University of Stuttgart
Institute for Theoretical Physics I

Wave functions and oscillator strengths in a two-band model for Rydberg excitons in cuprous oxide quantum wells

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Introduction

The Hamiltonian for an exciton in a hydrogen-like model with cylindrical coordinates in a quantum well with given quantum number m reads

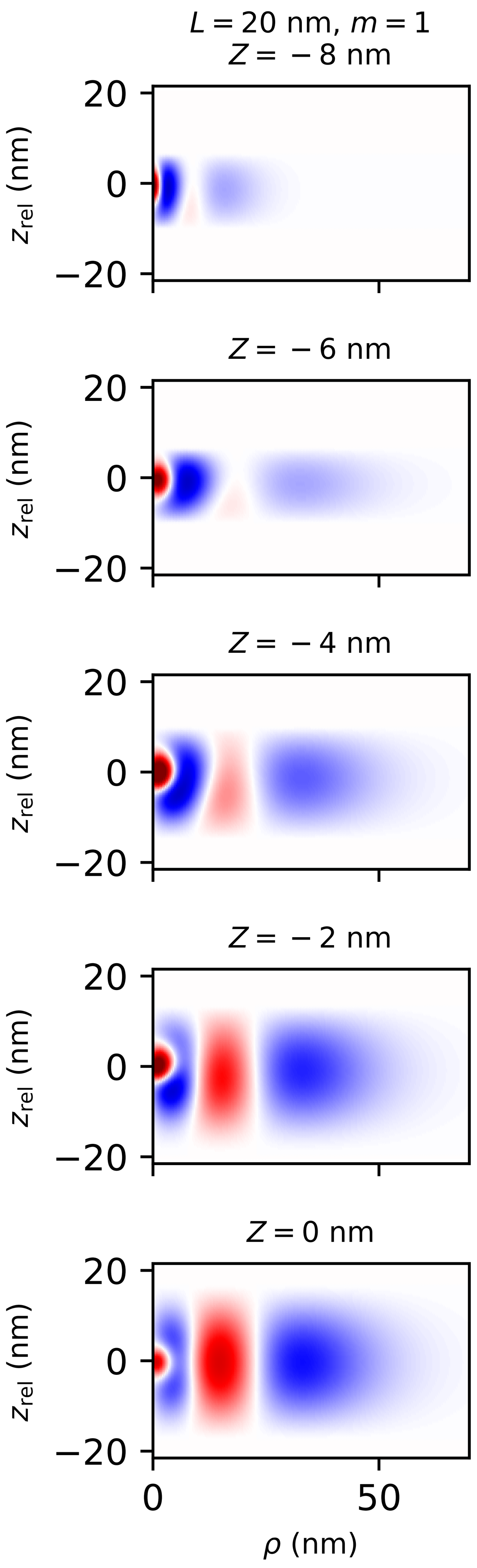
$$H = -\frac{\hbar^2}{2m_\mathrm{h}}\frac{\partial^2}{\partial z_\mathrm{h}^2} - \frac{\hbar^2}{2m_\mathrm{e}}\frac{\partial^2}{\partial z_\mathrm{e}^2} - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1/4 - m^2}{\rho^2}\right) - \frac{e^2}{4\pi\epsilon_0\epsilon\sqrt{\rho^2 + (z_\mathrm{e} - z_\mathrm{h})^2}}$$

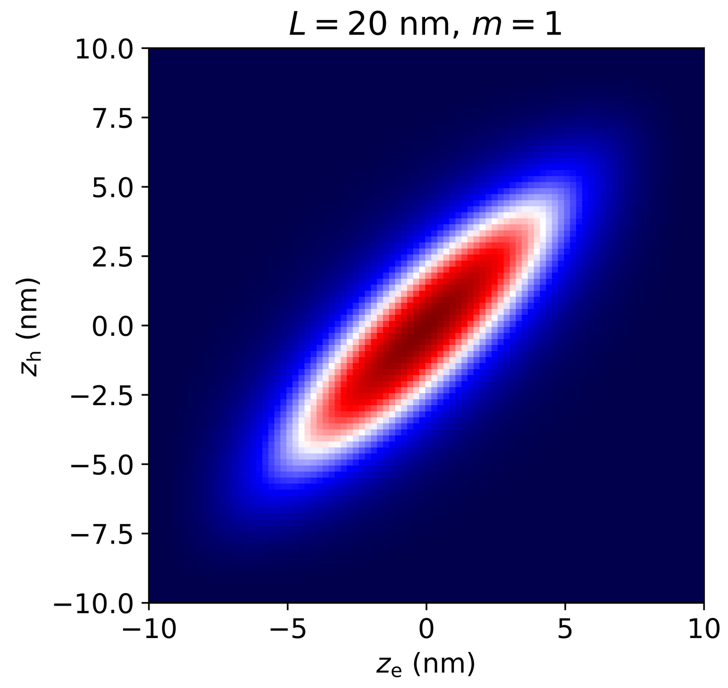
For the numerical calculation the wave function is approximated by B-splines

