University of Stuttgart
Institute for Theoretical Physics I

Resonance energies and linewidhts of Rydberg excitons in Cu$_2$0 quantum wells

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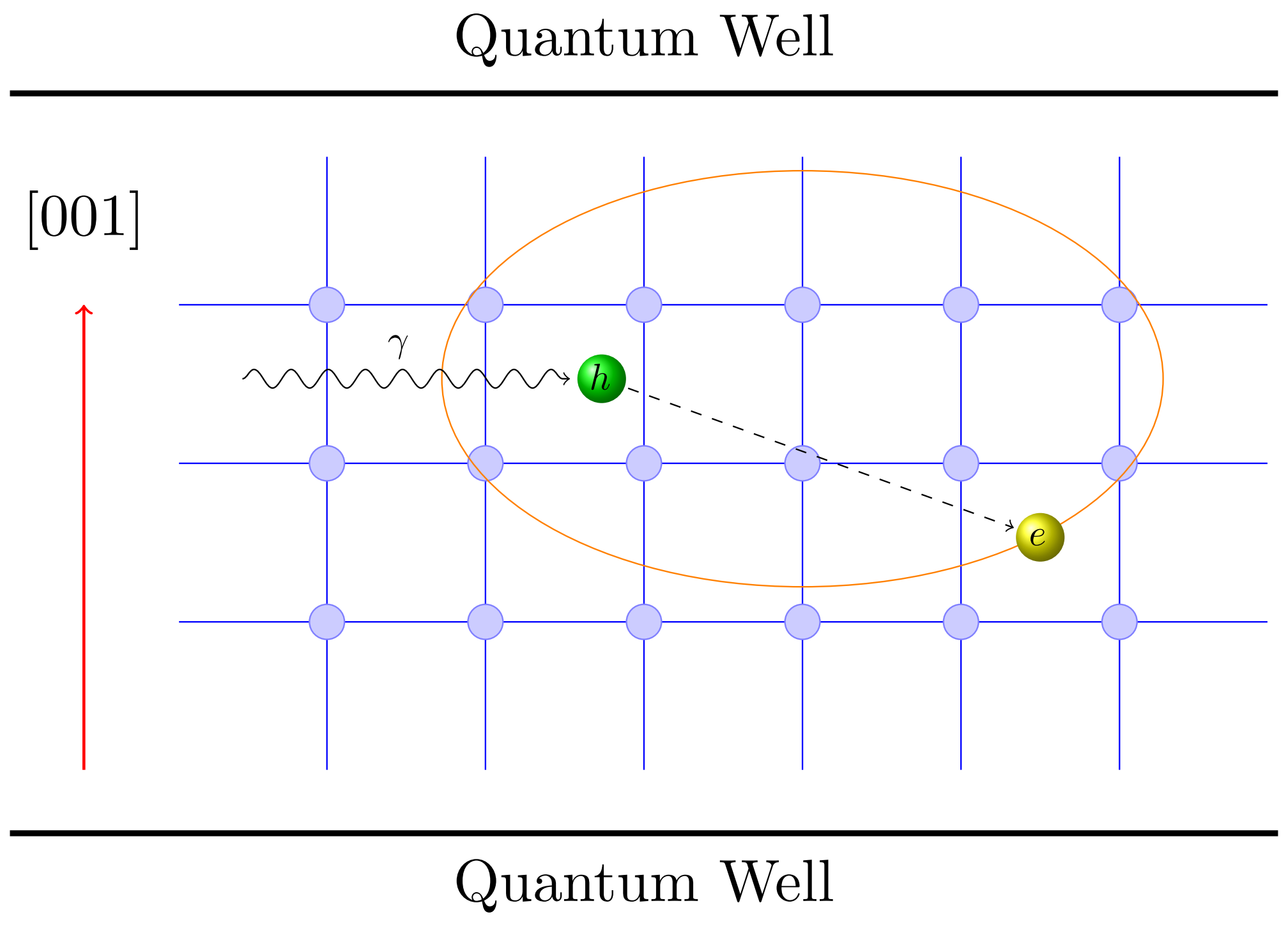
Hydrogenlike model for excitons in quantum wells

