modelling materials using quantum mechanics and digital computers

the plane-wave pseudo potential way

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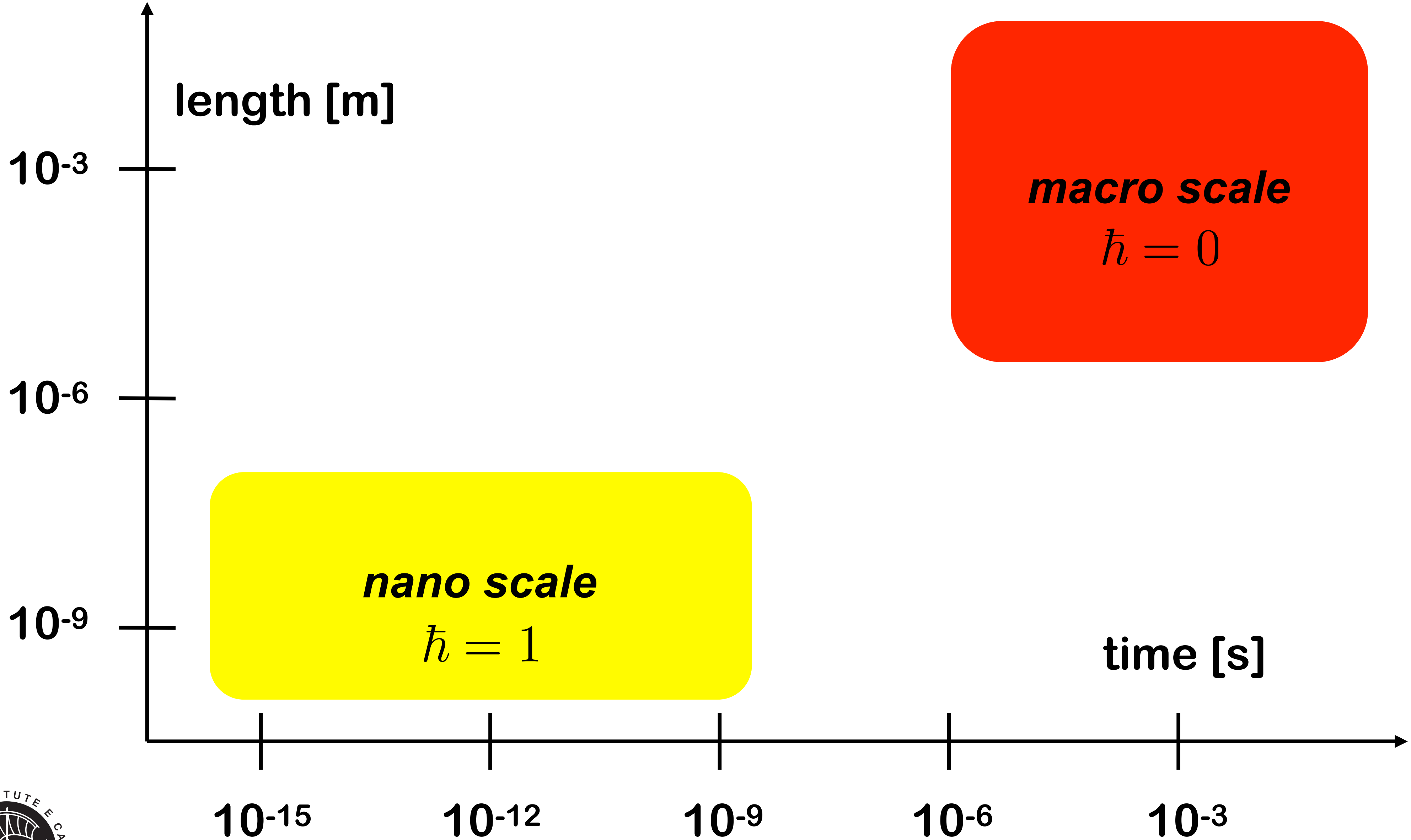
Jožef Stefan Institute, Ljubljana, September 16-20, 2019

the saga of time and length scales



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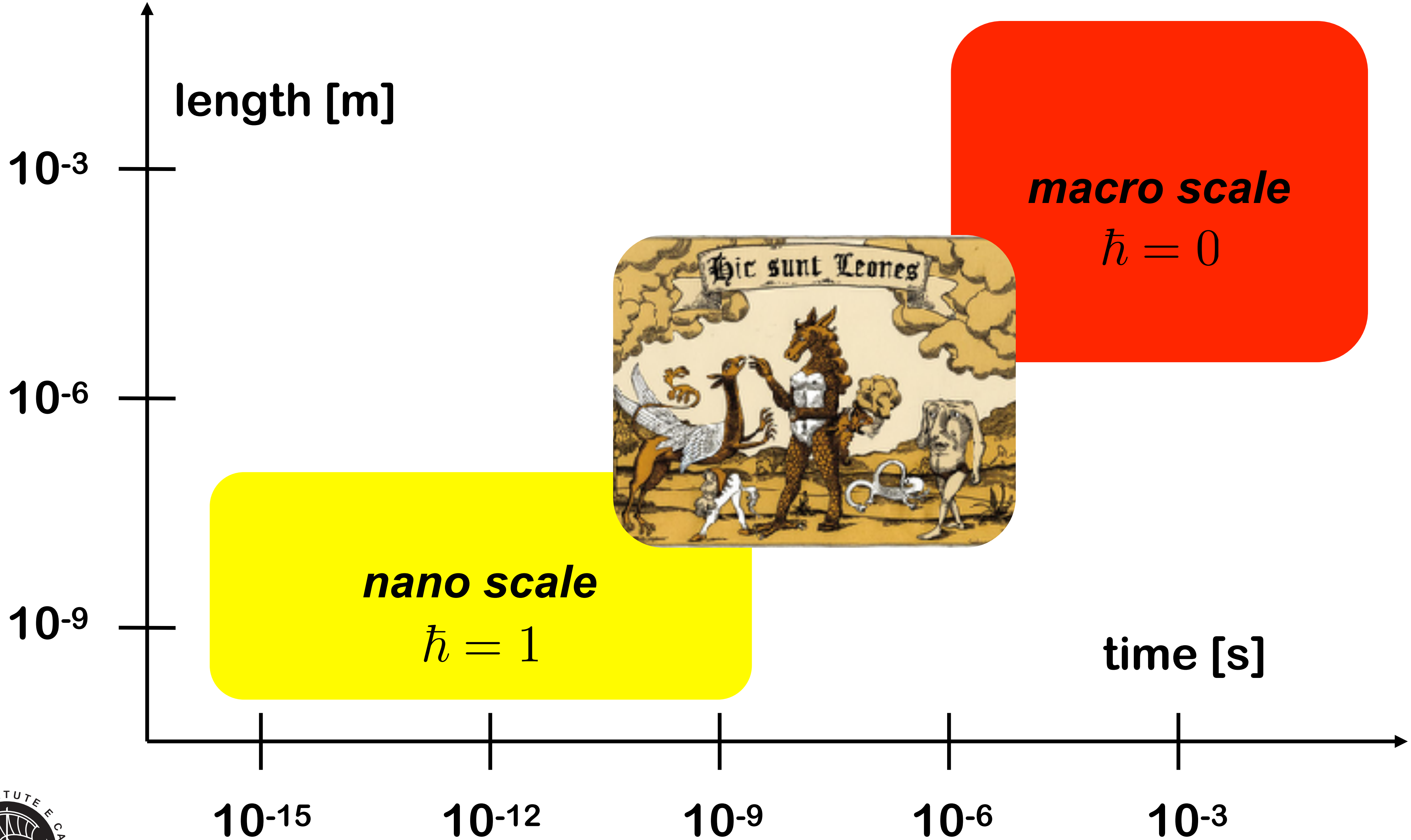

