Ultracold quantum scattering - Part II: bound states with discrete variable representation

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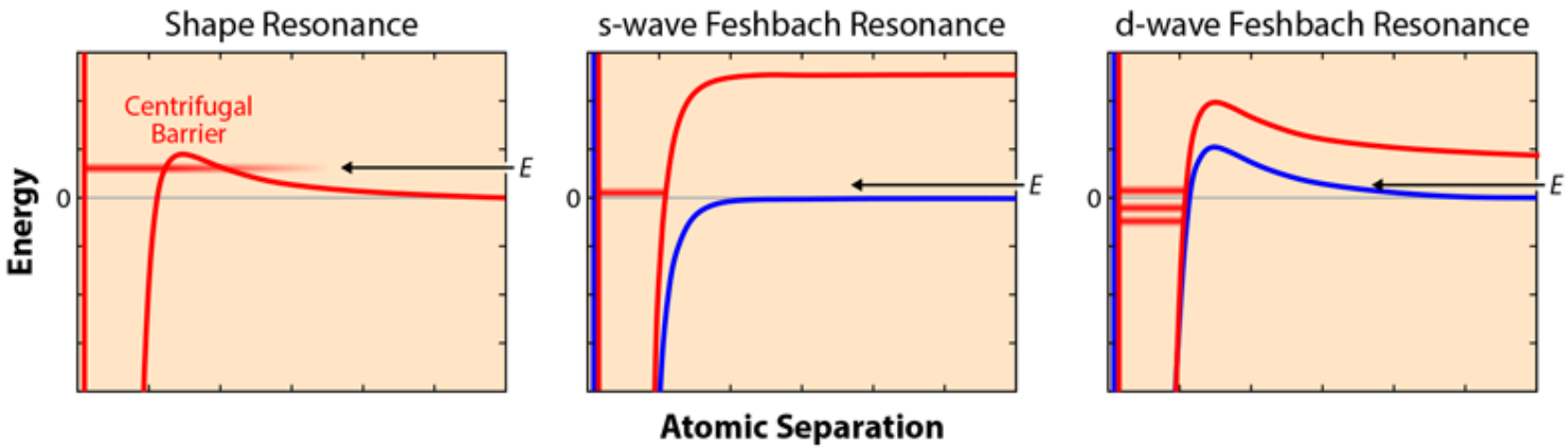
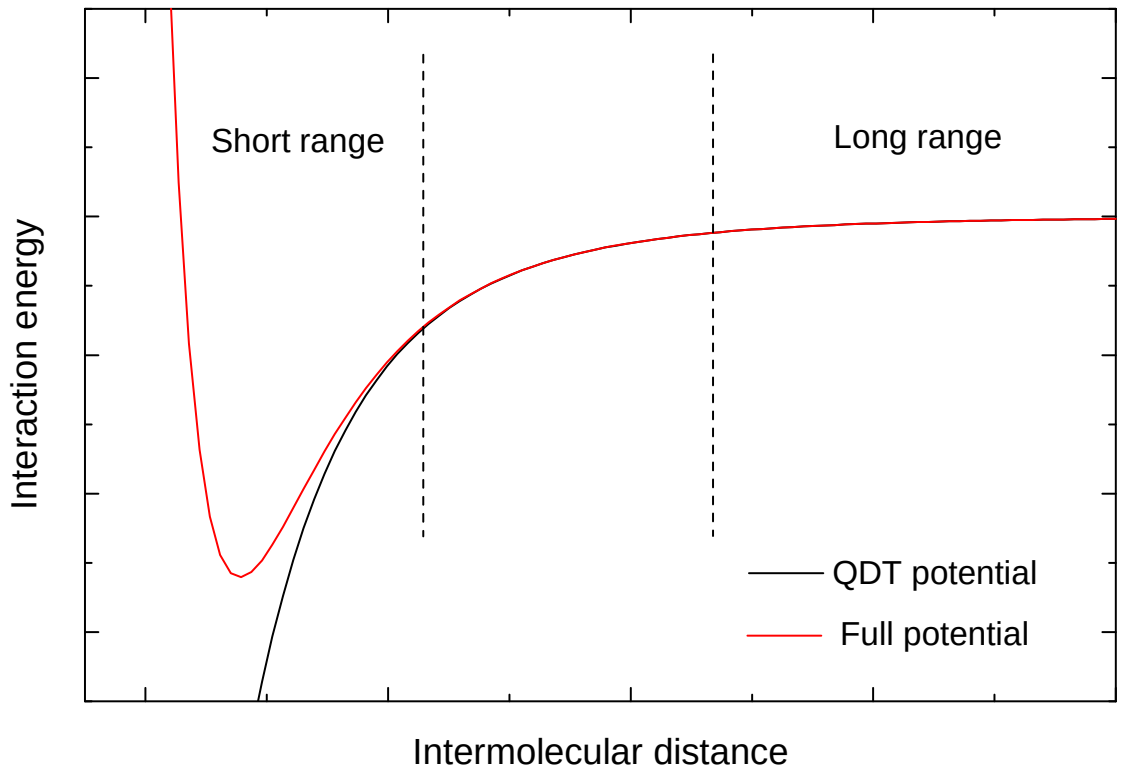
Resonances in ultracold collisions