In the hydrogenlike model for excitons in quantum wells the band structure is neglected. Due to the cylindrical symmetry in the Hamiltonian, the degrees of freedom can be reduced to the coordinates (ϱ, z_e, z_h) and reads

$$H = -\frac{\hbar^2}{2m_\mathrm{e}}\frac{\partial^2}{\partial z_\mathrm{e}^2} - \frac{\hbar^2}{2m_\mathrm{h}}\frac{\partial^2}{\partial z_\mathrm{h}^2} - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial \rho^2} - \frac{m^2-\frac{1}{4}}{\rho^2}\right) - \frac{1}{4\pi\varepsilon_0\varepsilon}\frac{e^2}{\sqrt{\rho^2+(z_\mathrm{e}-z_\mathrm{h})^2}}$$

for the wave function $\chi(\rho, z_\mathrm{e}, z_\mathrm{h}) = \sqrt{\rho}\Psi(\rho, z_\mathrm{e}, z_\mathrm{h})$ The well potential is included via the boundary condition $\chi(\rho, z_\mathrm{e,h} = \pm L/2) = 0$.

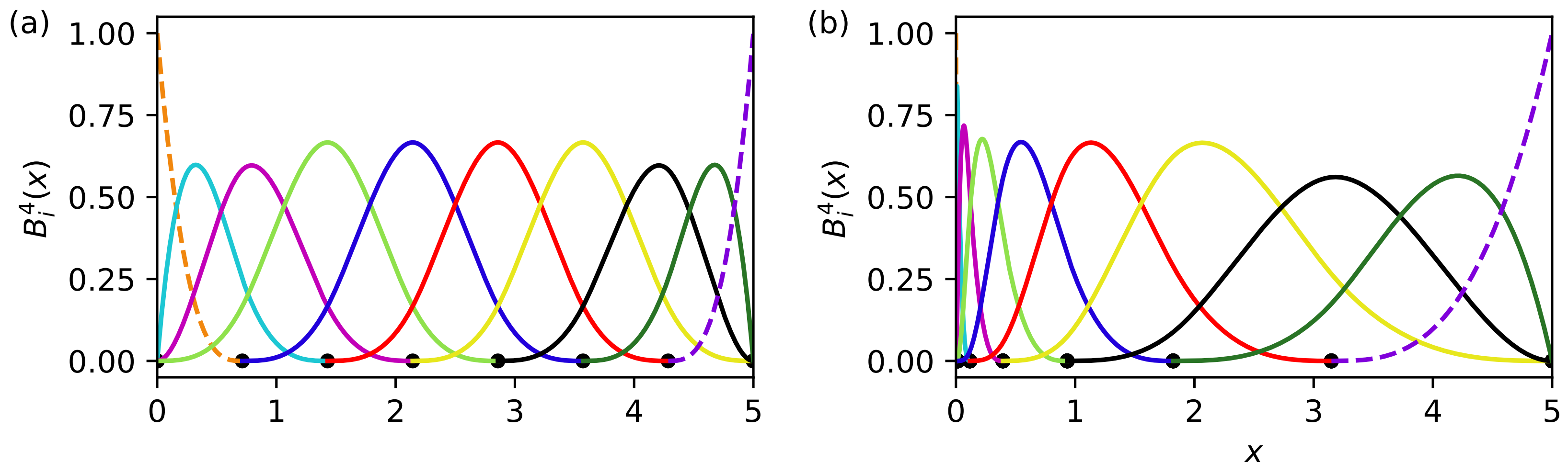


B-Spline method for energy calculations

In order to solve the time independent Schrödinger equation the wave function is expanded in terms of a finite B-spline basis

$$\chi(\rho, z_e, z_h) = \sum_{ijk} c_{ijk}\, B_i^k(\rho) B_j^k(z_e) B_k^k(z_h)$$

