# Tecniche di programmazione in chimica computazionale

## Examples

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# Matrix transpose

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

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- Transpose conjugated of a matrix: example tconjug.f90

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# Euler propagation

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using

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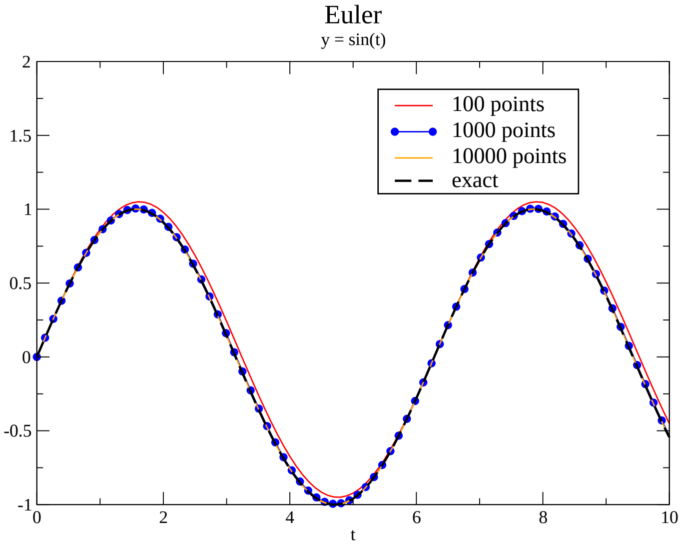
# Euler propagation: sin(t)



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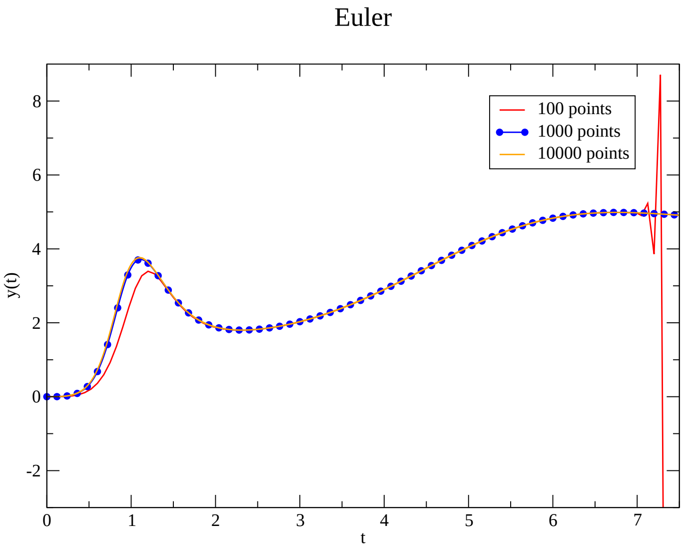

# Franck-Condon factors

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)
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Electronic contribution to transition dipole moment not varying with $q_N$

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$$S_{\nu,\nu'}^{e,e'} = \int dq_N \chi_\nu^{e,*}(q_N)\chi_{\nu'}^{e'}(q_N)$$
$$\mathrm{FC}_{\nu,\nu'}^{e,e'} = |S_{\nu,\nu'}^{e,e'}|^2$$

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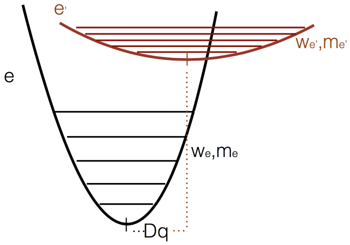
- Harmonic oscillator



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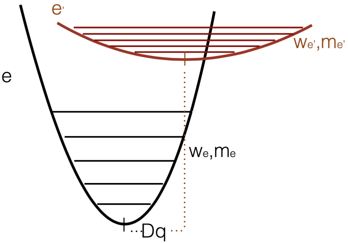


- Harmonic eigenfunctions

$$\chi_0^e(q_N) = \left(\frac{m_e\omega_e}{\pi}\right)^{1/4} \exp[-(m_e\omega_e)q_N^2/2]$$

$$\chi_1^e(q_N) = \sqrt{2}\left(\frac{m_e\omega_e}{\pi}\right)^{1/4} (m_e\omega_e q_N)\exp[-(m_e\omega_e)q_N^2/2]$$

$$\chi_2^e(q_N) = \frac{1}{\sqrt{2}}\left(\frac{m_e\omega_e}{\pi}\right)^{1/4} \left[2(m_e\omega_e q_N)^2 - 1\right]\exp[-(m_e\omega_e)q_N^2/2]$$

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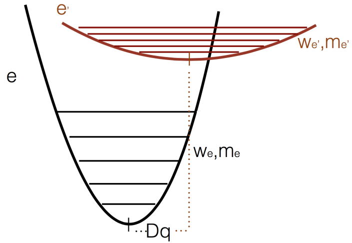


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- Example fc.f90

# Variational Monte Carlo (VMC)

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\begin{aligned}
E[\Psi_T] \equiv \langle \hat{\mathcal{H}} \rangle &= \frac{\int d\mathbf{x} \Psi_T^*(\mathbf{x}) \hat{\mathcal{H}}(\mathbf{x}) \Psi_T(\mathbf{x})}{\int d\mathbf{x} |\Psi_T(\mathbf{x})|^2} \geq E_0 \\
&= \frac{\int d\mathbf{x} \frac{\hat{\mathcal{H}}(\mathbf{x})\Psi_T(\mathbf{x})}{\Psi_T(\mathbf{x})} |\Psi_T(\mathbf{x})|^2}{\int d\mathbf{x} |\Psi_T(\mathbf{x})|^2} \\
&\simeq \frac{1}{N} \sum_{i=1}^{N} \frac{\hat{\mathcal{H}}(\mathbf{x}_i)\Psi_T(\mathbf{x}_i)}{\Psi_T(\mathbf{x}_i)}
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$$= \frac{\int d\mathbf{x} \frac{\hat{\mathcal{H}}(\mathbf{x})\Psi_T(\mathbf{x})}{\Psi_T(\mathbf{x})} |\Psi_T(\mathbf{x})|^2}{\int d\mathbf{x} |\Psi_T(\mathbf{x})|^2}$$

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- Trial wave function $\Psi_T$ and $\hat{\mathcal{H}}$ evaluated along $N$ random points in the configuration space (i.e., electronic coordinates)

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- Ground-state energy of the hydrogen atom

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R_{10}(r) &= (Z)^{3/2}\, 2 \exp\left[-Zr\right] \\
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