

Project 2 - Simulating with quantum dots

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1 Exercise 1

Open the notebook of example 1: 1D single dot 2025.ipynb. The hopping energy is given the description and both the hopping and potential energy are described in the model. What is the potential energy $V(x)$ with x in nm?

From the onsite definition

$$\varepsilon_i = 2t + Vi^2,$$

with $V = 4 \times 10^{-6}$ eV, lattice spacing $a = 5$ nm, and site position $x = ia$, we can express

$$i = \frac{x}{a} = \frac{x}{5 \text{ nm}}.$$

Substituting into $V(i) = Vi^2$ gives

$$V(x) = V\left(\frac{x}{5 \text{ nm}}\right)^2 = 1.6 \times 10^{-7} x^2 \text{ eV}.$$

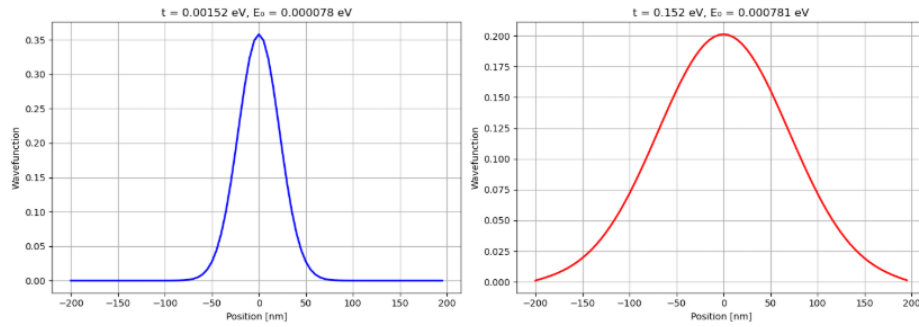
This relation shows that the onsite energy increases quadratically with the distance from the center, forming a parabolic confining potential. The constant $2t$ is only an energy offset and does not affect the shape of the potential, while the $V(x)$ term determines the confinement in the quantum dot.

2 Exercise 2

Plot the wave functions for the ground state (lowest eigen energy). Increase the hopping energy from 0.00152 to 0.152. Plot also the

ground state wave function for this situation. Explain what is happening.

Increasing hopping energy from 0.00152 to 0.152 eV makes the wavefunction to become more delocalized (its spread is wider), ground state energy increases with 100x. This is because larger t means easier hopping between sites, so the electron behaves more like a free particle. It is less confined by the potential, so we get broader wavefunction and higher energy.



3 Exercise 3

Change the hopping energy back to 0.00152. Calculate the ground state, first excited state and second excited state energy. Compare and verify these results with the analytical result of the harmonic oscillator.

```
Ground state energy (n=0): 0.000078 eV
First excited state (n=1): 0.000233 eV
Second excited state (n=2): 0.000387 eV
```

```
Analytical harmonic oscillator:
Energy spacing  $\hbar\omega$  = 0.000156 eV
E_0 (analytical) = 0.000078 eV
E_1 (analytical) = 0.000234 eV
E_2 (analytical) = 0.000390 eV
```

```
Comparison:
Numerical spacing E1-E0: 0.000155 eV
Numerical spacing E2-E1: 0.000154 eV
Analytical spacing  $\hbar\omega$ : 0.000156 eV
```

```
... Energy comparison (in eV):
```

| Level | Numerical | Analytical |
|--------------------------|--------------|--------------|
| ----- | ----- | ----- |
| E0 | 7.772355e-05 | 7.797435e-05 |
| E1 | 2.326657e-04 | 2.339231e-04 |
| E2 | 3.865931e-04 | 3.898718e-04 |
| Relative error E0: 0.32% | | |
| Relative error E1: 0.54% | | |
| Relative error E2: 0.84% | | |

The energy spacings are nearly equal and match the analytical harmonic oscillator prediction, confirming the system behaves as a quantum harmonic oscillator. The small difference comes from finite system size and boundary effects. The ground state is even and nodeless, while the first and second excited states show one and two nodes, respectively, consistent with the harmonic oscillator eigenfunctions.