Resonances in ultracold collisions

- **shape resonances**
- **Feshbach resonances**

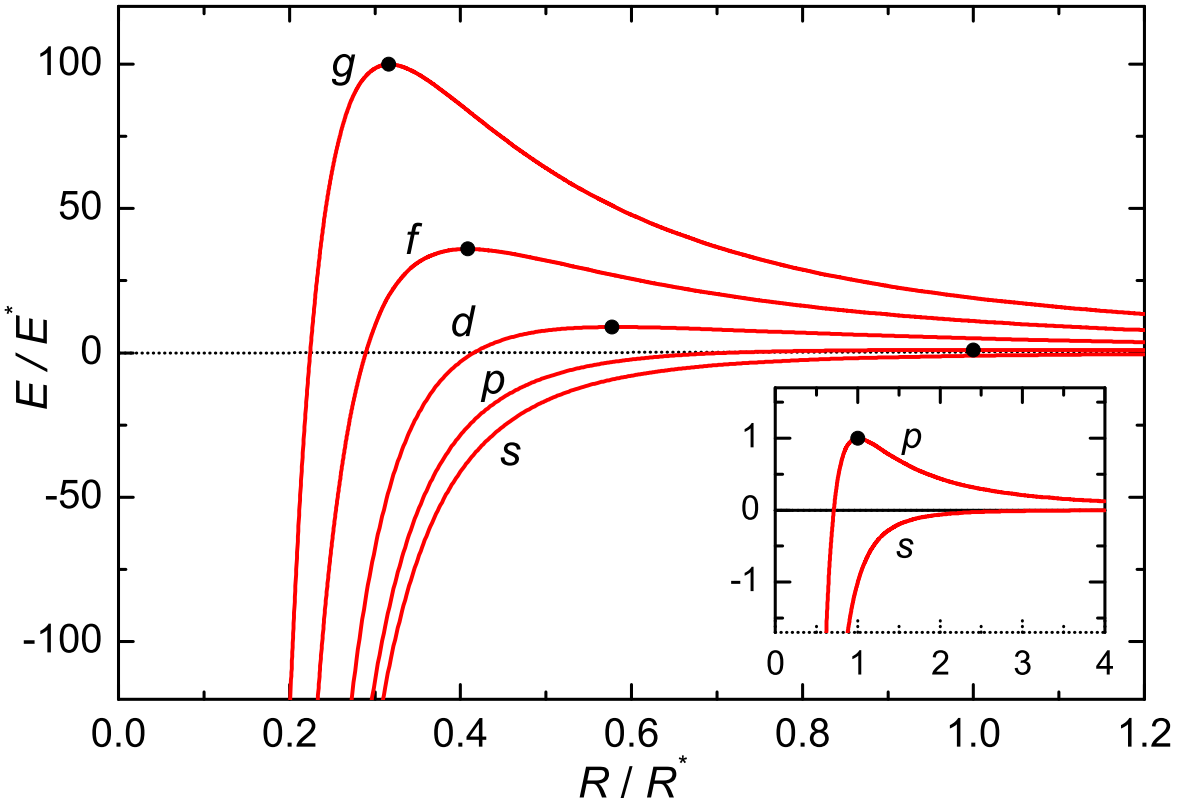


Interaction potential - isotropic case



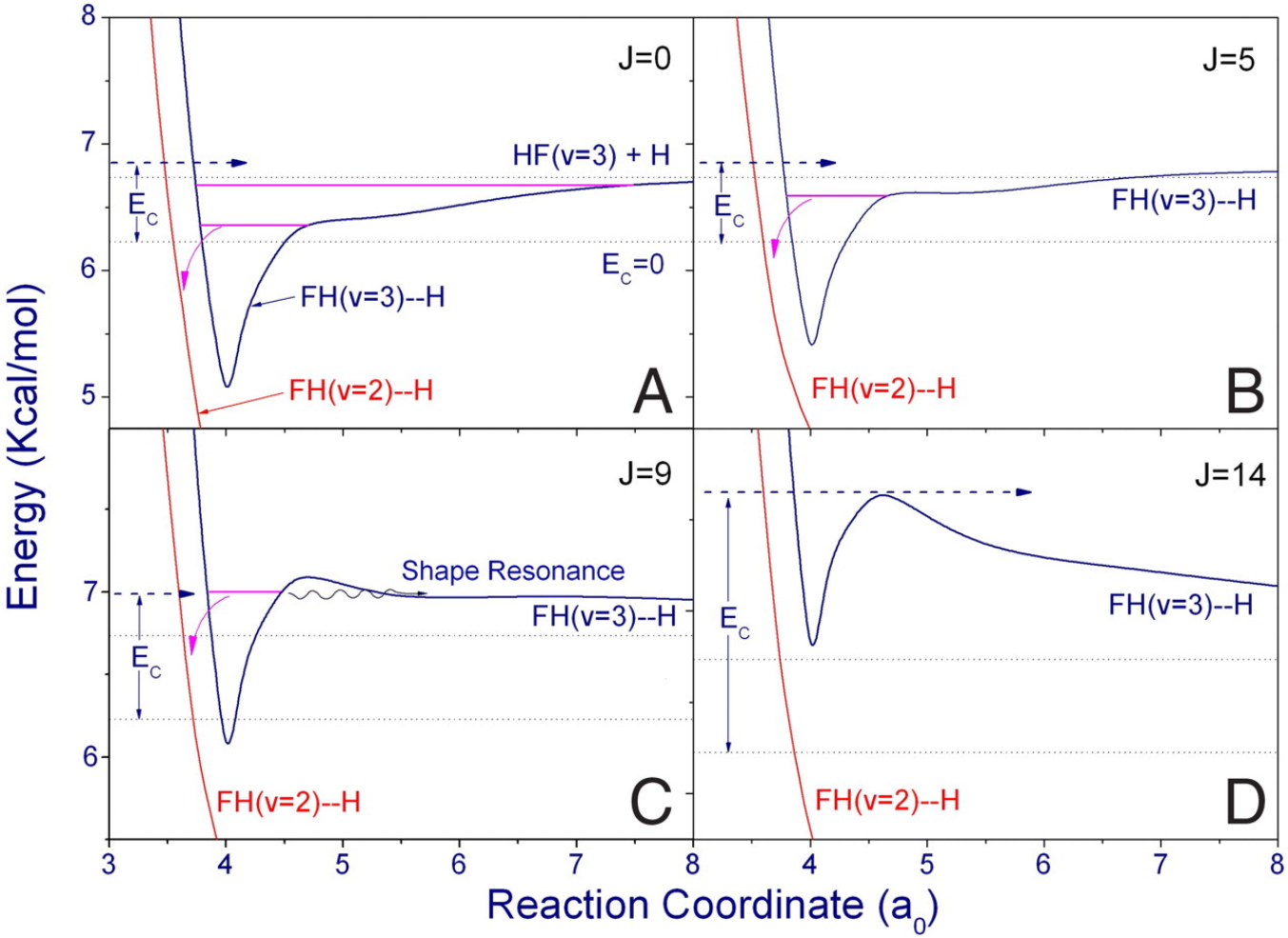
$$V_{\mathrm{tot}}(R) \xrightarrow{R\to\infty} \frac{\hbar^2 l(l+1)}{2\mu R^2} - \frac{C_6}{R^6}, \qquad k = \sqrt{2\mu E/\hbar^2}$$

