Tecniche di programmazione in chimica computazionale

Examples

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Matrix transpose

- Square matrix $\mathbf{A}$
- Transpose of $\mathbf{A} \rightarrow \mathbf{A}^T_{ij} = \mathbf{A}_{ji}$

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- Transpose conjugated of a matrix: example tconjug.f90

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- Example diag.f90

Franck-Condon factors

Born-Oppenheimer approximation

$$
\begin{aligned}
\Psi_{e\nu}(q_e, q_N) &= \psi_e(q_e; q_N)\chi_\nu^e(q_N) \\
\mu_{e,\nu;e',\nu'} &= \int dq_N \chi_\nu^{e,*}(q_N) M_{ee'} \chi_{\nu'}^{e'}(q_N) \\
M_{ee'} &= \int dq_e \psi_e^*(q_e; q_N)\hat{\mu}\psi_{e'}(q_e; q_N)
\end{aligned}
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Electronic contribution to transition dipole moment not varying with q_N

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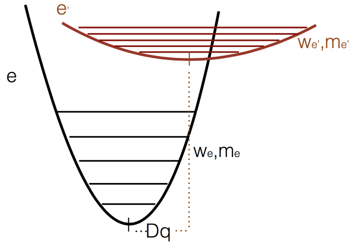
$$\mu_{e,\nu;e',\nu'} = M_{ee'}(\bar{q}_N)\int dq_N \chi_\nu^{e,*}(q_N)\chi_{\nu'}^{e'}(q_N)$$

$$\begin{aligned}S_{\nu,\nu'}^{e,e'} &= \int dq_N \chi_\nu^{e,*}(q_N)\chi_{\nu'}^{e'}(q_N) \\ FC_{\nu,\nu'}^{e,e'} &= |S_{\nu,\nu'}^{e,e'}|^2\end{aligned}$$

Franck-Condon factors

- Harmonic oscillator



Franck-Condon factors

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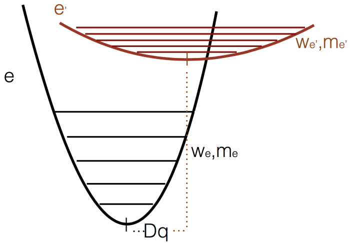

- Harmonic eigenfunctions

$$
\begin{aligned}
\chi_0^e(q_N) &= \left(\frac{m_e\omega_e}{\pi}\right)^{1/4} \exp[-(m_e\omega_e)q_N^2/2] \\
\chi_1^e(q_N) &= \sqrt{2}\left(\frac{m_e\omega_e}{\pi}\right)^{1/4} \left(\sqrt{m_e\omega_e}q_N\right) \exp[-(m_e\omega_e)q_N^2/2] \\
\chi_2^e(q_N) &= \frac{1}{\sqrt{2}}\left(\frac{m_e\omega_e}{\pi}\right)^{1/4} \left[2m_e\omega_e q_N^2 - 1\right] \exp[-(m_e\omega_e)q_N^2/2]
\end{aligned}
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Franck-Condon factors

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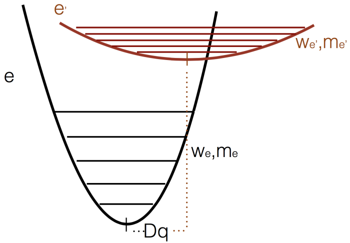

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- Example fc.f90

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- Given the same frequencies, displacement, reduced masses, how the FC factor changes with the vibrational quantum number ν (0, 1 or 2) of the electronic excited state?

Franck-Condon factors

- Given the same frequencies, displacement, reduced masses, how the FC factor changes with the vibrational quantum number ν (0, 1 or 2) of the electronic excited state?
- Given the same frequencies and reduced masses, how the FC factor changes with the displacement Δq (for a chosen ν)?