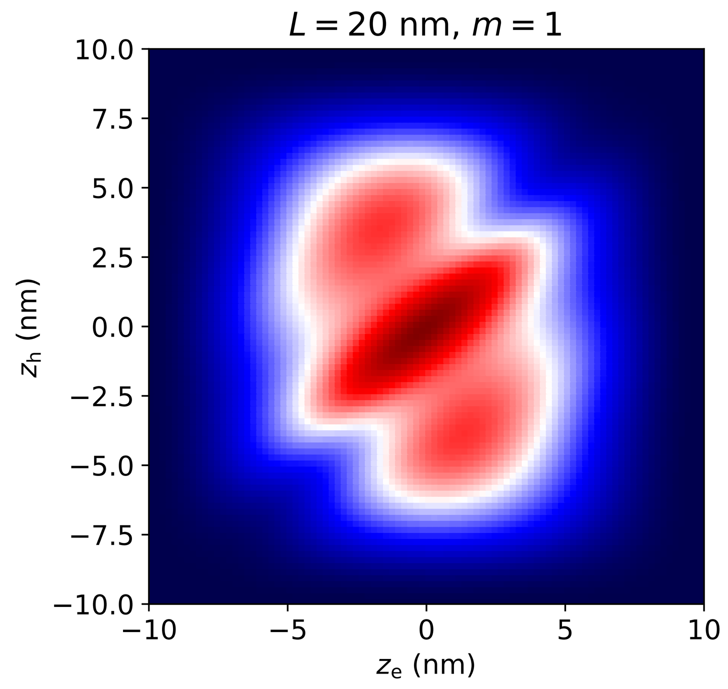
$$\chi(\rho, z_\mathrm{e}, z_\mathrm{h}) = \sum_{i=1}^{N_{z_\mathrm{h}}}\sum_{j=1}^{N_{z_\mathrm{e}}}\sum_{k=1}^{N_\rho} c_{ijk} B_i^n(z_\mathrm{h}) B_j^n(z_\mathrm{e}) B_k^n(\rho),$$

where $\chi(\rho, z_\mathrm{e}, z_\mathrm{h}) = \sqrt{\rho}\,\psi(\rho, z_\mathrm{e}, z_\mathrm{h})$. In a generalized eigenvalue problem the coefficients c_{ijk} are calculated for the different eigenvalues. The box potentials $V_\mathrm{e}(z_\mathrm{e})$ and $V_\mathrm{h}(z_\mathrm{h})$ are taken into account by boundary conditions $\chi(z_\mathrm{h,e} = \pm L/2) = 0$.