Centrifugal barrier

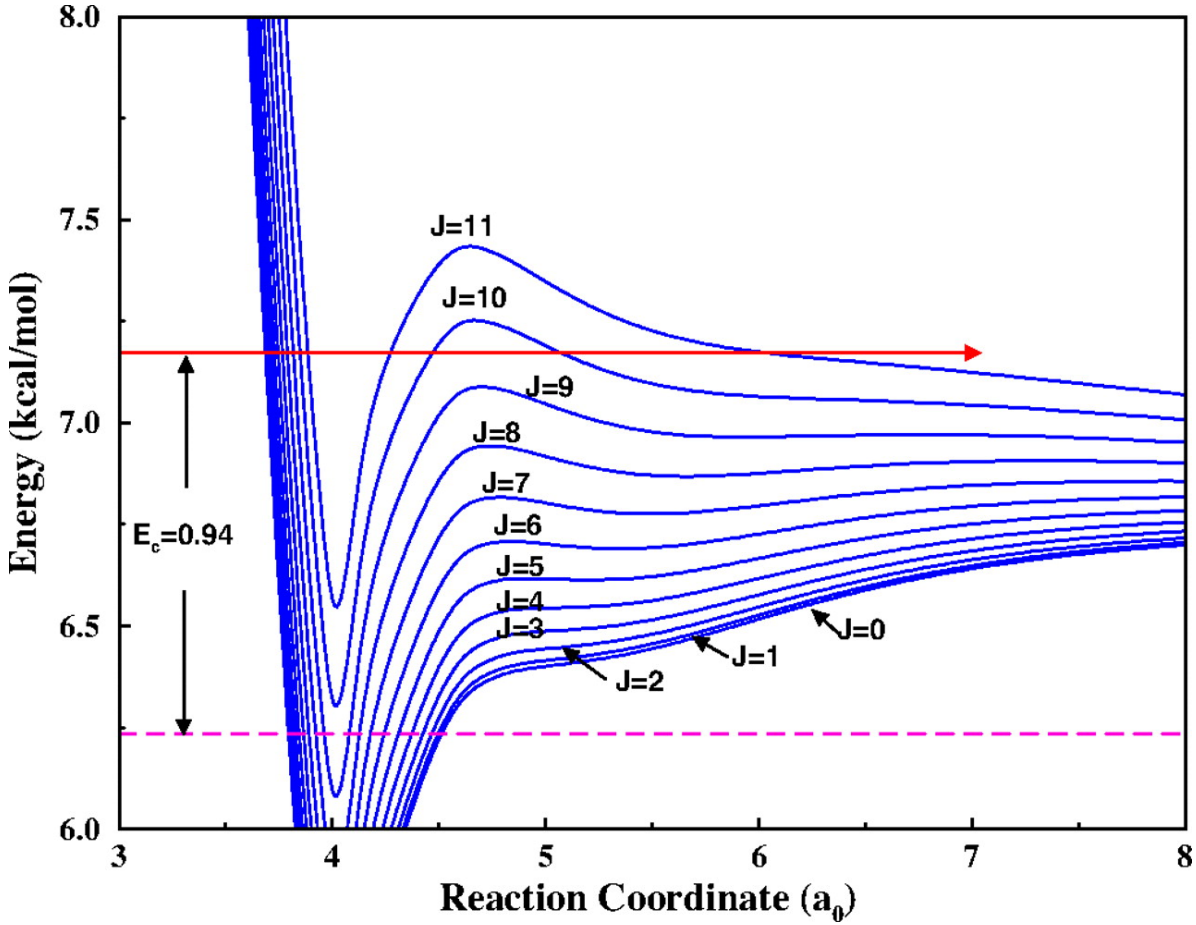


$$R_6 = \left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4}, \qquad E_6 = \frac{\hbar^2}{2\mu R_6^2}$$

