Homework 4b

Jahn-Teller model

(E×E) Jahn-Teller model describes vibrations of a molecule in two dimensional configuration space (x,y). The molecule can also flip between two electronic states $|1\rangle, |2\rangle$. The Hamiltonian reads

$\omega > 0$
$\varkappa \in \mathbb{R}$

$$\hat{H} = \frac{\omega}{2}\left[-\partial_x^2 - \partial_y^2 + x^2 + y^2\right]\hat{I} + \varkappa\left[x\hat{\sigma}_z - y\hat{\sigma}_x\right]$$

where $\hat{I} = |1\rangle\langle 1| + |2\rangle\langle 2|$ and $\hat{\sigma}_x = |1\rangle\langle 2| + |2\rangle\langle 1|$, $\hat{\sigma}_z = |1\rangle\langle 1| - |2\rangle\langle 2|$ are Pauli matrixes.

a) Transform the Hamiltonian in the circular basis $|\pm\rangle = |1\rangle \pm i|2\rangle$ and polar coordinates $(x,y) = \rho(\cos\varphi, \sin\varphi)$.

b) Show that the Hamiltonian commutes with the vibronic angular momentum operator

$$\hat{L} = -i\hat{I}\partial_\varphi - \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -|$$

c) Write the Hamiltonian as a matrix in the basis of eigenstates of 2 dimensional harmonic oscillator $|n\ell\rangle|\pm\rangle$ considering result of b).

d) Solve the stationary Schrödinger equation numerically and find the spectrum of $\hat{H}$ for suitable choice of ω and $\varkappa$.

Note: You can use cartesian or circular representation in numerical solution. If interested you can also draw wavefunctions and calculate photoionization spectrum (see lecture notes by W. Domcke).