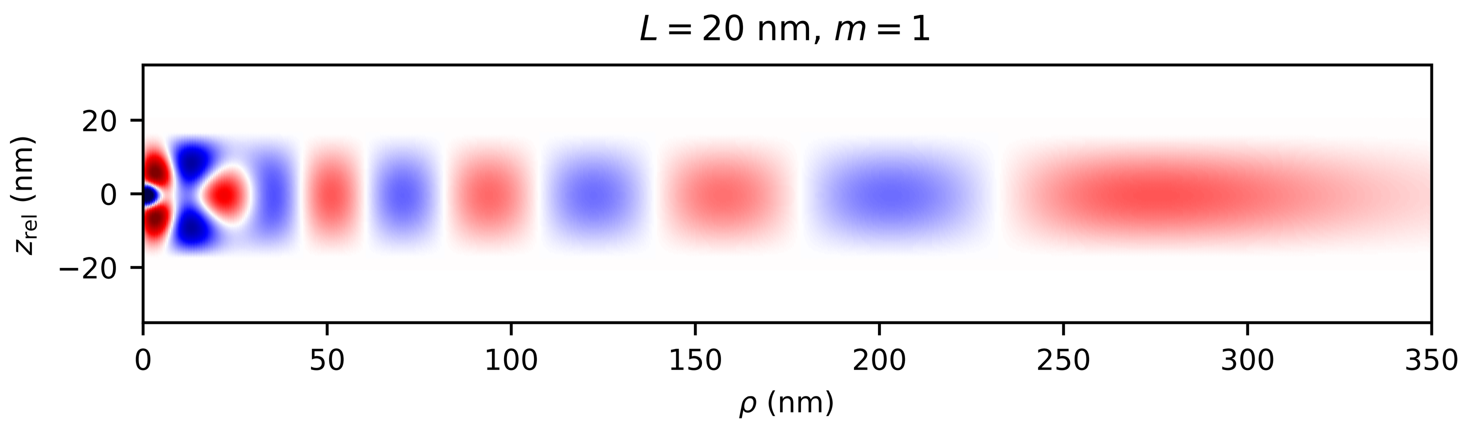
Wave functions

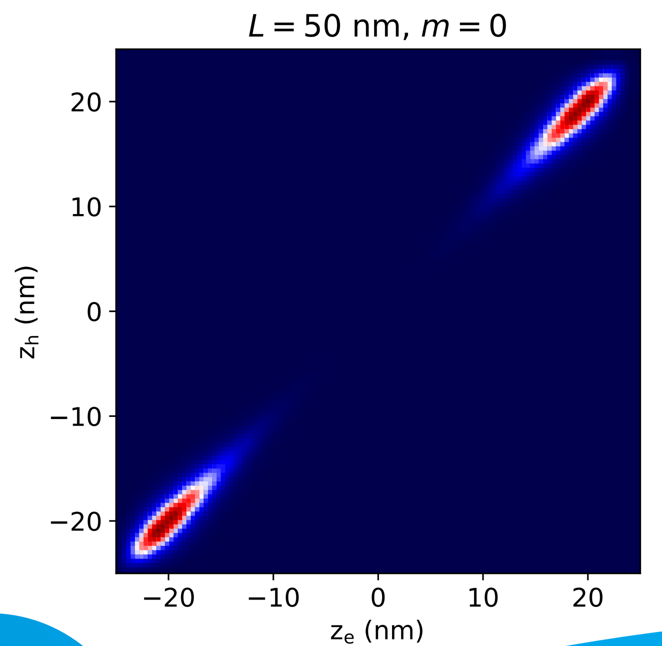






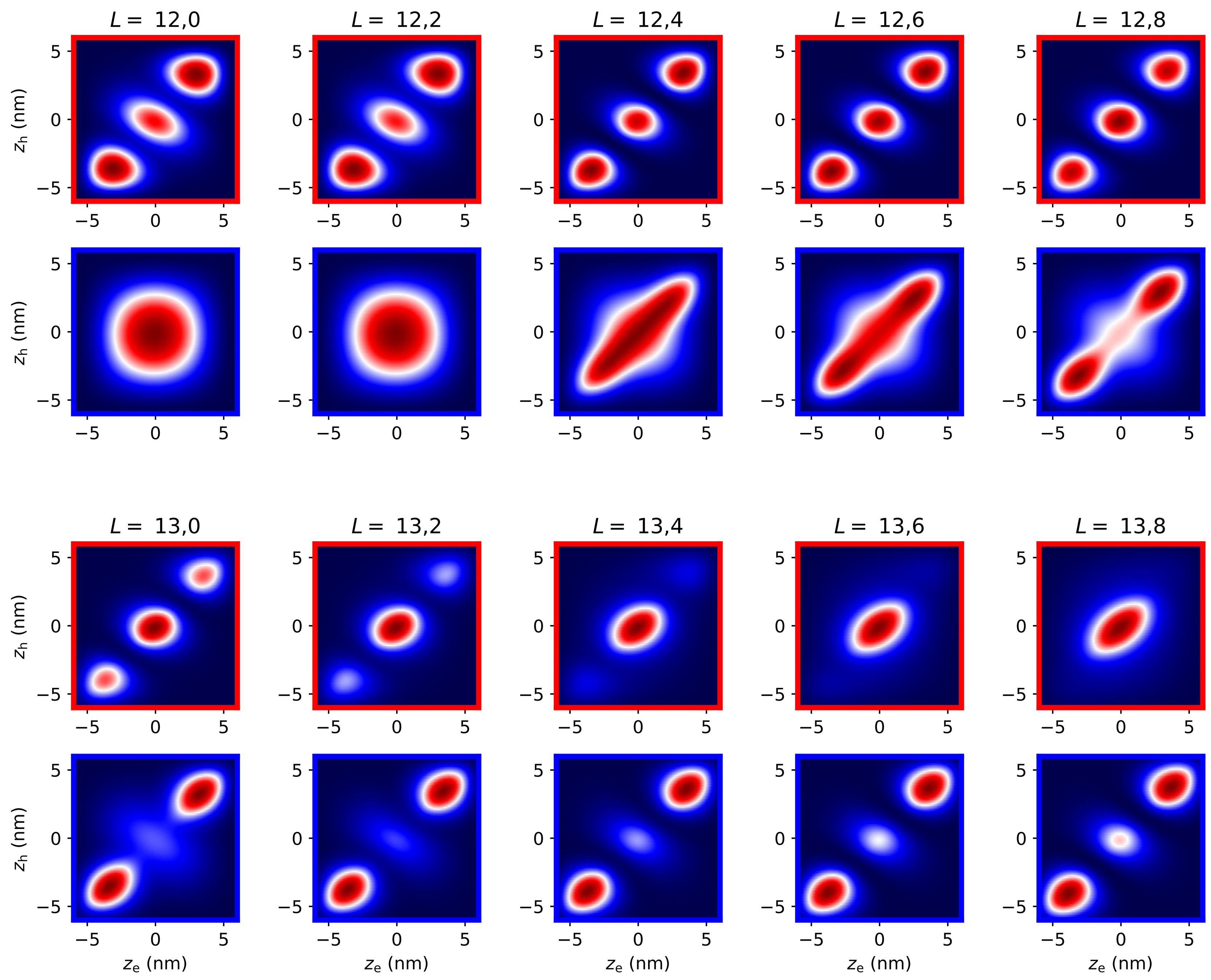
In the figures above $\int |\psi(z_\mathrm{e}, z_\mathrm{h}, \rho)|^2 \mathrm{d}\rho$ is shown in the $z_\mathrm{e}z_\mathrm{h}$-plane. The top figure shows the ground state for $m = 1$ in a well with width $L = 20\,\mathrm{nm}$. The right one is a higher excited state. The same state is also shown below. Here, $\psi(Z = 