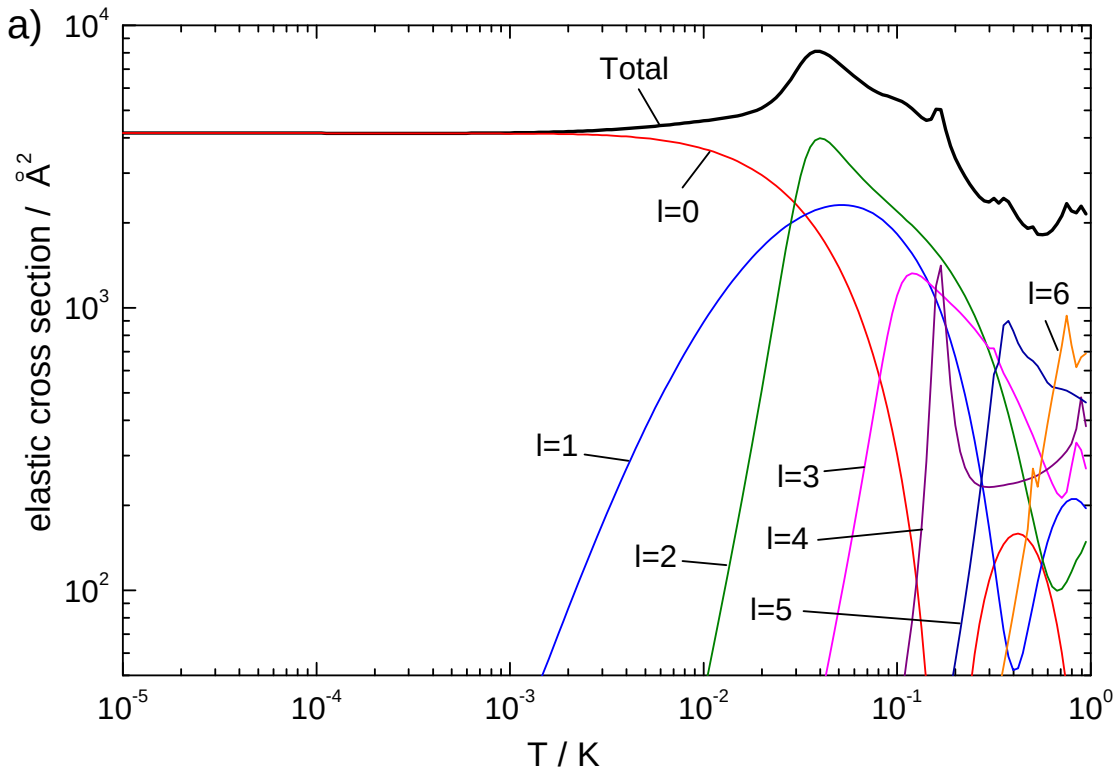
Shape resonances in collisions of HF+H



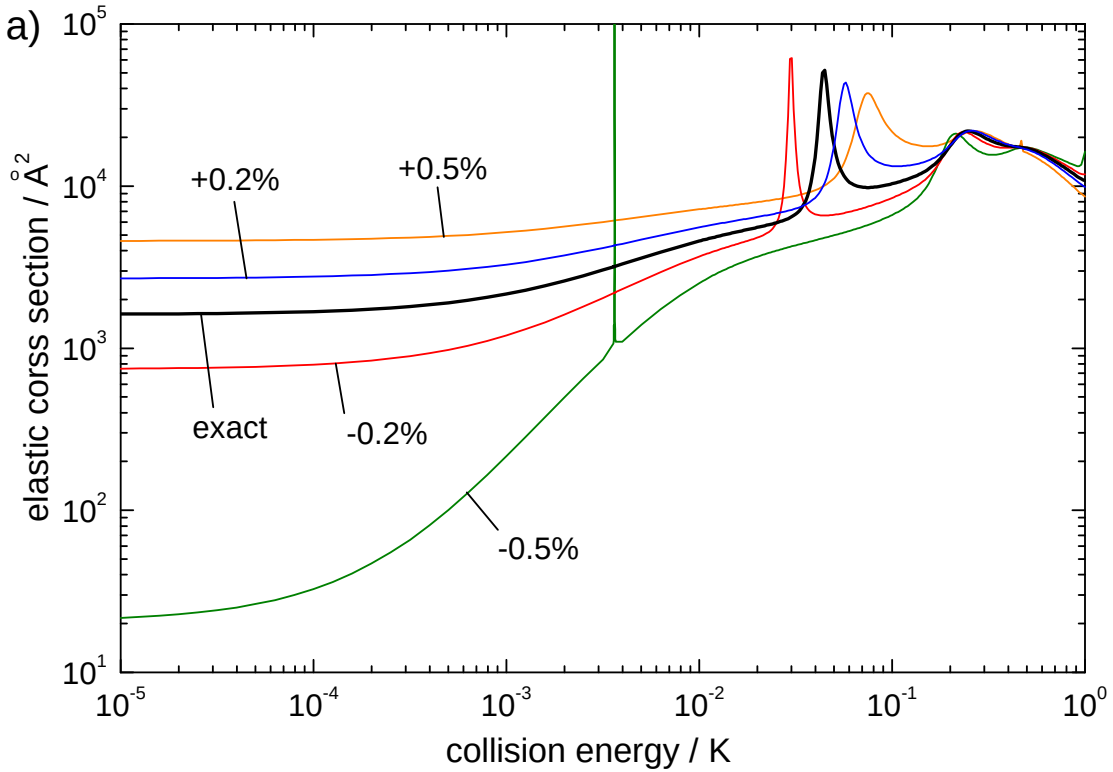
Shape resonances in collisions of HF+H



Shape resonances in collisions of LiH+Li

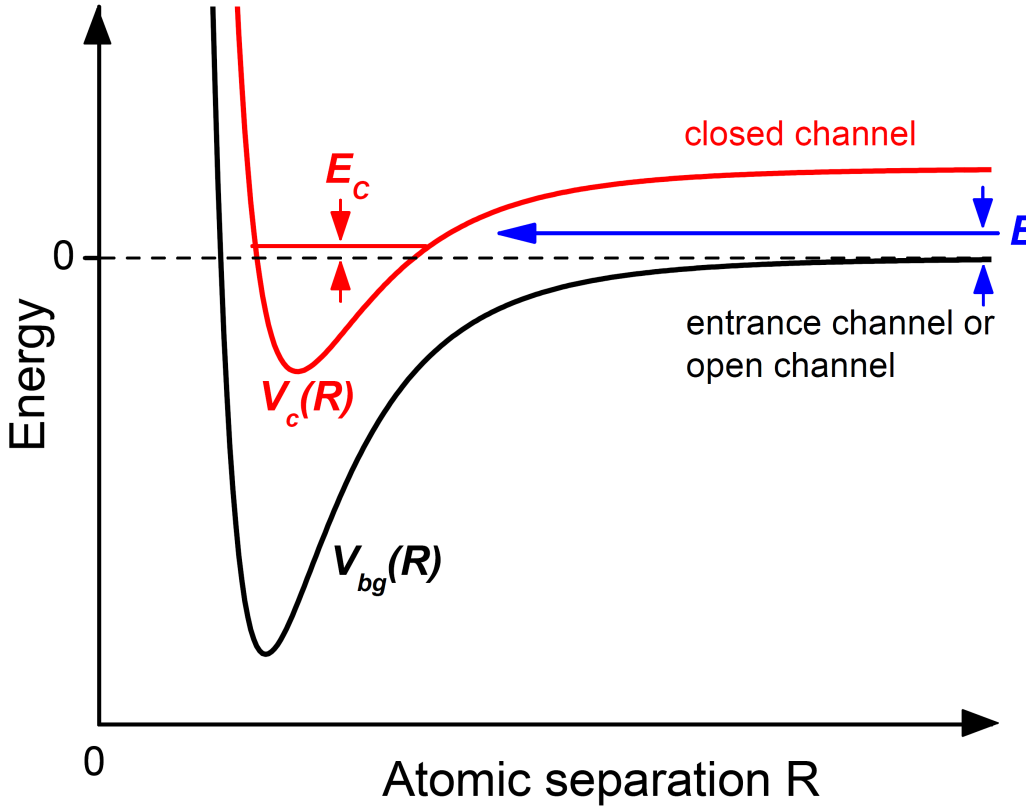


Controlling shape resonances in collisions of LiH+Li



Origin of Fesbhach resonances

Cold Molecules: Theory, Experiment, Applications.