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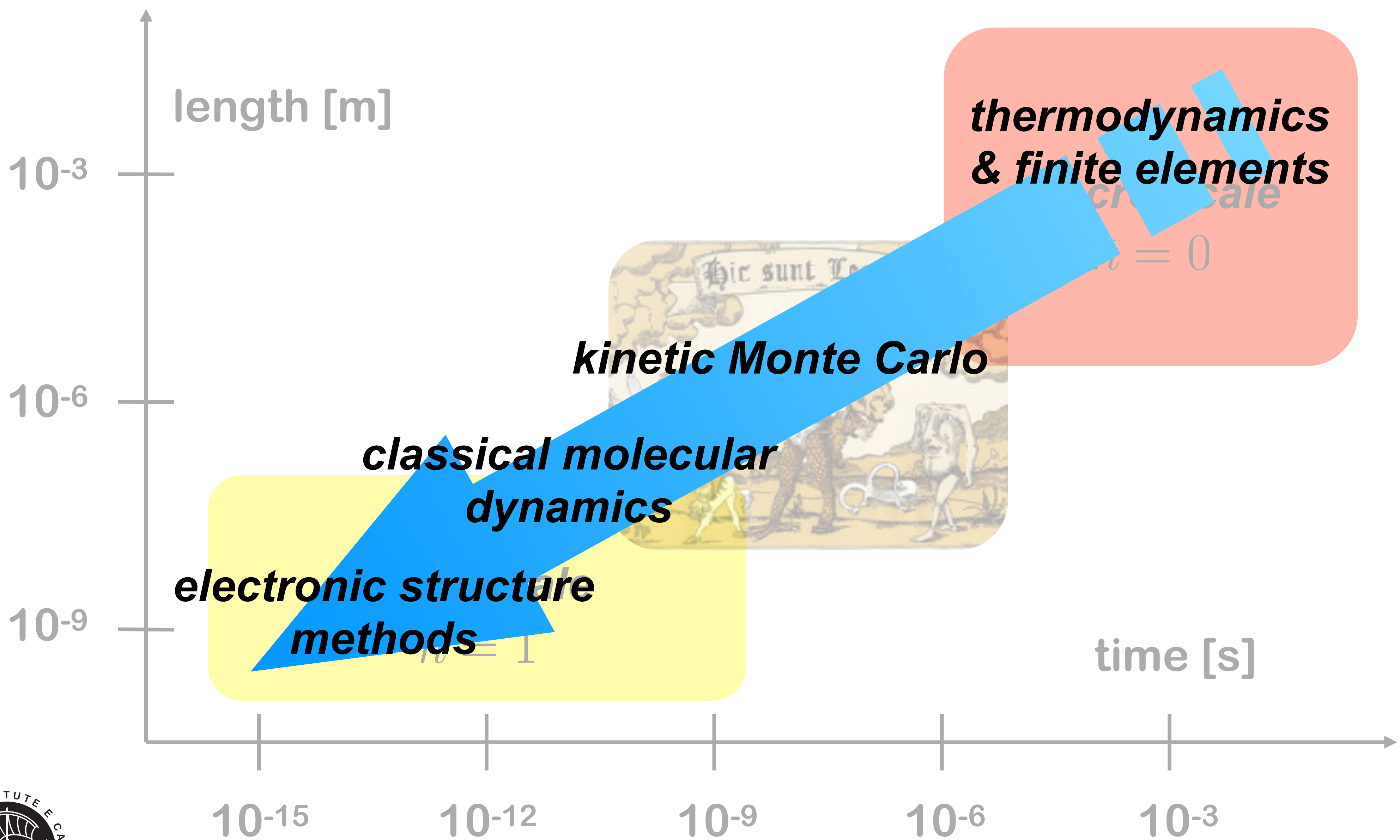
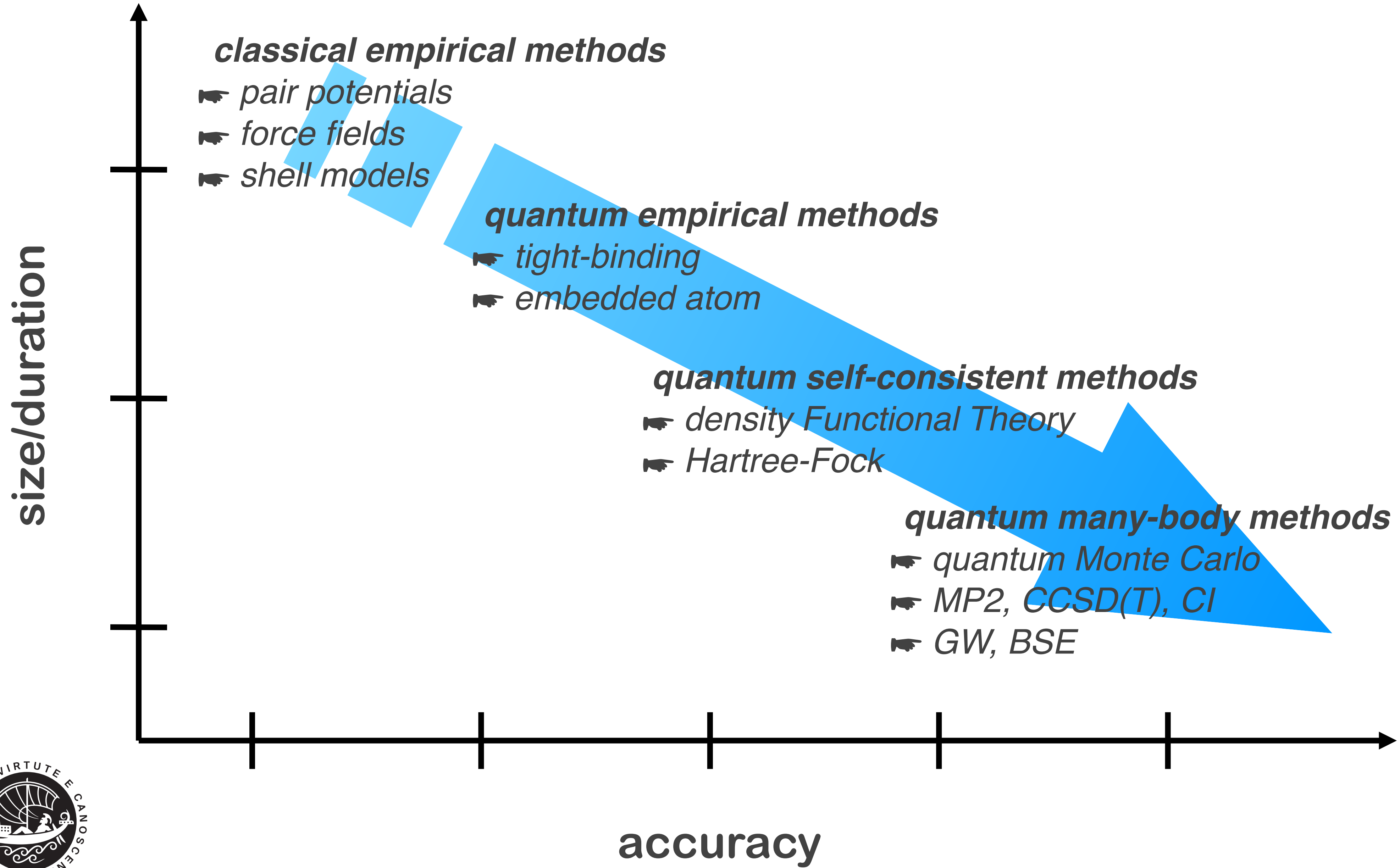