0\,\mathrm{nm}, z_\mathrm{rel}, \rho)$ is shown in the ρz_rel-plane. On the left side a state is shown for different center of mass coordinates.

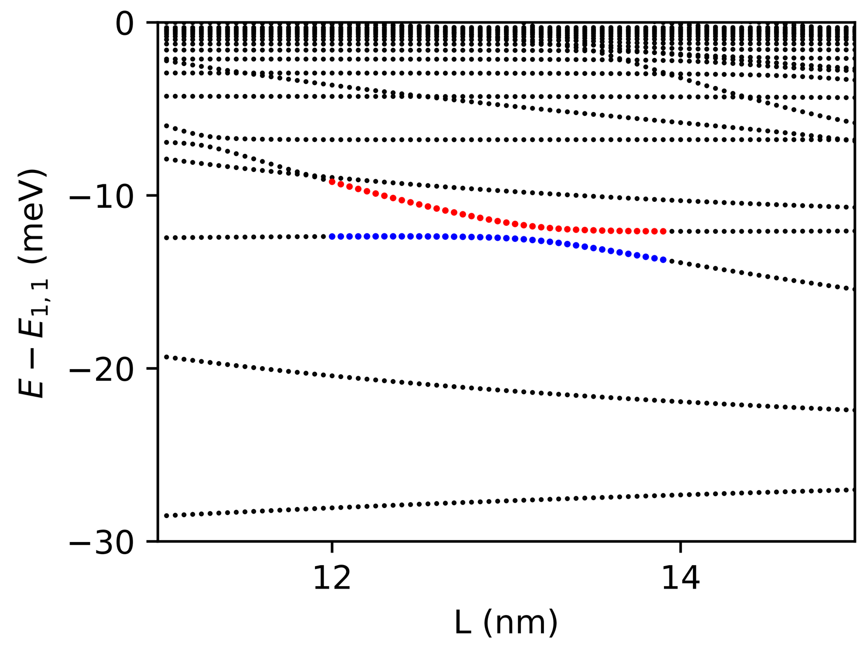




Here, $\int |\psi(z_\mathrm{e}, z_\mathrm{h}, \rho)|^2 \mathrm{d}\rho$ is shown for a state with $m = 0$. The calculation was done with the Rytova-Keldysh potential. This takes surface effects into account. The position of the maxima shows that the ground state is a surface-exciton state.