CRC Press, 2009



$|f_{1'}m_{1'}f_{2'}m_{2'}l'm_{l'}>$

$|f_1 m_1 f_2 m_2 l m_l>$

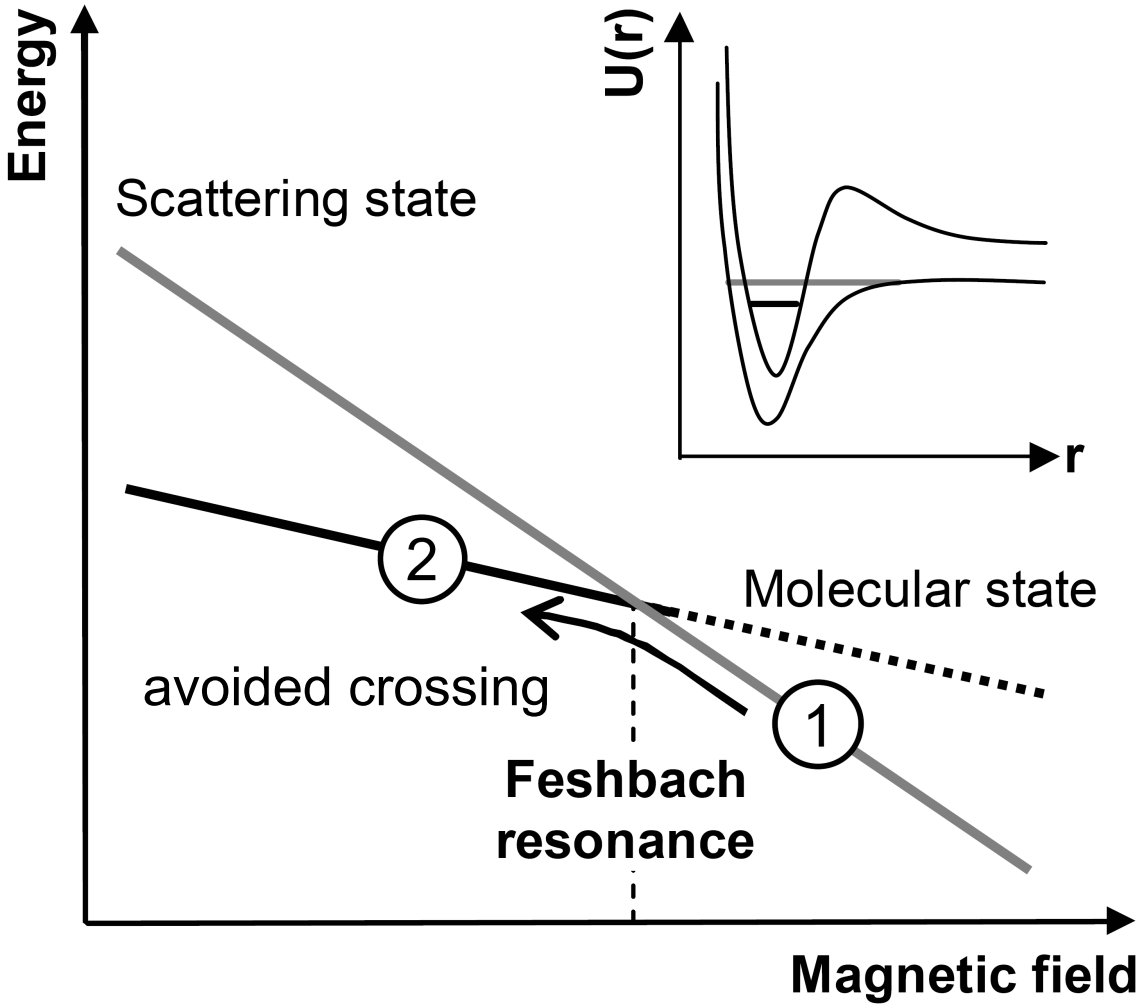
$|\alpha> \equiv |f_1 m_1 f_2 m_2 l m_l> \rightarrow |f_1 m_1> + |f_2 m_2>$

open: $E_\alpha = E_{f1m1} + E_{f2m2} < E_{total}$

closed: $E_\alpha = E_{f1m1} + E_{f2m2} > E_{total}$

Crossing between atomic and molecular states

Int. Rev. Phys. Chem. **25**(4), 496 (2006)