size vs. accuracy



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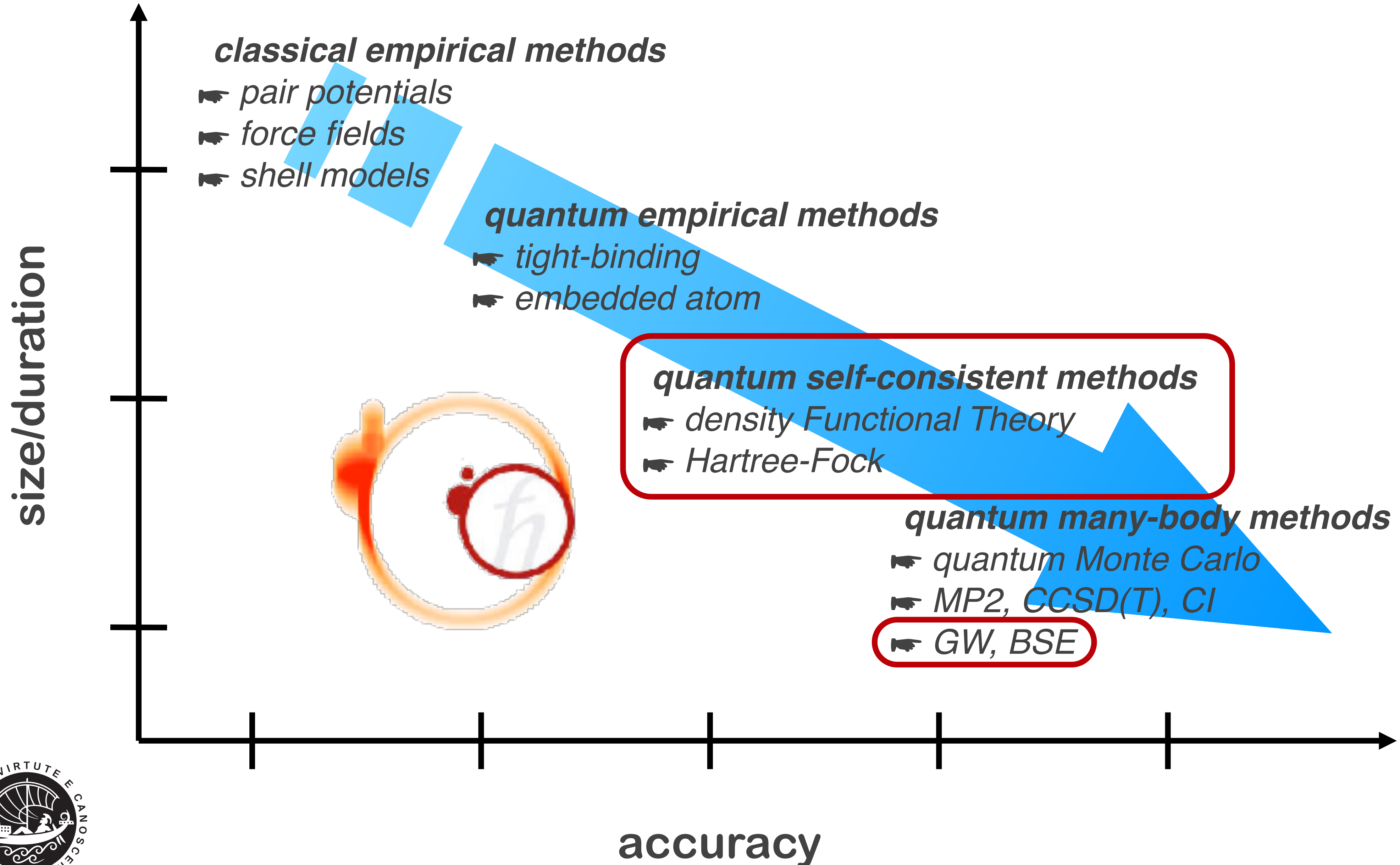

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why: they are accurate and *predictive*

when: if currently available approximations make the calculations feasible and the results meaningful (and no meaningful results can be obtained with cheaper methods)

how: using digital computers, clever algorithms, common sense, and *scientific rigor*

ab initio simulations

$$i\hbar\frac{\partial\Phi(\mathbf{r},\mathbf{R};t)}{\partial t}=\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\mathbf{R}^2}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}^2}+V(\mathbf{r},\mathbf{R})\right)\Phi(\mathbf{r},\mathbf{R};t)$$

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$M \gg m$

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M≫m: the Born-Oppenheimer approximation

$$M\ddot{\mathbf{R}} = -\frac{\partial E(\mathbf{R})}{\partial \mathbf{R}}$$

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + V(\mathbf{r}, \mathbf{R}) \right) \Psi(\mathbf{r}|\mathbf{R}) = E(\mathbf{R}) \Psi(\mathbf{r}|\mathbf{R})$$

density-functional theory

$$V(\mathbf{r},\mathbf{R}) = \frac{e^2}{2}\frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} - \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{e^2}{2}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

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DFT

$$V(\mathbf{r}, \mathbf{R}) \rightarrow \frac{e^2}{2} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} + v_{[\rho]}(\mathbf{r})$$

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Kohn-Sham Hamiltonian

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$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + v_{[\rho]}(\mathbf{r})\right)\psi_v(\mathbf{r}) = \epsilon_v \psi_v(\mathbf{r})$$

functionals

$$G[f] : \{f\} \longmapsto \mathbb{R}$$

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examples:

$$G[f] = f(x_0)$$

$$G[f] = \int_a^b f^2(x)dx$$

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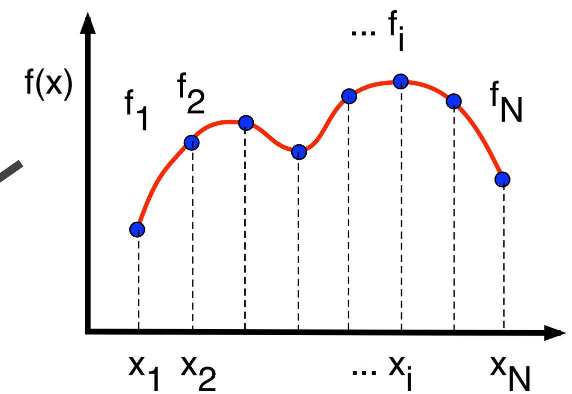

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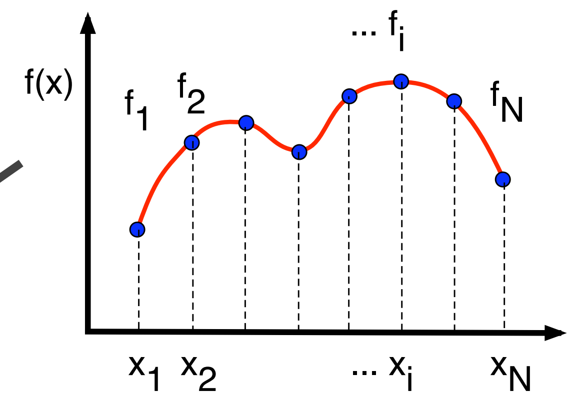

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$$f(x) \approx \sum_n c_n \phi_n(x)$$

functional derivatives

$$G[f_0 + \epsilon f_1] = G[f_0] + \epsilon \int f_1(x) \left. \frac{\delta G}{\delta f(x)} \right|_{f=f_0} dx + \mathcal{O}\left(\epsilon^2\right)$$