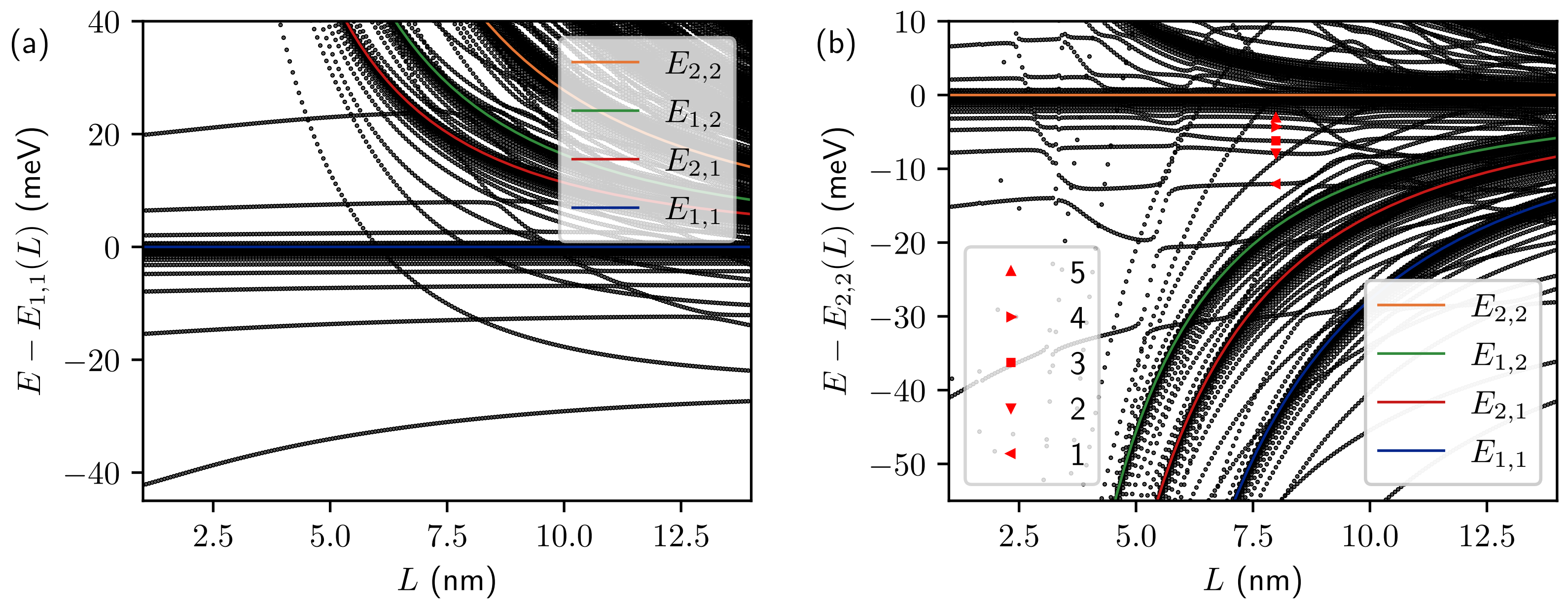
The B-splines are piecewise continuous polynomials, that are nonzero only in a certain interval. This expansion leads to generalized eigenvalue problem with sparse matrices.



For $L \rightarrow 0$ the problem can be solved analytically. The spectrum contains Rydberg series below each threshold associated to the confinement states with the energies