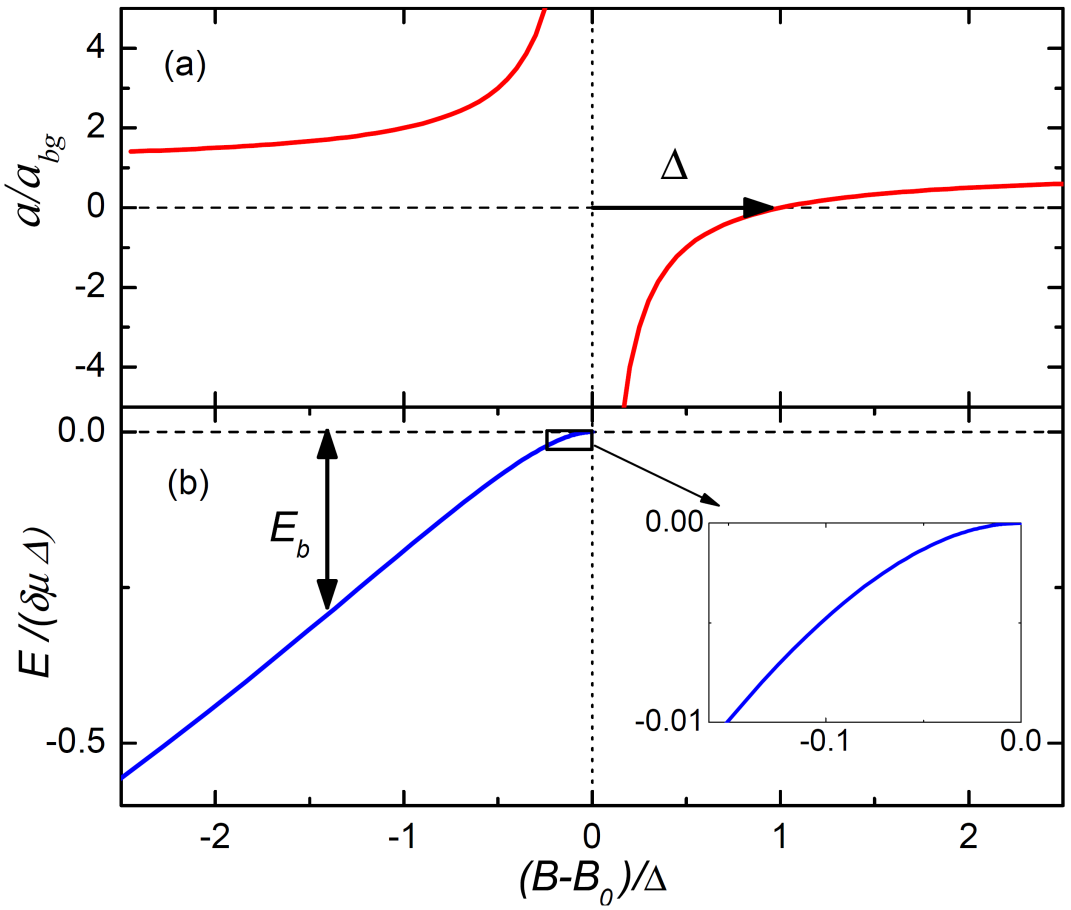


$E=\Sigma \mu_i B_i$

$\mu_{open} \neq \mu_{closed}$

Scattering length and binding energy

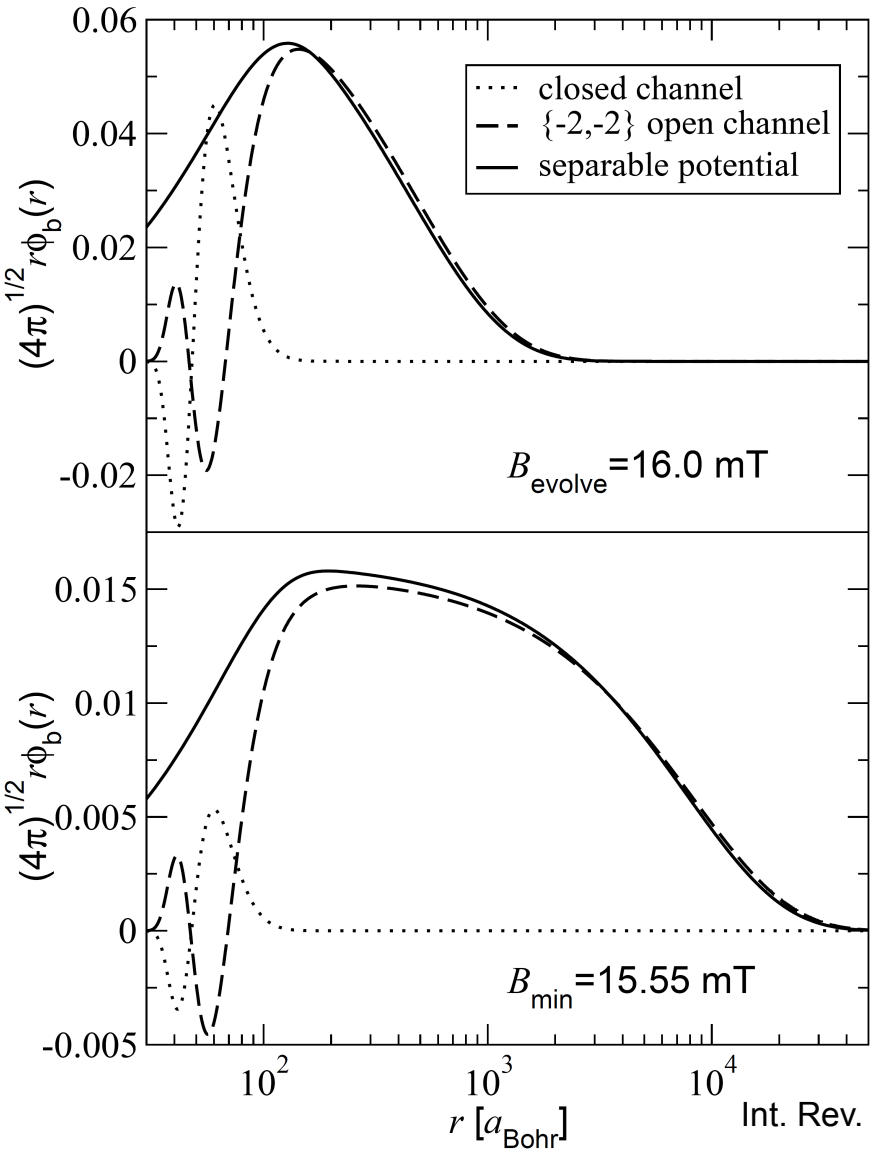
Cold Molecules: Theory, Experiment, Applications.
CRC Press, 2009