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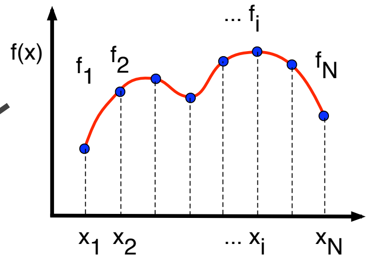

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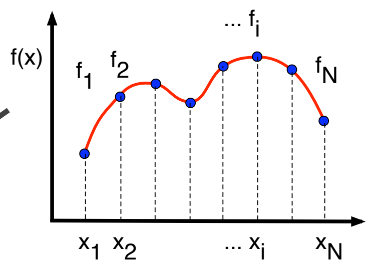

$$\frac{\delta G}{\delta f(x)} \text{“} = \text{”} \lim_{\epsilon \to 0} \frac{G[f(\bullet) + \epsilon \delta(\bullet - x)] - G[f(\bullet)]}{\epsilon}$$

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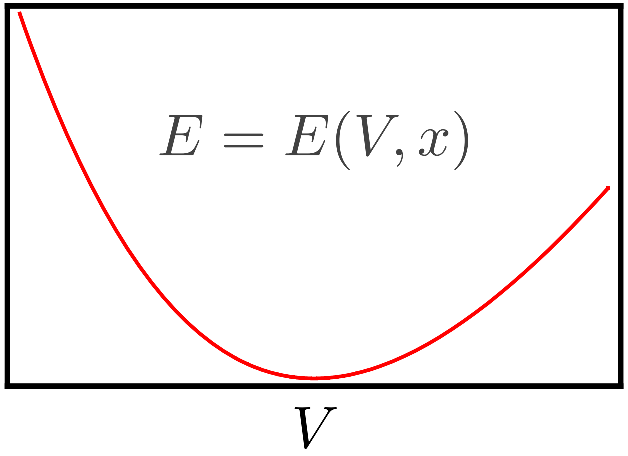
conjugate variables & Legendre



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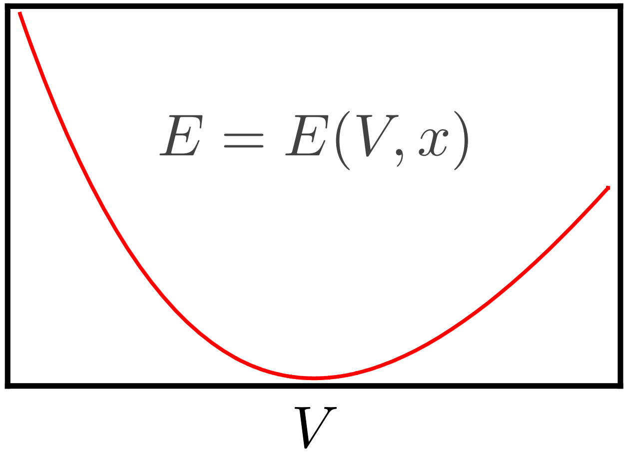

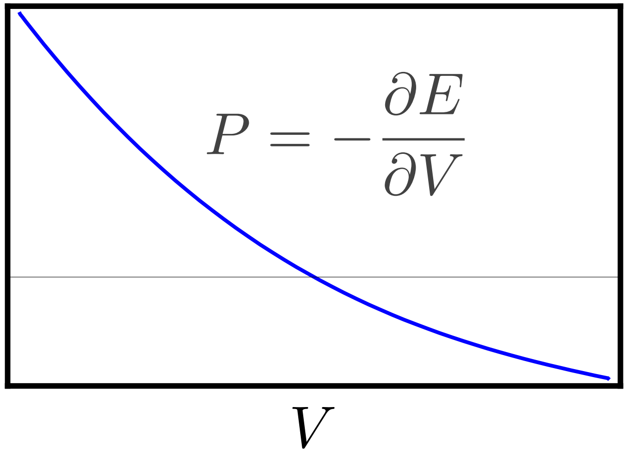

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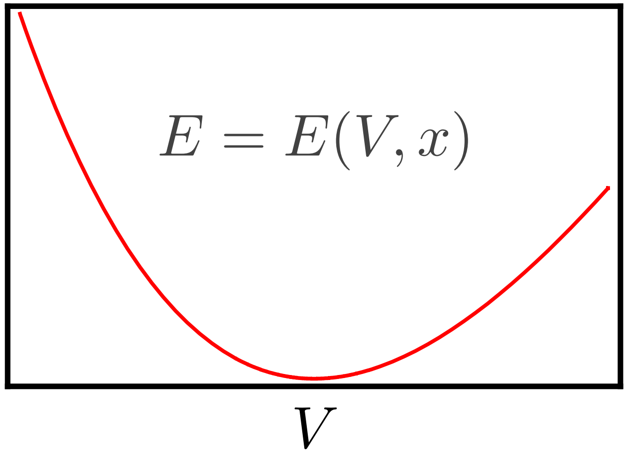

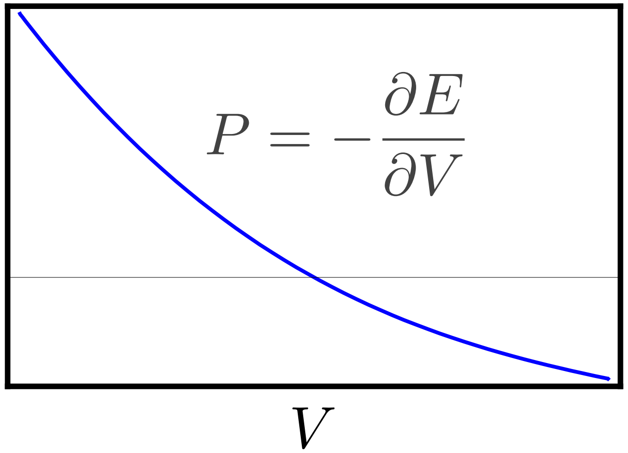

Legendre transform: $H(P, x) = E + PV$

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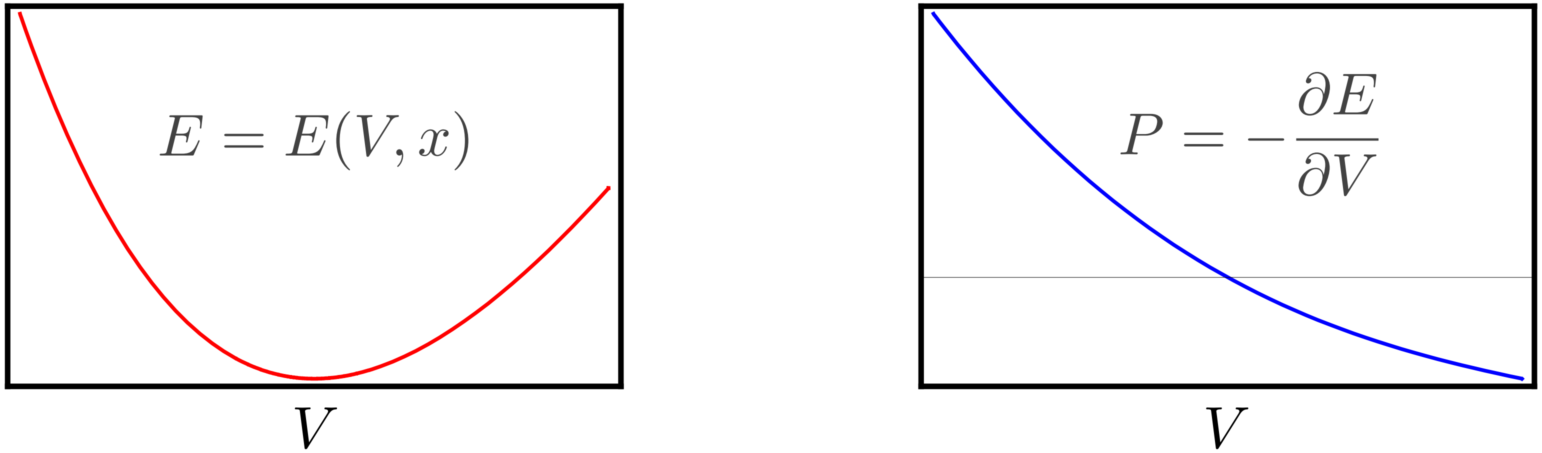

