Exercises Quantum Physics (GEMF) – Model systems

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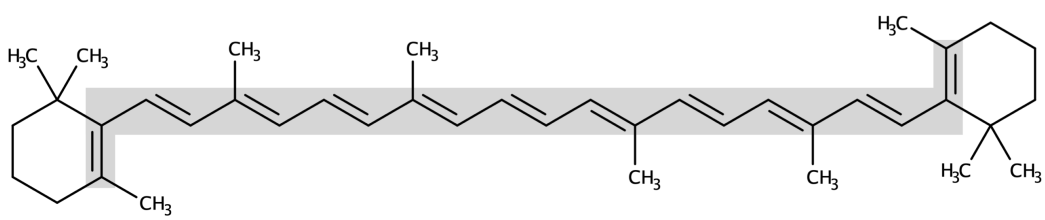
last modification: December 25, 2022

1. **Particle in a box of length 2L:** Solve the particle in a box problem for

$$V(x) = \begin{cases} \infty \text{ for } x \leq -L \text{ and } x \geq L \\ 0 \text{ for } -L < x < L \end{cases}$$

2. **Spectroscopy:** β-carotene is a pigment that plays an important role in the colour of many plants, for example the orange colour of carrots. The structure depicted below consist of a long carbon chain capped with two six-membered carbon rings. The central part is the active part in the process of absorbing light and can be described to some extent with the particle in a box approach. There are 22 carbon atoms in this box with a length of approximately 22 Å. Each of those carbon atoms has one electron that is delocalized over the whole box, occupying levels that have a certain resemblance with the particle-in-a-box solutions. Estimate the wave length of the lowest optically allowed transition.



Two useful mathematical relations

$$2\sin(nx)\sin(mx) = \cos(n-m)x - \cos(n+m)x$$
$$\int x\cos ax = \frac{\cos ax}{a^2} + \frac{x\sin ax}{a}$$

3. **Potential step:** Calculate the reflection coefficient for a particle with energy E moving along the x-axis towards a potential step at $x = 0$ of height V_0 with $E < V_0$. ($V(x) = 0$ for $x < 0$ and V_0 for $x \geq 0$. Calculate the relative probability of finding the particle at $x = 1$ and $x = 2$ for $E = \frac{1}{4}V_0$, $0.1V_0$ and $0.01V_0$.

4. **Tunneling:** Calculate the transmission probability for particle with $m = 1$ au and $E = 0.01$ au for tunnelling through a potential energy barrier of length $L = 1$ au and height $V_0 = 1$ au. Repeat the calculation by doubling one by one each of the four parameters and establish which parameter affects most strongly the tunnelling probability.

5. **Classical allowed region:** Calculate the probability to find a particle outside the classically allowed region of a one-dimensional harmonic oscillator when the state vector of the particle corresponds to the ground state vector.

6. **Heisenberg's matrix mechanics:** As an alternative for solving the Schrödinger equation to obtain information about quantum systems, one can also follow the matrix description of Heisenberg, developed a couple a years before the wave mechanics of Schrödinger. This problem illustrates how this works for the harmonic oscillator.

   (a) Represent $\langle n|\hat{N}|n'\rangle$ in a matrix form, or in other words, find the matrix representation of $\hat{N}$.

   (b) Do the same for the operators $\hat{a}^\dagger$ and $\hat{a}$.

   (c) Use the matrix representations of $\hat{a}^\dagger$ and $\hat{a}$ to obtain those of $\hat{P}$ and $\hat{X}$.

   (d) Check that the matrix presentations of $\hat{P}$ and $\hat{X}$ fulfil the relation $[\hat{X}, \hat{P}] = i\hbar$.

   (e) Calculate $\hat{P}^2$ and $\hat{X}^2$ and from there the matrix representation of the Hamiltonian.

   (f) Do the eigenvalues of the Hamiltonian coincide with the relation derived from solving the Schrödinger equation?