$$a(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right)$$

$$E_{top} = \frac{-h^2}{2\mu a^2}$$

Very weakly bound states



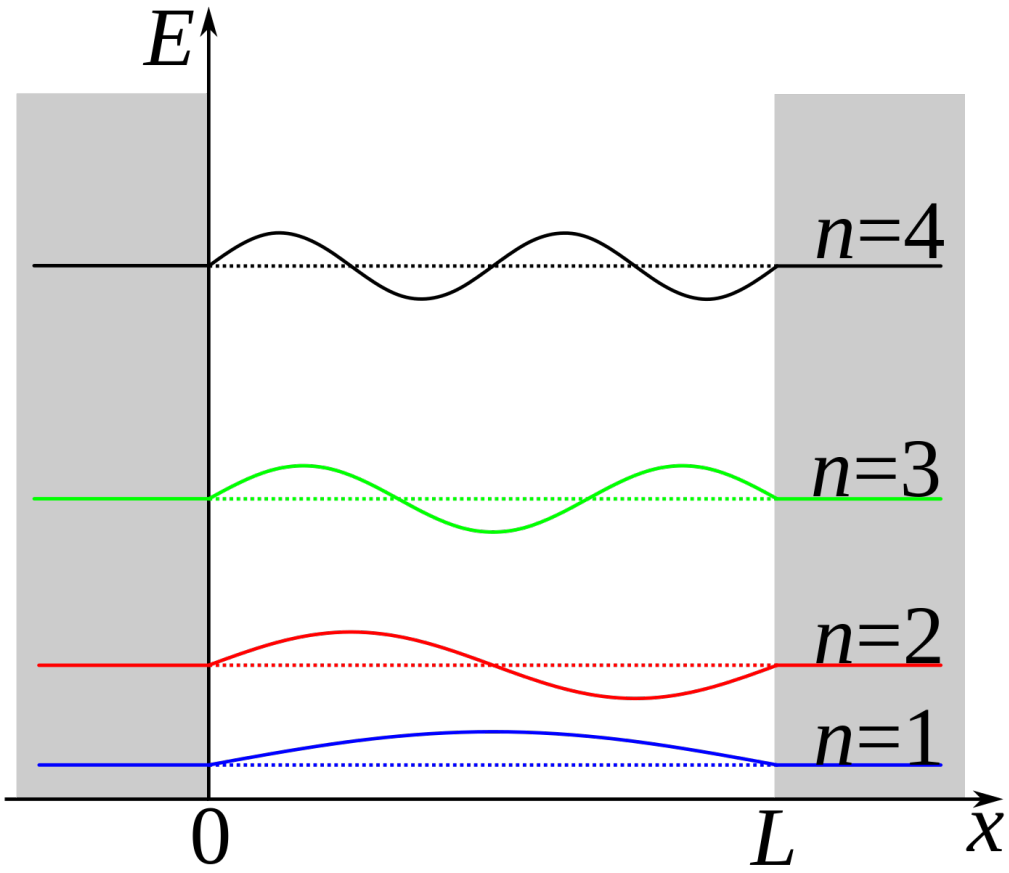
Int. Rev. Phys. Chem. **25**(4), 496 (2006)

Quantum bound state calculations

Schrödinger equation for a particle in 1D

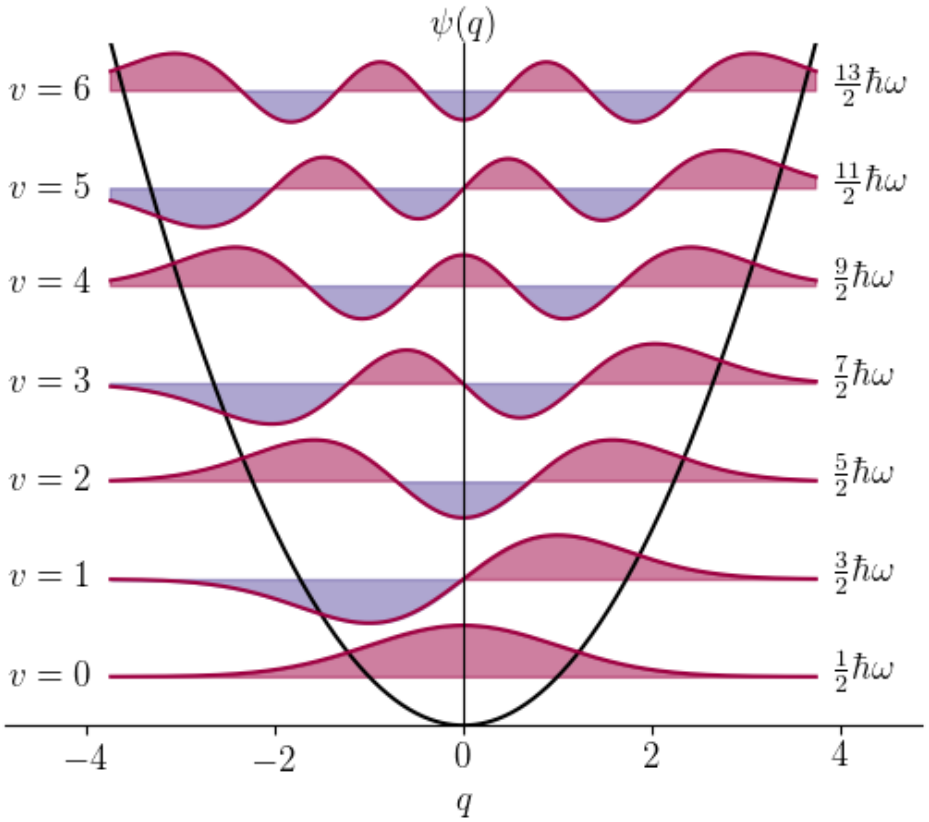
$$\left(\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + V(R)\right)\Psi_n(R) = E_n\Psi_n(R) \tag{1}$$