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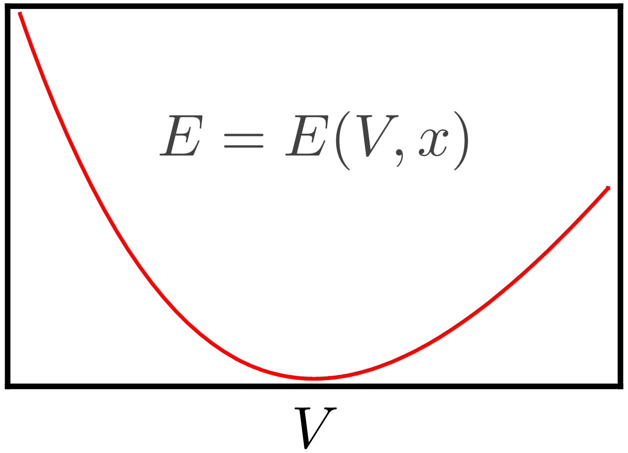

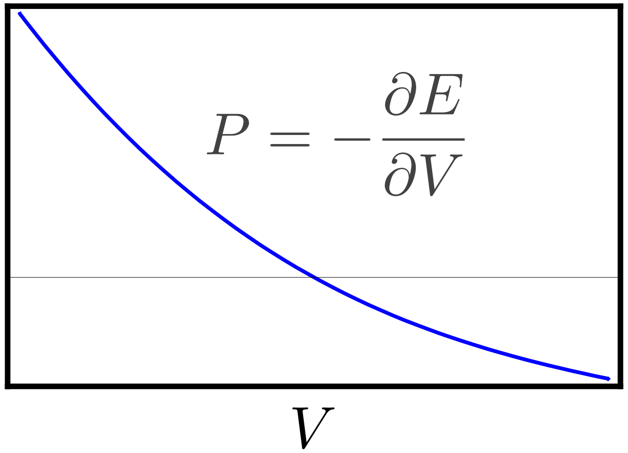

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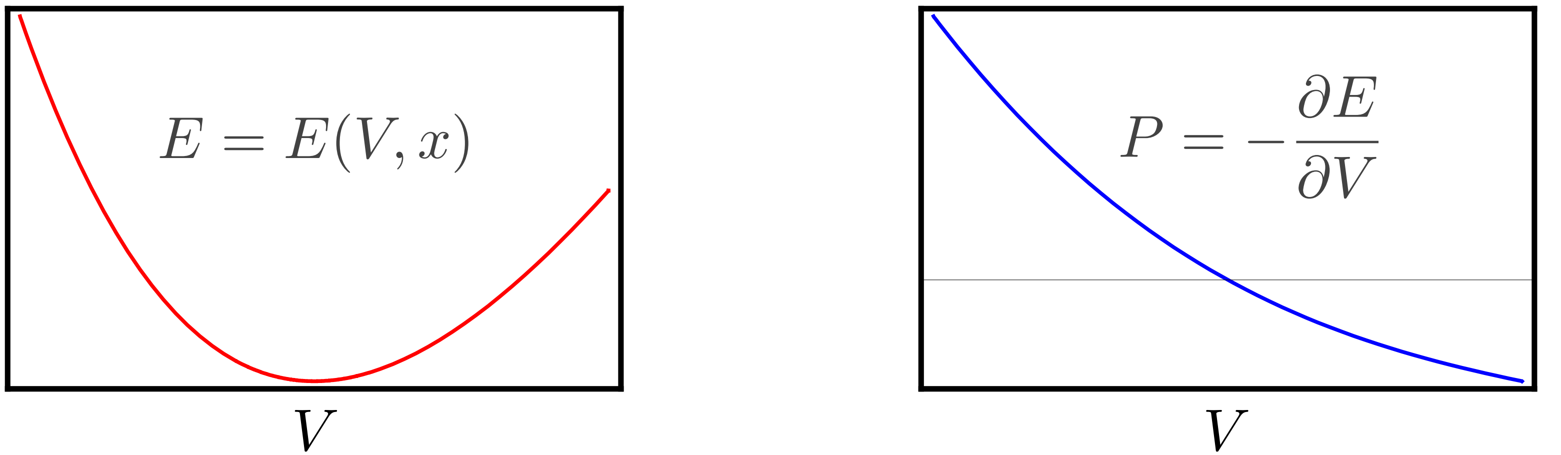

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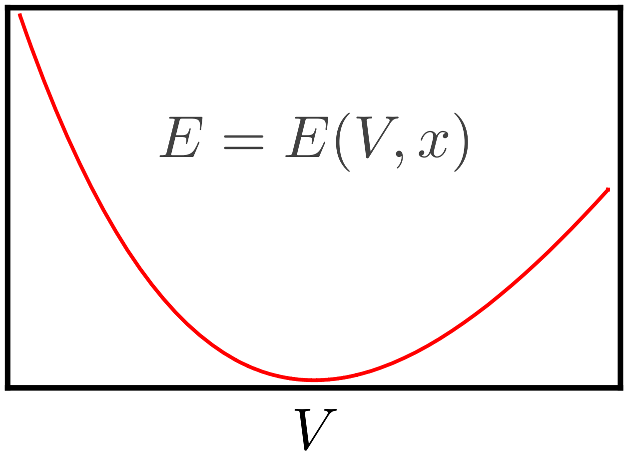