4 Exercise 4

To get a better accuracy with the numerical modelling, change the parameters as below. Show that these results are in better agreement.

```
Ground state energy (n=0): 0.000078 eV
First excited state (n=1): 0.000234 eV
Second excited state (n=2): 0.000389 eV

Analytical harmonic oscillator:
Energy spacing  $\hbar\omega$  = 0.000156 eV
E_0 (analytical) = 0.000078 eV
E_1 (analytical) = 0.000234 eV
E_2 (analytical) = 0.000390 eV

Comparison:
Numerical spacing E1-E0: 0.000156 eV
Numerical spacing E2-E1: 0.000155 eV
Analytical spacing  $\hbar\omega$ : 0.000156 eV
```

Energy comparison (in eV):

| Level | Numerical | Analytical |
|--------------------------|--------------|--------------|
| E0 | 7.791180e-05 | 7.797435e-05 |
| E1 | 2.336101e-04 | 2.339231e-04 |
| E2 | 3.890575e-04 | 3.898718e-04 |
| Relative error E0: 0.08% | | |
| Relative error E1: 0.13% | | |
| Relative error E2: 0.21% | | |

The parameters were adjusted to $t = 0.00608$ eV, $V = 1 \times 10^{-6}$ eV, and the new length is $i \in [-80, 80]$. These new values maintain the same harmonic-oscillator shape because $\hbar\omega = 2\sqrt{tV}$ remains constant. Both t and V were changed so that the product tV remained constant. Increasing t smooths the lattice approximation and decreases numerical errors, while the smaller V and the larger system size reduce boundary effects, leading to results that agree more closely with the analytical values.

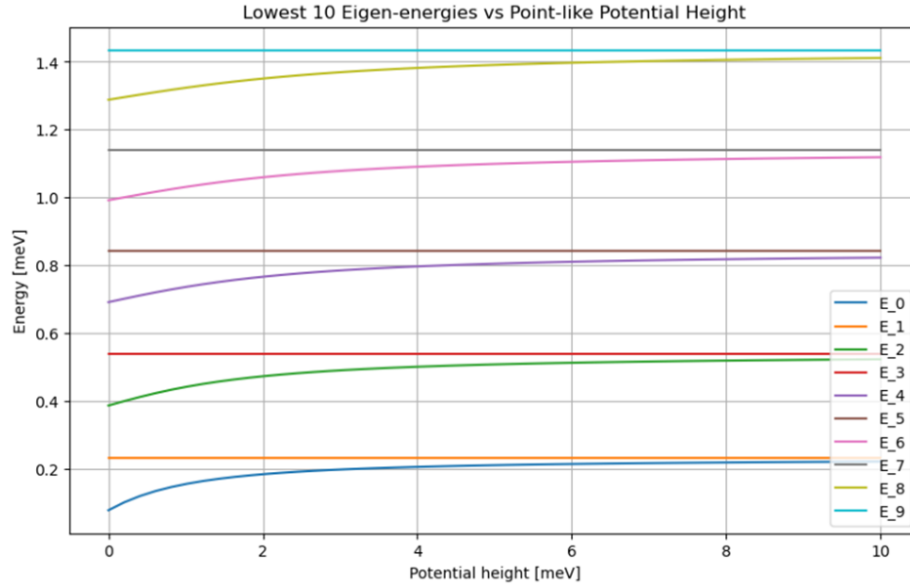
The new eigenenergies are $E_0 = 7.79 \times 10^{-5}$ eV, $E_1 = 2.34 \times 10^{-4}$ eV, $E_2 = 3.89 \times 10^{-4}$ eV, while the analytical prediction of the harmonic-oscillator remains

the same. The relative errors drop below 0.3%, showing a better agreement with the analytical result of the harmonic oscillator.

5 Exercise 5

Modify the code in example 1: add a point-like potential (add for one point a non-zero value) at the center of the potential well. Plot the lowest 10 eigen-energies as a function of the height of the potential.

A localized potential U was added at the center site ($i = 0$) of the 1D quantum dot. For each value of U , the Hamiltonian was diagonalized to obtain the ten lowest eigenenergies. The plot below shows how these energies change as the point-like potential increases from 0 to 10 meV



6 Exercise 6

Compare the results with the point-like potential with the original results. Which level changes the most, which level changes the least? Explain the results.

