PHOT 301: Quantum Photonics

Project topics: project 3

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Introduction

There are three projects to be performed during the PHOT 301 course of this semester. This file contains the project topics for the third project. The projects are meant to focus more on applied "real world" problems.

You can and are encouraged to work together on projects, further, you can ask help from me and Yağız (asking help will not influence your project grade). However, your project report and any figures containing plots and/or schematics should be made individually and not copied from others or online resources. Please cite any sources that you used and where you used them (you don't have to cite this document).

Type of report for project 3

The report should be between one and two pages (one sheet) including figures. Please ask help to your instructors on time, we might have not enough time to help you at the last day before the deadline of the report.

Grading of the project

This project will count for one third of 40% of your grade. During this semester three projects will be made in total, corresponding to 40% of your total grade.

Project topics

Next is a list of problems out of which you can choose for your project together with their task description. You only have to solve one problem for your project. Please inform me if the problem description contains any errors or anything is unclear.

You can use the code snippets in the separate document: `phot301_guidelines_for_the_projects.pdf` to construct any numerical methods required for your problem: transfer matrix method, finite basis method, tight-binding method, etc. There are also some code snippets provided for creating visualizations/plots. The code snippets are in Python, please inform me if you need help within another program (such as MATLAB).

Problem 1: Band structure of a chain of atoms (Tight-binding method)

Calculate the bandstructure for the following tight-binding Hamiltonian of a linear chain of carbon atoms:

$$\hat{H} = \sum_{n}^{N} \left(\varepsilon_0 |n\rangle\langle n| \, - \, t|n+1\rangle\langle n| \, - \, t|n-1\rangle\langle n| \right),$$

where N is the number of atoms in the chain, $|n\rangle$ is the atomic orbital of the nth atom in the chain, ε_0 is the atomic orbital (on-site) energy, and $-t$ is the hopping integral (approximate $t \approx 2.74$ eV). Hereby, we assumed that the basis is orthonormal basis, i.e., $\langle n|m\rangle = \delta_{mn}$.

The time-independent Schrodinger equation with this Hamiltonian can be solved by writing the Hamiltonian in matrix form and solving the eigenvalue equation. For example for $N = 2$ atoms we have:

$$\begin{pmatrix} \varepsilon_0 & -t \\ -t & \varepsilon_0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = E \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

where ϕ_n are the amplitudes in the superposition of the original atom orbital eigenstates. The wave function for the whole chain ψ can be written as a superposition $\psi = \phi_1|1\rangle + \phi_2|2\rangle$. This is an eigenvalue problem with solutions:

$$E_{\pm} = \varepsilon_0 \mp t, \qquad \psi_{\pm} = \frac{1}{\sqrt{2}} \left(|1\rangle \pm |2\rangle \right)$$

for the eigenenergies and eigenstates, and where $|n\rangle$ is the atomic orbital eigenstate of the nth atom.

If the chain would consist of N atoms we obtain an $N \times N$ matrix:

$$\begin{pmatrix} \varepsilon_0 & -t & & & \\ -t & \varepsilon_0 & -t & & \\ & \ddots & \ddots & \ddots & \\ & & -t & \varepsilon_0 & -t \\ & & & -t & \varepsilon_0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N-1} \\ \phi_N \end{pmatrix} = E \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{N-1} \\ \phi_N \end{pmatrix}$$

Where similarly the wave function for the whole chain ψ can be written as a superposition $\psi = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \phi_n |n\rangle$. This is again an eigenvalue problem with N eigenenergies and eigenstates.

Tasks to be performed:

- Calculate and plot the eigenenergies for different values of N: you can use for example 2, 3, 13, and 200.
- How do the eigenvalues change if you adapt the value of ε_0? How do they change when you adapt the value for t?

Problem 2: Electron interactions in a Helium atom (Variational theory)

A Helium atom has two electrons and a positive nucleus with charge equal to two: Z = 2. Unlike Hydrogen this system has two electrons which will interact with eachother. Here we will look at how electron interaction changes the ground state of the atom.

The Hamiltonian incorporates two electrons, each of charge e, that orbit a nucleus of charge $Ze = 2e$:

$$\hat{H} = \frac{\vec{p}_1^{\,2}}{2m_0} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_1} + \frac{\vec{p}_2^{\,2}}{2m_0} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_2} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

This Hamiltonian is similar to the sum of two Hydrogen Hamiltonians (with double nucleus charge), and an extra interaction term between the two electrons (the last term). If we ignore that last term, the Hamiltonian consists of two independent hydrogen atom Hamiltonians. In that case its eigenstates simply could be written as the product of Hydrogen atom eigenstates (with the correction for Z):

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_{n_1,l_1,m_1}(\vec{r}_1)\, \psi_{n_2,l_2,m_2}(\vec{r}_2)$$

with independent quantum numbers for each electron n, l, m. We will ignore any spin interaction here. We will look the ground state and assume that the electrons have opposite spin. When ignoring the interaction term we obtain the following eigenenergies and eigenstates:

$$E_{n_1,n_2} = -Z^2\left(\frac{1}{n_1^2} + \frac{1}{n_2^2}\right)\text{Ry}$$

Specifically for the ground state ($n_1 = n_2 = 1$ and remember $Z = 2$):

$$E_0 \equiv E_{1,1} = -8\text{ Ry} \approx -109\text{ eV} \qquad \text{with} \quad \psi_{100}(\vec{r}) = \sqrt{\frac{Z^3}{\pi a_0^3}}\, e^{-Zr/a_0}$$

This value is too low, the true ground state has an energy value of approximately $E_0 \approx -79.0$ eV.

To approximate the true ground state we will use the variational approach here: in this method the true *unknown* wave function is approximated by another parameterized function for which we then minimize the energy. Although the ground state energy of the parameterized function probably is still larger than the true ground state (unless we by accident choose the exact solution), it provides an upper bound to the true ground state energy (for a description of the variational method see page 178 in Miller's book [1]).

Use the approach of [2] where the following parameterized wave function for the ground state is used:

$$\Psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_1;\, \alpha)\psi(\vec{r}_2;\, \alpha)$$

where the parameterized function $\psi(\vec{r};\, \alpha)$ is obtained by replacing $Z \longrightarrow \alpha$ in the ground state $\psi_{100}(\vec{r})$:

$$\psi(\vec{r};\, \alpha) = \sqrt{\frac{\alpha^3}{\pi a_0^3}}\, e^{-\alpha r/a_0}$$

Task to be performed:

- Calculate the ground state energy by following the approach in [2], where a full explanation is given. The most relevant part is provided starting from page 146 of Chapter 6 in the course materials of David Tong.
- Plot the expectation value of the ground state energy as function of parameter α.

References

[1] David A. B. Miller, *Quantum Mechanics for Scientists and Engineers*, Cambridge University Press, USA, 2008.

[2] David Tong, *Lectures on Applications of Quantum Mechanics*, Chapter 6, part of his personal online course materials, Cambridge University, 2017.