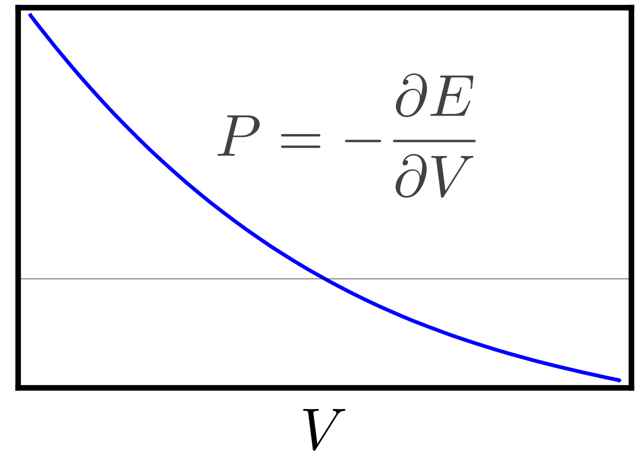

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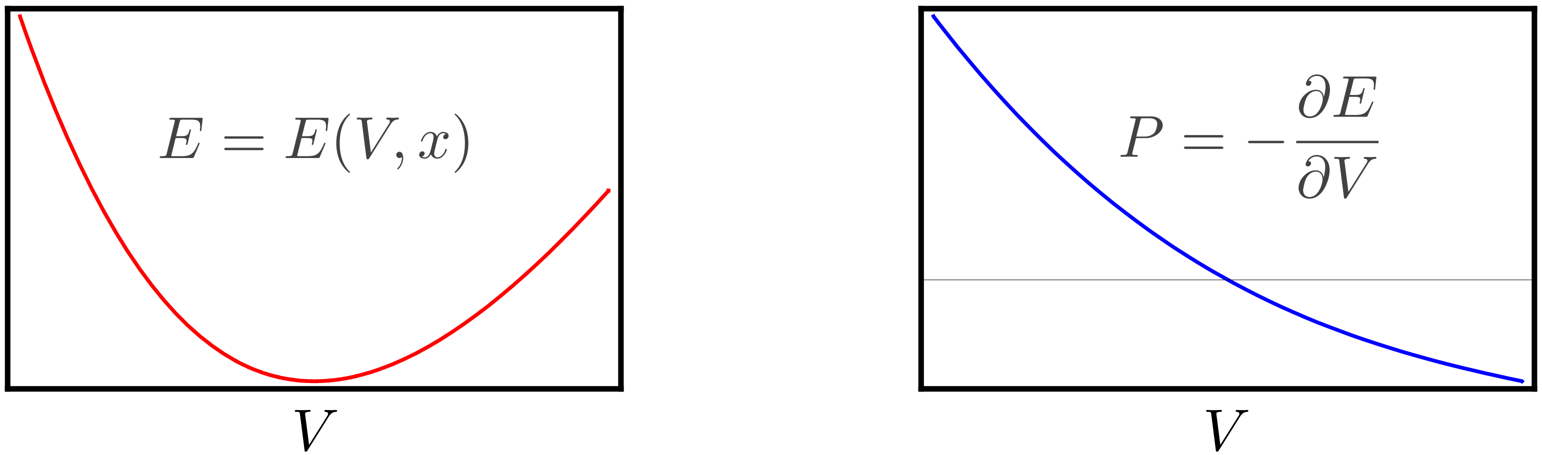

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Hohenberg-Kohn DFT

$$H = -\frac{\hbar^2}{2m}\sum_i \frac{\partial^2}{\partial \mathbf{r}_i^2} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_i V(\mathbf{r}_i)$$

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consequences:

- $V(\mathbf{r}) \rightleftarrows \rho(\mathbf{r})$ (1st *HK theorem*)
- $F[\rho] = E - \int V(\mathbf{r})\rho(\mathbf{r}) d\mathbf{r}$ is the Legendre transform of E
- $E[V] = \min_\rho \left[F[\rho] + \int V(\mathbf{r})\rho(\mathbf{r}) d\mathbf{r} \right]$ (2nd *HK theorem*)

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$$\frac{\delta T_0}{\delta\rho(\mathbf{r})} + e^2\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{xc}}{\delta\rho(\mathbf{r})} + V(\mathbf{r}) = \mu$$

Kohn-Sham DFT

$$F[\rho] = T_0[\rho] + \frac{e^2}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}' + E_{xc}[\rho]$$

$$\frac{\delta T_0}{\delta\rho(\mathbf{r})} + \overbrace{e^2\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \frac{\delta E_{xc}}{\delta\rho(\mathbf{r})} + V(\mathbf{r})}^{v_{KS}[\rho](\mathbf{r})} = \mu$$

MA PER SEGUIR VIRTUTE E CANOSCENZA

Kohn-Sham DFT

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$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{KS}[\rho](\mathbf{r})\right)\psi_v(\mathbf{r}) = \epsilon_v \psi_v(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum_v |\psi_v(\mathbf{r})|^2 \theta(\epsilon_v - \mu)$$

XC energy functionals

- LDA (Kohn & Sham, 60's)

$$E_{xc}[\rho] = \int \epsilon_{xc}(\rho(\mathbf{r}))\rho(\mathbf{r})d\mathbf{r}$$

- GGA (Becke, Perdew, *et al.*, 80's)

$$E_{xc} = \int \rho(\mathbf{r})\epsilon_{GGA}(\rho(\mathbf{r}), |\nabla\rho(\mathbf{r})|)\, d\mathbf{r}$$

- DFT+U (Anisimov *et al.*, 90's)

$$E_{DFT+U}[\rho] = E_{DFT} + Un(n-1)$$

- hybrids (Becke *et al.*, 90's)

$$E_{hybr} = \alpha E^{x}_{HF} + (1-\alpha)E^{x}_{GGA} + E^{c}$$

- meta-GGA (Perdew, early 2K's)

$$E_{mGGA} = \int \rho(\mathbf{r})\times \epsilon_{mGGA}(\rho(\mathbf{r}), |\nabla\rho(\mathbf{r})|, \tau_s(\mathbf{r}))\, d\mathbf{r}$$

$$\tau_s(\mathbf{r}) = \frac{1}{2}\sum_i |\nabla^2\psi_i(\mathbf{r})|^2$$

- VdW (Langreth & Lundqvist, 2K's)

$$E_{VdW} = \int \rho(\mathbf{r})\rho(\mathbf{r}')\times \Phi_{VdW}[\rho](\mathbf{r},\mathbf{r}')d\mathbf{r}d\mathbf{r}'$$

- ...

the Local-Density Approximation

on the blackboard

KS equations from functional

$$E[\{\psi\},\mathbf{R}] = -\frac{\hbar^2}{2m}\sum_v \int \psi_v^*(\mathbf{r})\frac{\partial^2\psi_v(\mathbf{r})}{\partial\mathbf{r}^2}dr + \int V(\mathbf{r},\mathbf{R})\rho(\mathbf{r})d\mathbf{r}+$$

$$\frac{e^2}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}' + E_{xc}[\rho]$$

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$$E(\mathbf{R}) = \min_{\{\psi\}}\Big(E[\{\psi\},\mathbf{R}]\Big)$$

$$\int \psi_u^*(\mathbf{r})\psi_v(\mathbf{r})d\mathbf{r} = \delta_{uv}$$

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$$\longrightarrow \quad \frac{\delta E_{KS}}{\delta\psi_v^*(\mathbf{r})} = \sum_{uv}\Lambda_{vu}\psi_u(\mathbf{r})$$

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KS equations from functional

$$E[\{\psi\},\mathbf{R}] = -\frac{\hbar^2}{2m}\sum_v \int \psi_v^*(\mathbf{r})\frac{\partial^2\psi_v(\mathbf{r})}{\partial\mathbf{r}^2}dr + \int V(\mathbf{r},\mathbf{R})\rho(\mathbf{r})d\mathbf{r} +$$

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$$\frac{\delta E_{KS}}{\delta\psi_v^*(\mathbf{r})} = \sum_{uv}\Lambda_{vu}\psi_u(\mathbf{r})$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{KS}[\rho](\mathbf{r})\right)\psi_v(\mathbf{r}) = \epsilon_v\psi_v(\mathbf{r})$$

MA PER SEGUIR VIRTUTE E CANOSCENZA

solving the Kohn-Sham equations

$$\psi_v(\mathbf{r}) = \sum_j c(j,v)\varphi_j(\mathbf{r})$$

$$\psi_v(\mathbf{r}) \rightleftarrows c(j,v)$$

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$$\frac{\delta E_{KS}}{\delta\psi_v^*(\mathbf{r})} = \sum_{uv} \Lambda_{vu}\psi_u(\mathbf{r})$$

$$\dot{c}(i,v) = -\sum_j h_{KS}[c](i,j)c(j,v) + \sum_u \Lambda_{vu} c(i,v)$$

requirements

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- (effective) completeness of the basis set easily checked and systematically improved