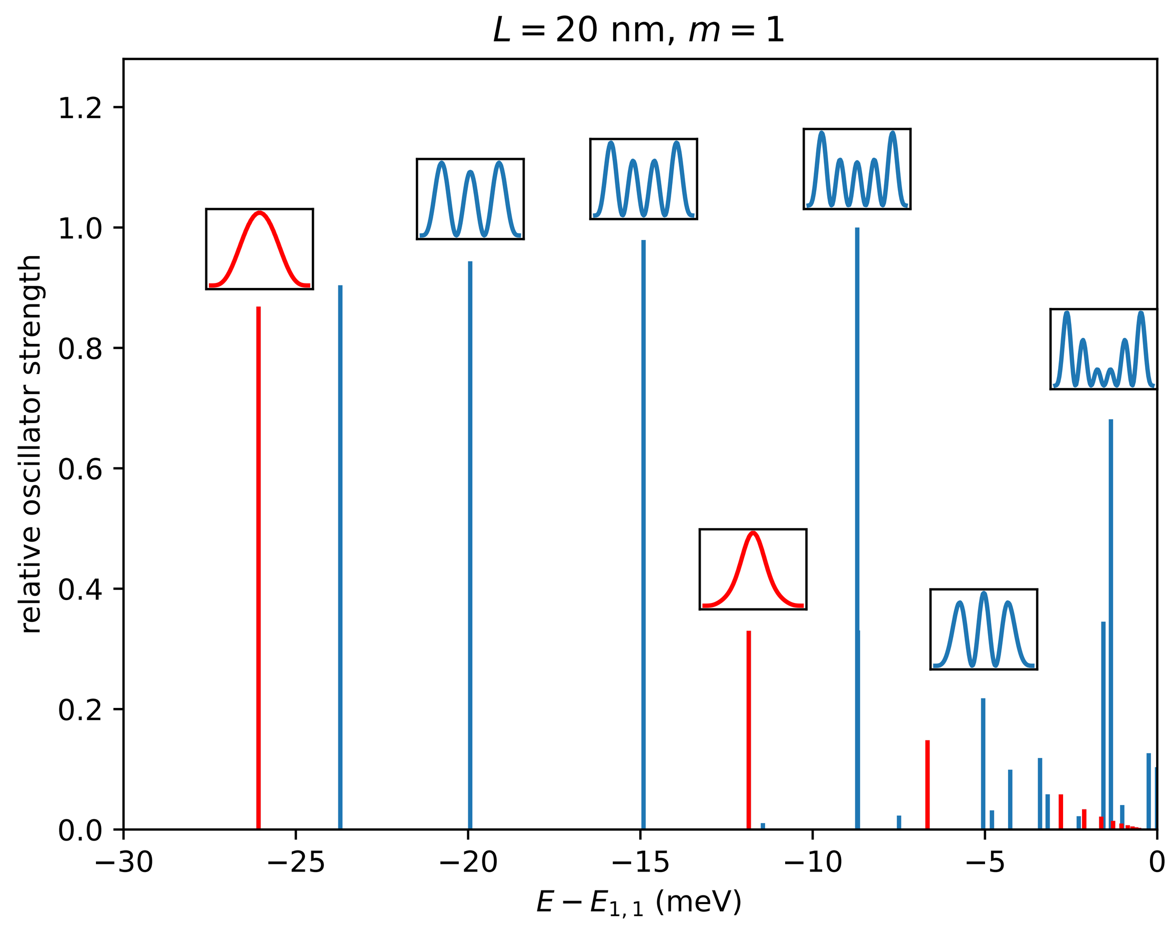
Avoided crossing





Here, two states can be seen with different quantum well widths. A transition from one state to the other can be seen along the avoided crossing, which is displayed in the figure on the left. One can see the different excitations in the number of knots along the diagonal.

Oscillator strengths



The relative oscillator strength for $m = 1$ is proportional to

$$f_\mathrm{rel} \sim \left|\lim_{\rho\to 0}\frac{1}{\rho}\psi(\rho, Z, z_\mathrm{rel} = 0)\right|^2.$$

In the figure one can see the relative oscillator strength of states in a cuprous oxide quantum well with width $L = 20\,\mathrm{nm}$ and magnetic quantum number $m = 1$. The inserted plots show the relative oscillator strength over the center of mass coordinate along the z-axis. The states that are marked in red, are the ones with only a single peak along the center of mass coordinate.