeed, the black plot in Fig. 19.2 does confirm this assumption. However, we also see that with a narrower momentum distribution, the relation between w and V_0 is not monotonic for the parameters in question. In the plot we have also included the special case of a fully rectangular barrier and an incoming wave with a sharply defined momentum. In this special case, we have an exact analytical expression for the transmission probability, see Eq. (6.4).

19.2.2 The fundamental commutator – numerically

The implementation from Exercise 2.2.2 is a convenient starting point for checking to what extent the momentum and position operators actually abide by Eq. (2.43) in a numerical context. When we check this for specific choices of wave functions, this is not anything which would come close to any sort of proof. Still, it is reassuring to see that the theory adds up as numerics improve.

In Fig. 19.3 we demonstrate how this is actually the case for the wave function of Eq. (1.15b) with both the midpoint rule, Eq. (1.23), and a five point formula:

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \mathcal{O}(h^4) \quad .$$

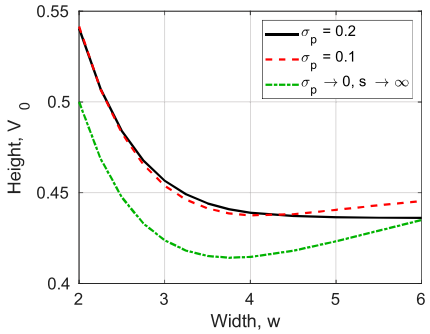

Fig. 19.2 These graphs demonstrate the relation between the width w and the height V_0 of the barrier, given in Eq. (2.30), that a wave function collides with such that it is split equally between a transmitted wave and a reflected one. The black curve corresponds to a Gaussian initial wave with mean momentum $p_0 = 1$ unit and with $\sigma_p = 0.2$ units. The red, dashed one is the same, except that the momentum width is 0.1 in that case. The green curve corresponds to an initial wave with a definite momentum hitting a fully rectangular barrier.

As expected, the error falls off more quickly with the five point formula than is the case for the three point formula.

The error when using the FFT approximation to the momentum operator, on the other hand, reaches machine accuracy very quickly – as long as the domain is chosen large enough so that also $\psi(\pm L/2)$ is no greater than machine accuracy. Actually, this would require a vely large L indeed for the wave functions in Eqs. (1.15a) and (1.15b).

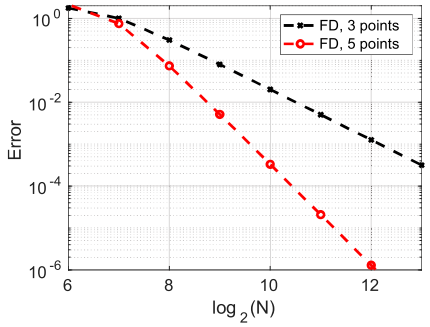

Fig. 19.3 The expectation value of $[X, P] - \mathrm{i}\hbar I_N$, where the matrices X and P approximates the position and momentum operators, as a function of the number N of points in our numerical grid. This particular case is calculated for the wave function of Eq. (1.15b) using three point and five point finite difference approximations on a grid extending from -25 to 25 length units.

19.3 Exercises for Chapter 3

19.3.1 A two-dimensional ground state

a) With the wave function written as a product, Eq. (18.11), the double derivatives in the Hamiltonian reads

$$\frac{\partial^2}{\partial x^2}\psi(x,y) = \frac{\partial^2\psi_x}{\partial x^2}\cdot\psi_y(y)$$
$$\frac{\partial^2}{\partial y^2}\psi(x,y) = \psi_x(x)\cdot\frac{\partial^2\psi_y}{\partial y^2} \quad .$$

With this, the time-independent Schrödinger equation may be written

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} + V_x(x)\psi_x(x)\right)\cdot\psi_y(y) +$$
$$\psi_x(x)\cdot\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} + V_y(y)\psi_y(y)\right) = \varepsilon\psi_x(x)\cdot\psi_y(y)$$

We divide both side by $\psi(x,y) = \psi_x(x)\cdot\psi_y(y)$ and separate the terms in purely x-dependent and y-dependent ones:

$$\frac{1}{\psi_x\psi_y}\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} + V_x(x)\psi_x(x)\right)\cdot\psi_y(y) + \right.$$
$$\left.\psi_x(x)\cdot\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} + V_y(y)\psi_y(y)\right)\right] = \frac{1}{\psi_x\psi_y}\cdot\varepsilon\psi_x(x)\cdot\psi_y(y) = \varepsilon$$
$$-\frac{1}{\psi_x(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} + V_x(x) = \varepsilon + \frac{1}{\psi_y(y)}\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} + V_y(y)$$

Since the left hand side above depends on x exclusively, and the right hand side depends on only y, they must both equal the same constant, which we, conveniently, will call ε_x:

$$-\frac{1}{\psi_x(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} + V_x(x) = \varepsilon_x$$
$$\varepsilon + \frac{1}{\psi_y(y)}\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} + V_y(y) = \varepsilon_x \quad ,$$

or, with $\varepsilon_y = \varepsilon - \varepsilon_x$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} + V_x(x)\psi_x(x) = \varepsilon_x\,\psi_x(x)$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} + V_y(y)\psi_y(y) = \varepsilon_y\,\psi_y(y) \quad .$$

In other words, the fact that our potential has the particular form of Eq. (18.10) allows us to recast a two-dimensional time-independent Schrödinger equation into two one-dimensional ones. And the full, two-dimensional eigenstate is, indeed, of the form of Eq. (18.11).