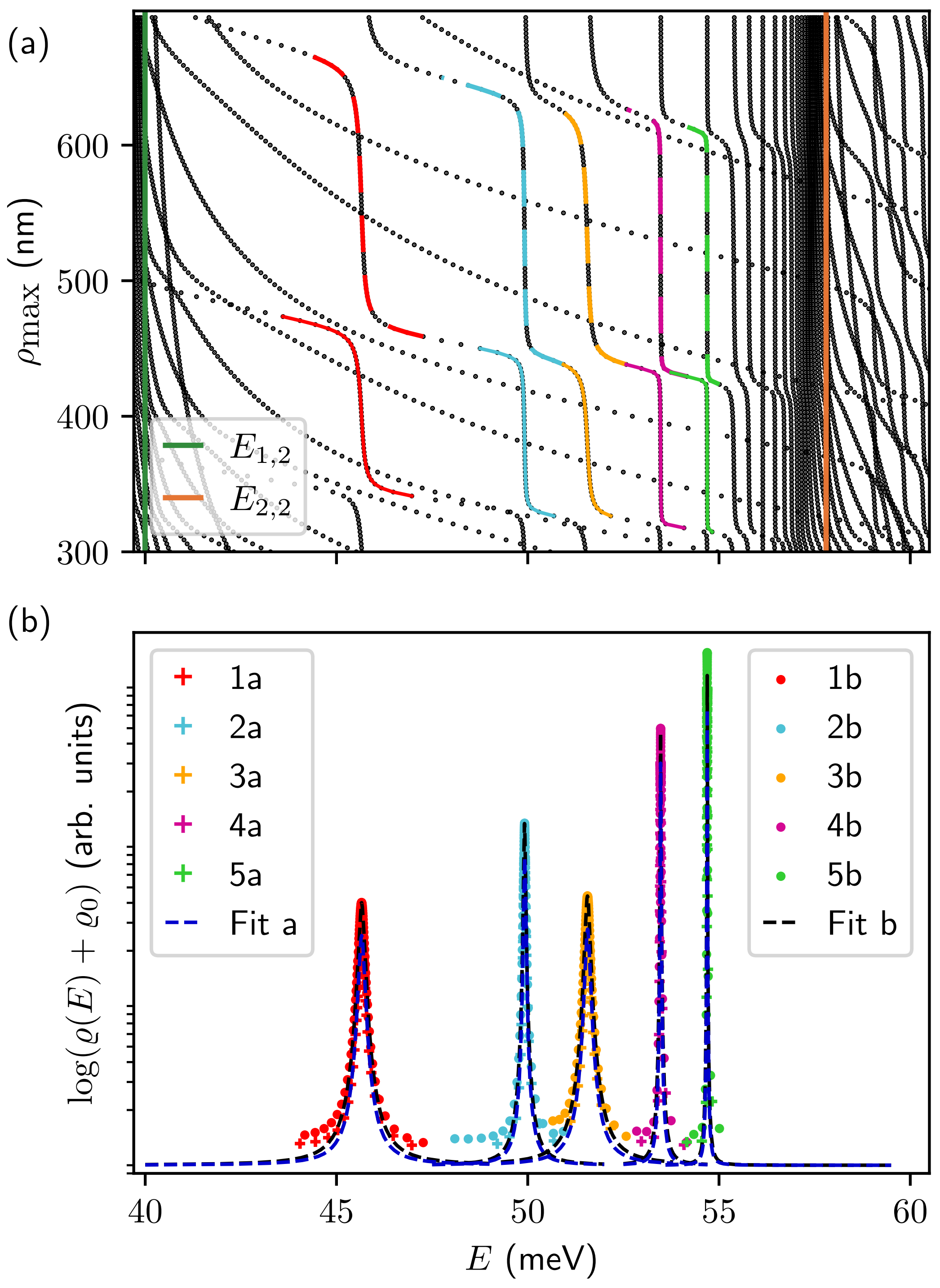
$$E_{i,j}(L) \equiv E_{\mathrm{e}i}(L) + E_{\mathrm{h}j}(L) = \frac{\hbar^2(i\pi)^2}{2m_\mathrm{e}L^2} + \frac{\hbar^2(j\pi)^2}{2m_\mathrm{h}L^2}.$$

For finite well widths, there is a coupling between the states belonging to different thresholds. This results in the occurrence of resonant states.



N. Scheuler, P. Rommel, J. Main, and P. A. Belov, Phys. Rev. B **109**, 165440 (2024)

Stabilization method



The stabilization method uses the real-valued spectrum of the Hamiltonian to calculate the complex eigenenergies $E = E_\mathrm{res} - i\Gamma/2$. Calculating the spectrum for different values of the stabilization parameter ρ_max yields the stability diagram. Bound states are independent of the parameter, while resonant states stabilize in certain regions. The density of states can be extracted from the branches in the stability diagram using the relationship

$$\varrho(E) = \left|\frac{\mathrm{d}E_\mathrm{b}(\rho_\mathrm{max})}{\mathrm{d}\rho'_\mathrm{max}}\right|^{-1}_{E_j(\rho'_\mathrm{max})=E},$$