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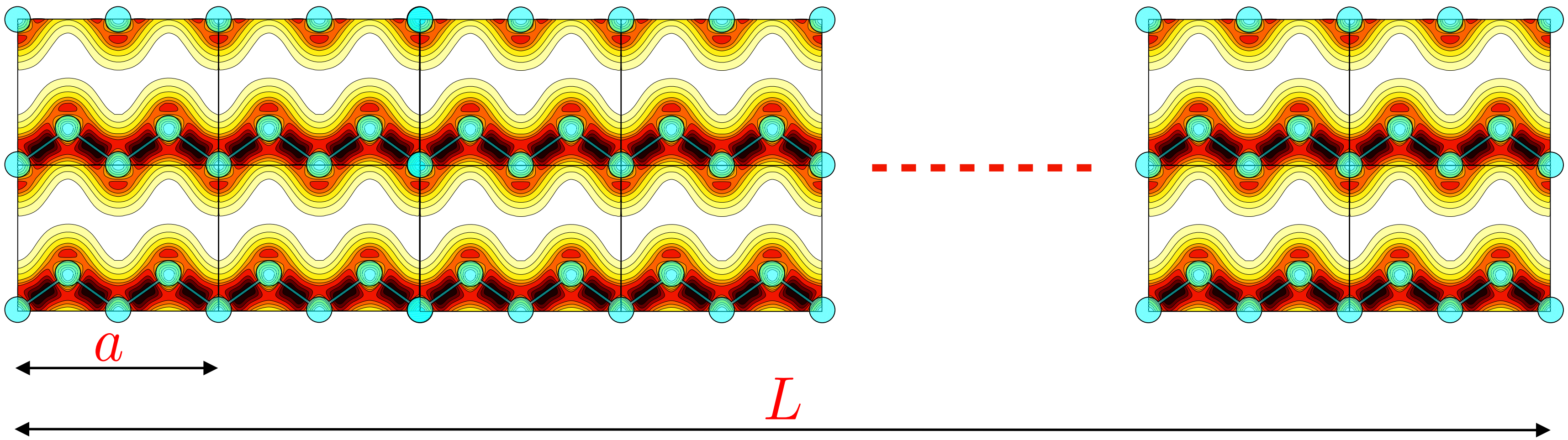
- (effective) completeness of the basis set easily checked and systematically improved
- matrix elements easy to calculate and/or $H\psi$ products easily calculated on the fly
- Hartree and XC potentials easy to represent and calculate
- orthogonality is a plus

the Bloch theorem & plane waves

infinite crystals



$$\psi(x+L) = \psi(x)$$

Born — von Kármán PBC

the Bloch theorem & plane waves

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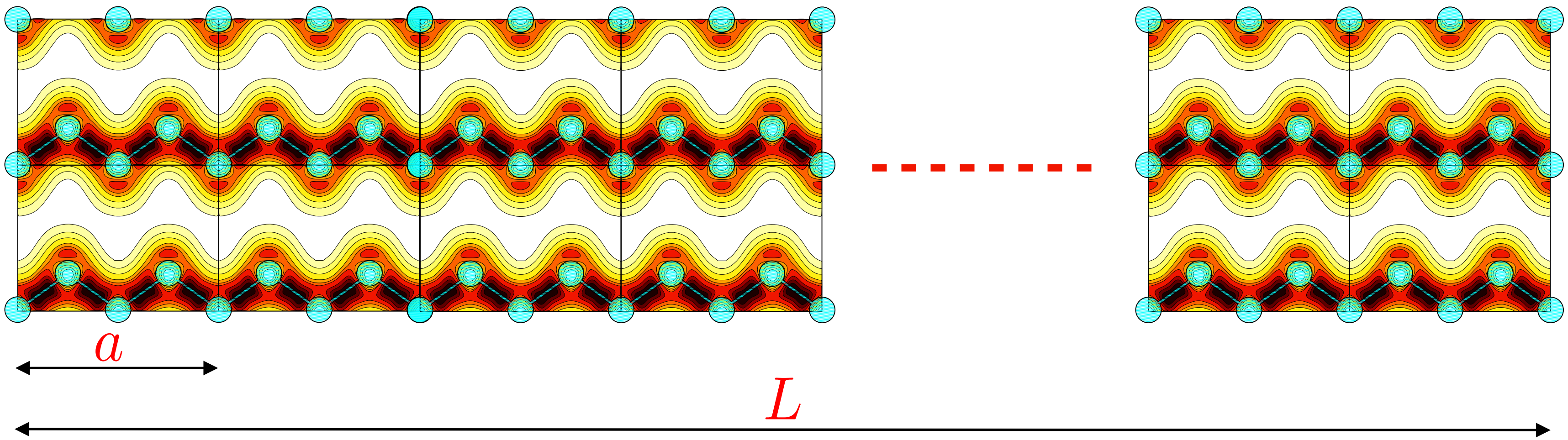

$$\psi(x+L) = \psi(x)$$ Born — von Kármán PBC

$$\left.\begin{aligned} \psi_k(x+a) &= \mathrm{e}^{ika}\psi_k(x) \\ \psi_k(x) &= \mathrm{e}^{ikx}u_k(x) \\ u_k(x+a) &= u_k(x) \end{aligned}\right\}$$ Bloch theorem

$$u_k(x) = \sum_n c_k(n)\mathrm{e}^{i\frac{2n\pi}{a}x}$$

plane-wave basis sets

$$\psi(\mathbf{r}) = \sum_j c(j)\varphi_j(\mathbf{r})$$

$$\varphi_j(\mathbf{r}) = \frac{1}{\sqrt{\Omega}}\mathrm{e}^{i\mathbf{q}_j\cdot\mathbf{r}}$$

$$\frac{\hbar^2}{2m}\mathbf{q}_j^2 \leq E_{cut}$$

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periodic boundary conditions

$$\varphi(x+\ell) = \varphi(x) \to q_j = \frac{2\pi}{\ell} j$$

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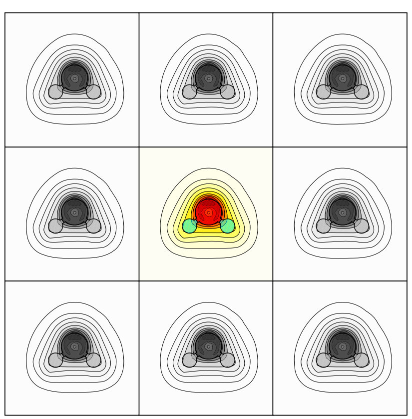
finite systems $(\ell = a)$



$$\mathbf{q} = \mathbf{G}$$

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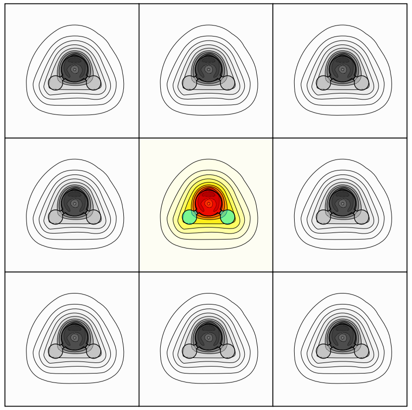
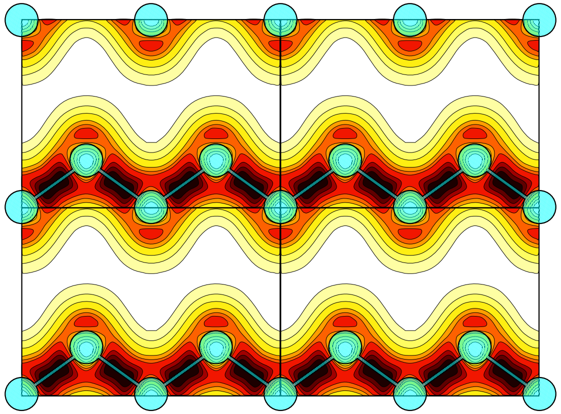