Quantum particle in a box



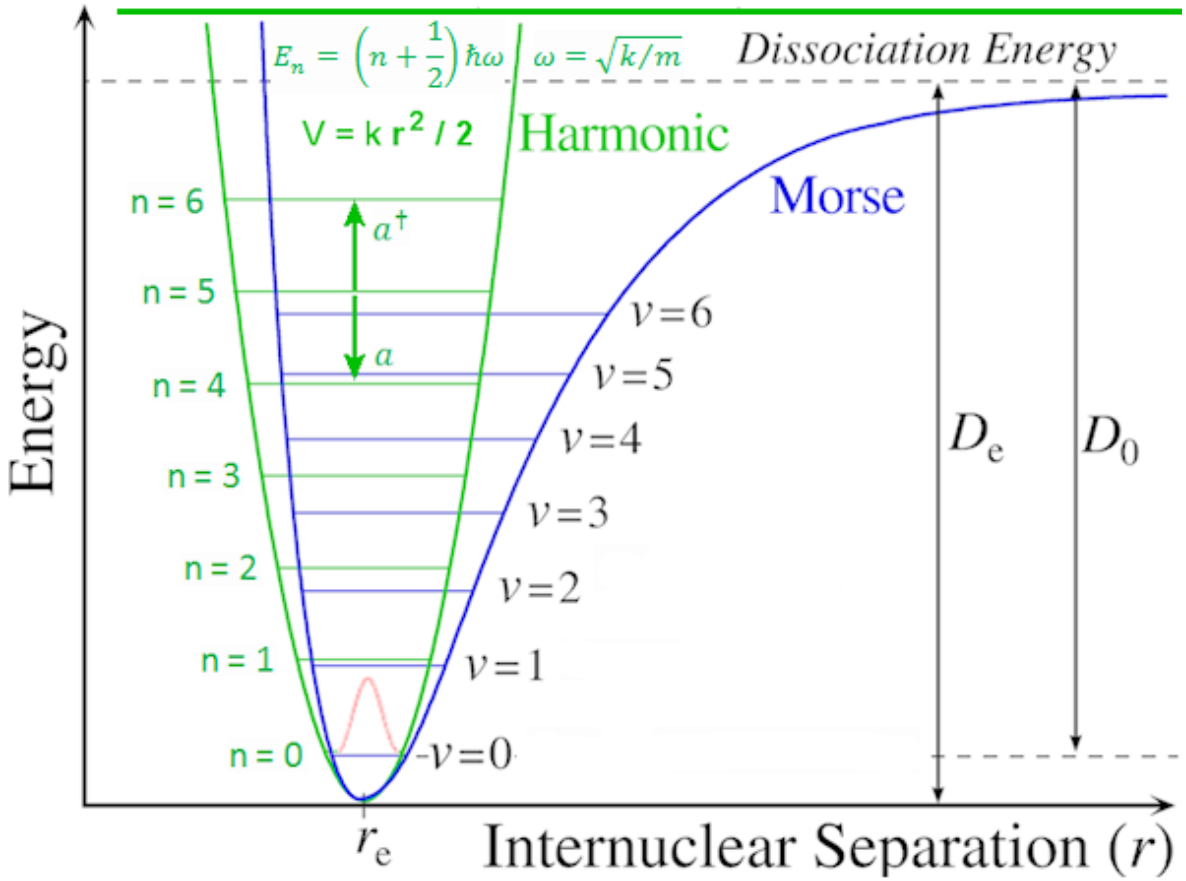
$$E_n = \frac{n^2 \pi^2 \hbar^2}{2\mu L^2} \tag{2}$$

Quantum harmonic oscillator



$$E_v = \hbar\omega_0 \left(\frac{1}{2} + v \right) \tag{3}$$

Molecular potential



$$E_v = \hbar\omega_0 \left(\frac{1}{2} + v\right) - \chi\hbar\omega_0 \left(\frac{1}{2} + v\right)^2 + \ldots \qquad (4)$$

Discrete variable representation

Schrödinger equation for a diatomic molecule

$$\hat{H}\Psi_{v,j}(R) = E_{v,j}\Psi_{v,j}(R) \tag{5}$$

$$\left(\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \frac{\hbar^2}{2\mu}\frac{j(j+1)}{R^2} + V_{\text{int}}(R)\right)\Psi_{v,j}(R) = E_{v,j}\Psi_{v,j}(R) \tag{6}$$

$$\hat{H} = \frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \frac{\hbar^2}{2\mu}\frac{j(j+1)}{R^2} + V_{\text{int}}(R) \tag{7}$$

DVR method

The DVR methods are pseudo-spectral methods, where the Schrödniger equation (6) is discretized on a finite grid of collocation distances R_i,

$$H_{ij} = T_{ij} + V_{ij}\,, \tag{8}$$

and eigenenergies and eigenstates are found by the diagonalization of the **H** matrix.
The simplest DVR method is the Fourier grid representation, which is based on the eigenfunctions of a particle in a box. In this methods, the equidistant collocation distances R_i between R_0 and R_N are employed

$$R_i = R_0 + \frac{i(R_N - R_0)}{N} \tag{9}$$

for i between 1 and $N-1$.

DVR method

The kinetic energy operator is given by

$$T_{ii} = \frac{\hbar^2\pi^2\left(\frac{1}{3}(2N^2+1) - \sin^{-2}\left(\frac{\pi i}{N}\right)\right)}{4\mu(R_N - R_0)^2} \tag{10}$$

for $i = j$ and

$$T_{ij} = \frac{\hbar^2\pi^2(-1)^{i-j}\left(\sin^{-2}\left(\frac{\pi(i-j)}{2N}\right) - \sin^{-2}\left(\frac{\pi(i+j)}{2N}\right)\right)}{4\mu(R_N - R_0)^2} \tag{11}$$

for $i \neq j$. The potential energy operator is diagonal and simply given by

$$V_{ij} = \delta_{ij}\left(\frac{\hbar^2 j(j+1)}{2\mu R_i^2} + V_{\text{int}}(R_i)\right) . \tag{12}$$

Computer laboratory

Molecular bound states

Task I (1 pt.): Calculate and plot wavefunctions and binding energies of molecular bound states of the K_2 molecules in the $a^3\Sigma_u^+$ electronic state. Analyze the isotopic effect (change in spectra due to selecting different isotopes), rotational effect (change in spectra due to selecting different rotational state), and anharmonicity effect (difference between molecular spectrum and spectrum of the harmonic oscillator with the same curvature at the equilibrium distance).

Task* II (0.2 pt.): Calculate the average interatomic distance for vibrational states of $^{39}K_2$ molecule.

Molecular bound states

Interaction potential for the K_2 in the $a^3\Sigma_u^+$ electronic state:

$$V(R) = D_e \left[\left(\frac{R_e}{R} \right)^{12} - 2 \left(\frac{R_e}{R} \right)^{6} \right],$$

where $D_e = 0.0011141$ a.u., $R_e = 10.98$ a.u.

$m_{^{39}\mathrm{K}}$=38.963707 u
$m_{^{40}\mathrm{K}}$=39.963999 u
$m_{^{41}\mathrm{K}}$=40.961825 u
1 u = 1822.888 a.u.

use atomic units: $\hbar = m_e = 1$