while it is expected to behave as

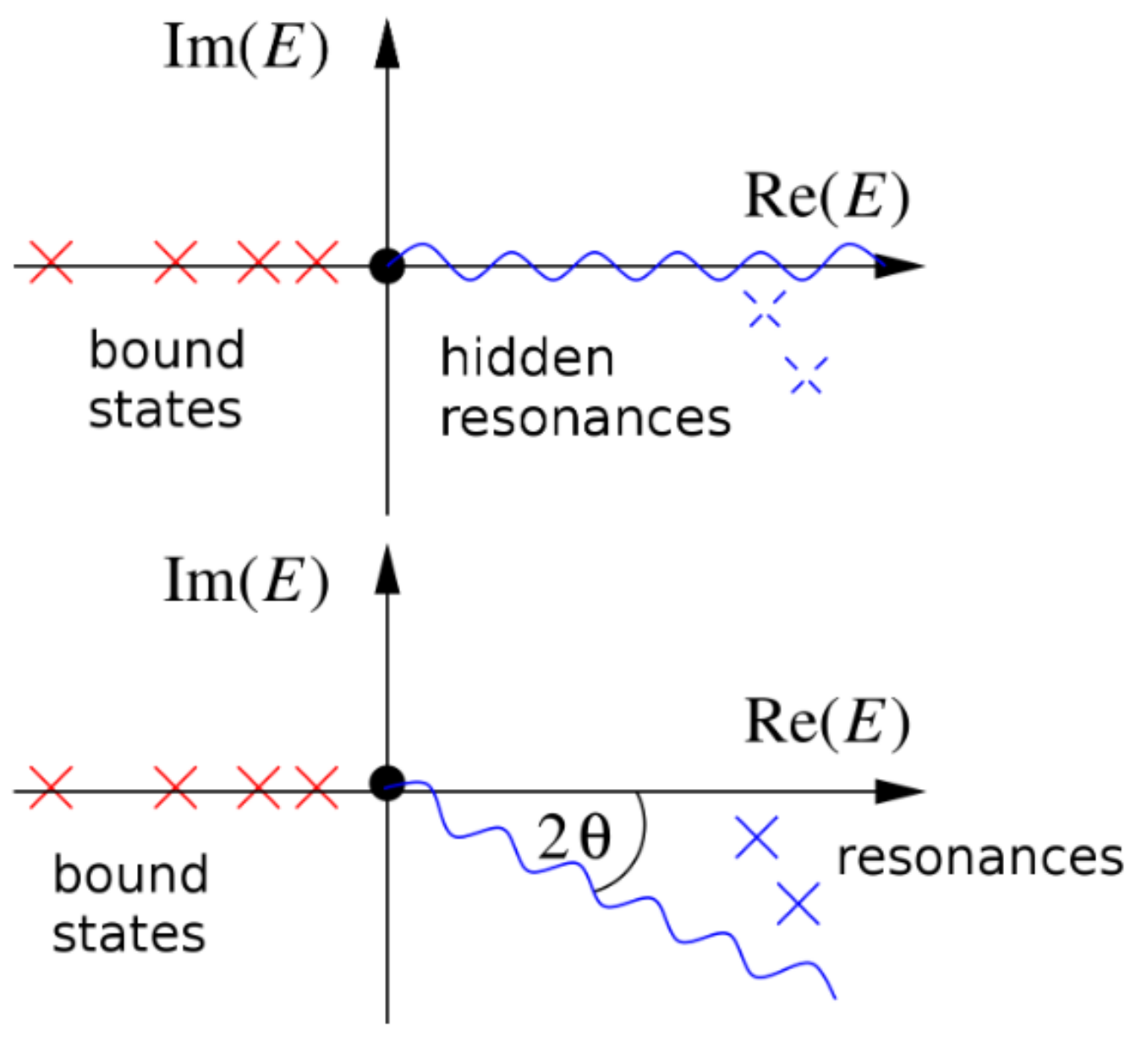
$$\varrho(E) \simeq \pi^{-1}\frac{\Gamma/2}{(E_\mathrm{res}-E)^2+\Gamma^2/4}.$$