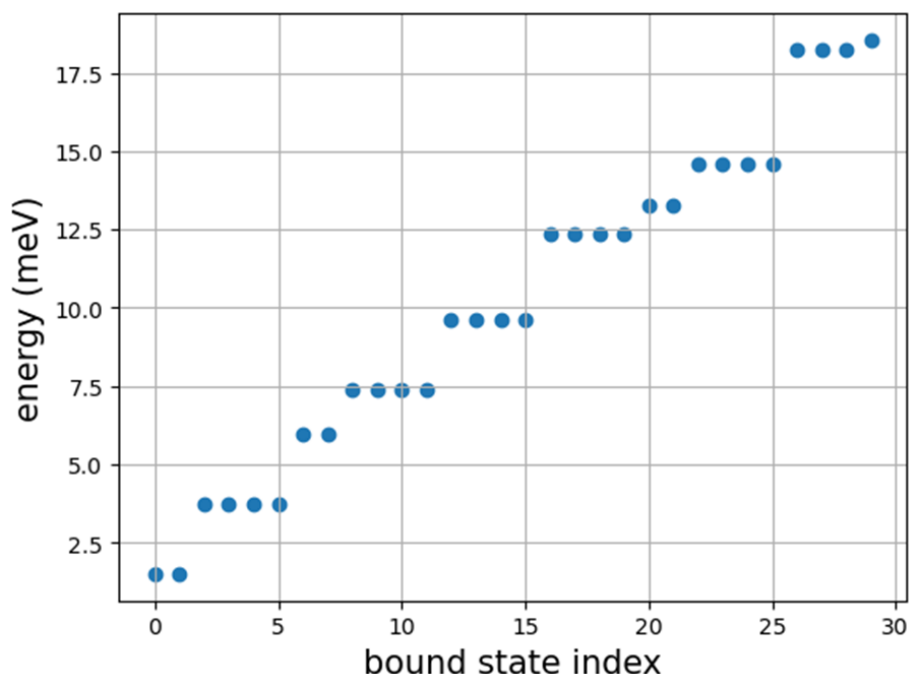
As the point-like potential U at the center of the well increases, the even-parity energy levels (E_0, E_2, E_4, E_6, E_8) shift upward noticeably, while the odd-parity levels (E_1, E_3, E_5, E_7, E_9) remain almost unchanged. This behavior follows from the spatial symmetry of the wavefunctions. Even states are symmetric and have a nonzero amplitude at the center ($x = 0$), so the added potential di-

rectly increases their energy. Odd states, on the other hand, have a node at the center, giving nearly zero overlap with the perturbation and thus negligible energy shifts. The alternating pattern of affected and unaffected levels therefore reflects the alternating parity of the wavefunctions in the quantum dot.

The ground state shows the largest shift because its probability density is maximal at the center. Higher even states have smaller amplitude at $x=0$, so their energy shifts are progressively weaker.

7 Exercise 7

Open the notebook: 2D single dot 2025.ipynb. Using section 1.2, print the first 30 energy levels. Look at the accompanying wave functions for visualization and to acquire a better understanding of what is happening. Describe the resulting pattern and relate this to the notion of quantum dots being called artificial atoms.



The figure shows the first 30 bound-state energies of the two-dimensional quantum dot. The energy levels appear in distinct groups or shells, where several states have nearly the same energy. This shell structure is very similar to the electronic energy levels in natural atoms.

The lowest level corresponds to the s-like ground state, followed by a pair of nearly degenerate p-like states, then a set of d-like states, and so on. These

degeneracies arise from the circular symmetry of the confining potential in two dimensions, which leads to multiple states sharing the same total energy.

Connection to artificial atoms is based on the following reasons:

- The quantum dot has discrete, quantized energy levels, just like real atoms.
- It shows a shell structure with increasing degeneracy, similar to atomic orbitals (s, p, d, f).
- The 2D circular confinement creates states with well-defined angular momentum, same as orbitals in atoms.
- The properties of the system are tunable (for example, by changing its size or potential), making it an artificial atom rather than a natural one.