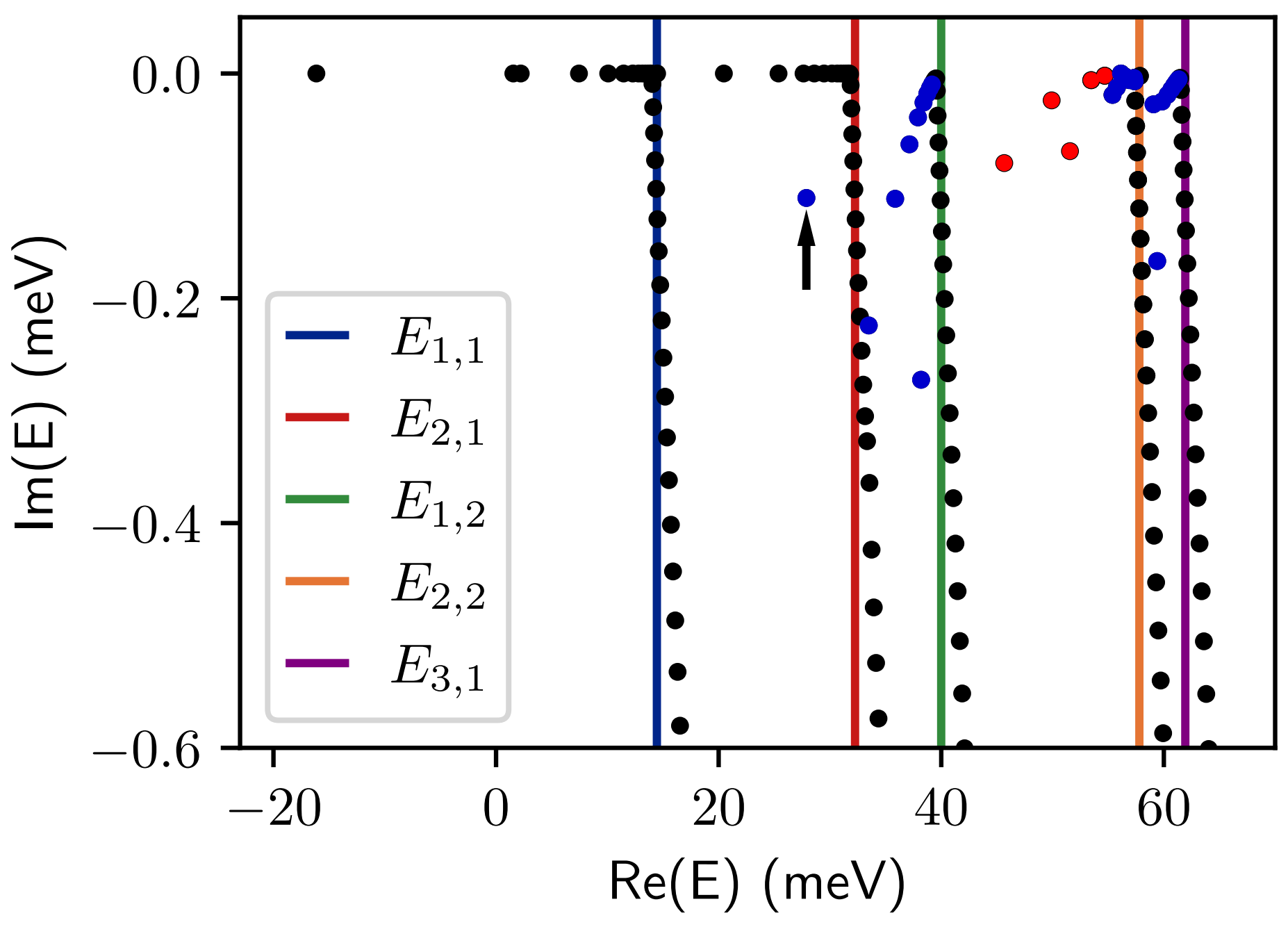
The complex energy is then determined by a fit to Lorentzian profile.

V. A. Mandelshtam, H. S. Taylor, V. Ryaboy, and N. Moiseyev, Phys. Rev. A **50**, 2764–2766 (1994)

Complex-coordinate-rotation method

The transformation $\rho \rightarrow \rho\exp(i\Theta)$ makes the Hamiltonian non-Hermitian. Bound and resonant state energies are invariant under this transformation, while the discretized continuum energies are rotated in the lower half of the complex plane by the angle 2Θ. This reveals the hidden resonances.





W. P. Reinhardt, Annual Review of Physical Chemistry **33**, 223–255 (1982)

Comparison of the results

				Stabilization method		Complex rotation	
i	j	n	segment	Re E	Im E	Re E	Im E
2	2	3	1a	45.6577	-0.0815	45.6607	-0.0798
			1b	45.6547	-0.0812		
2	2	4	2a	49.9181	-0.0242	49.9189	-0.0239
			2b	49.9164	-0.0229		
3	1	3	3a	51.5645	-0.0670	51.5665	-0.0691
			3b	51.5613	-0.0705		
2	2	5	4a	53.4736	-0.0060	53.4738	-0.0060
			4b	53.4738	-0.0062		
2	2	6	5a	54.6914	-0.0020	54.6915	-0.0020
			5b	54.6914	-0.0019		