$$\mathbf{q} = \mathbf{G}$$

infinite crystals $(\ell = L)$



$$\mathbf{q} = \mathbf{k} + \mathbf{G}; \quad \mathbf{k} \in BZ$$

plane-wave expansion of LCAO orbitals

on the blackboard

using plane waves

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}} c_{n\mathbf{k}}(\mathbf{G}) \mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}}$$

using plane waves

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}} c_{n\mathbf{k}}(\mathbf{G}) \mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}}$$

$$-\nabla^2 \psi_{n\mathbf{k}}(\mathbf{r}) \longmapsto |\mathbf{k}+\mathbf{G}|^2 c_{n\mathbf{k}}(\mathbf{G})$$

$$V(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r}) \longmapsto \frac{1}{\Omega}\int \mathrm{e}^{-i\mathbf{G}\cdot\mathbf{r}} V(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r}$$

using plane waves

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$$\rho(\mathbf{r}) = \sum_{v\mathbf{k}} |u_{v\mathbf{k}}(\mathbf{r})|^2$$

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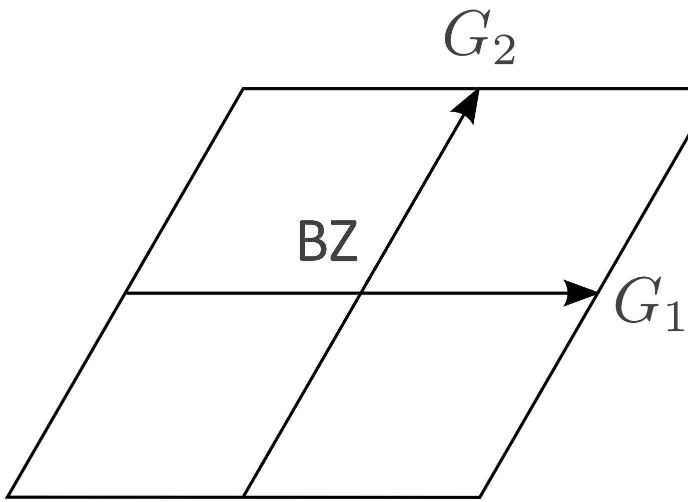
$$\begin{aligned} V_{xc}(\mathbf{r}) &= \mu_{xc}\big(\rho(\mathbf{r})\big) \\ V_H(\mathbf{r}) &= e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' \\ &= e^2 \sum_{\mathbf{G}\neq 0} \mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}} \frac{4\pi}{G^2} \tilde{\rho}(\mathbf{G}) \end{aligned}$$

sampling the Brillouin zone: special points

$$\rho(\mathbf{r}) = \sum_{v\mathbf{k}\in \mathrm{BZ}} |u_{v\mathbf{k}}(\mathbf{r})|^2$$



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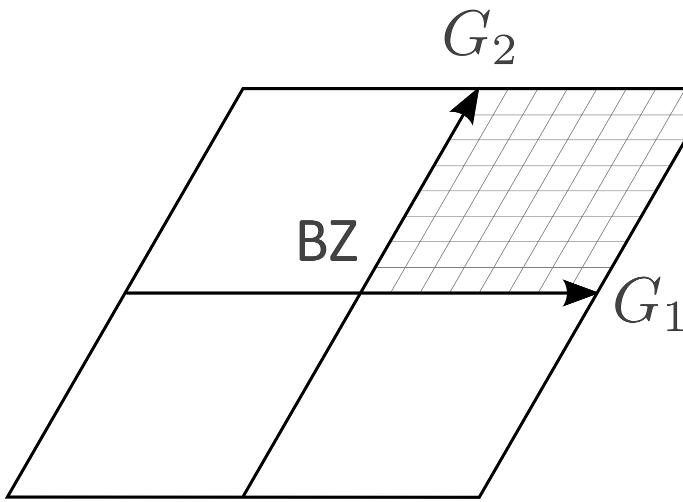

sampling the Brillouin zone: special points

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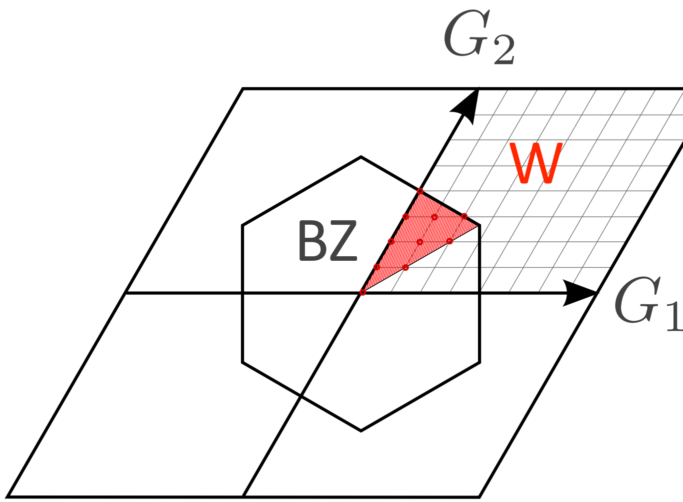

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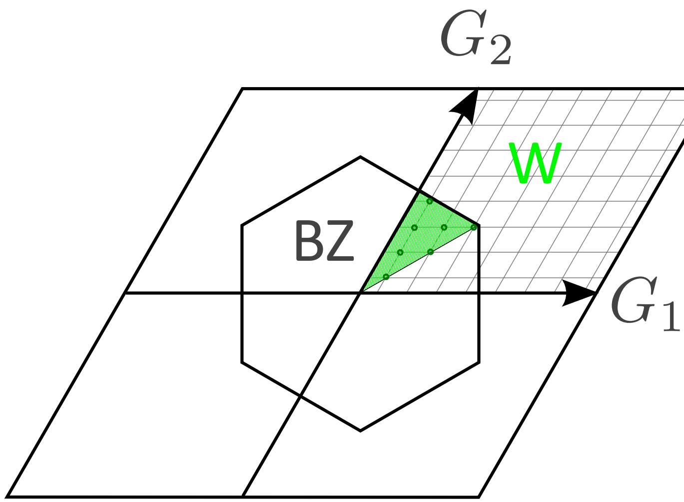
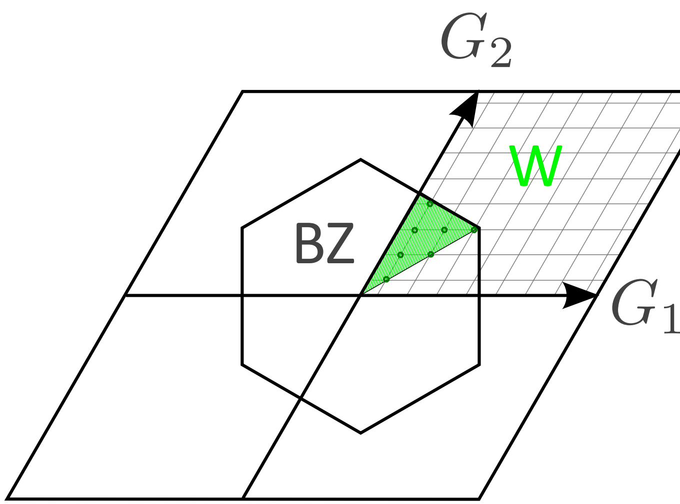


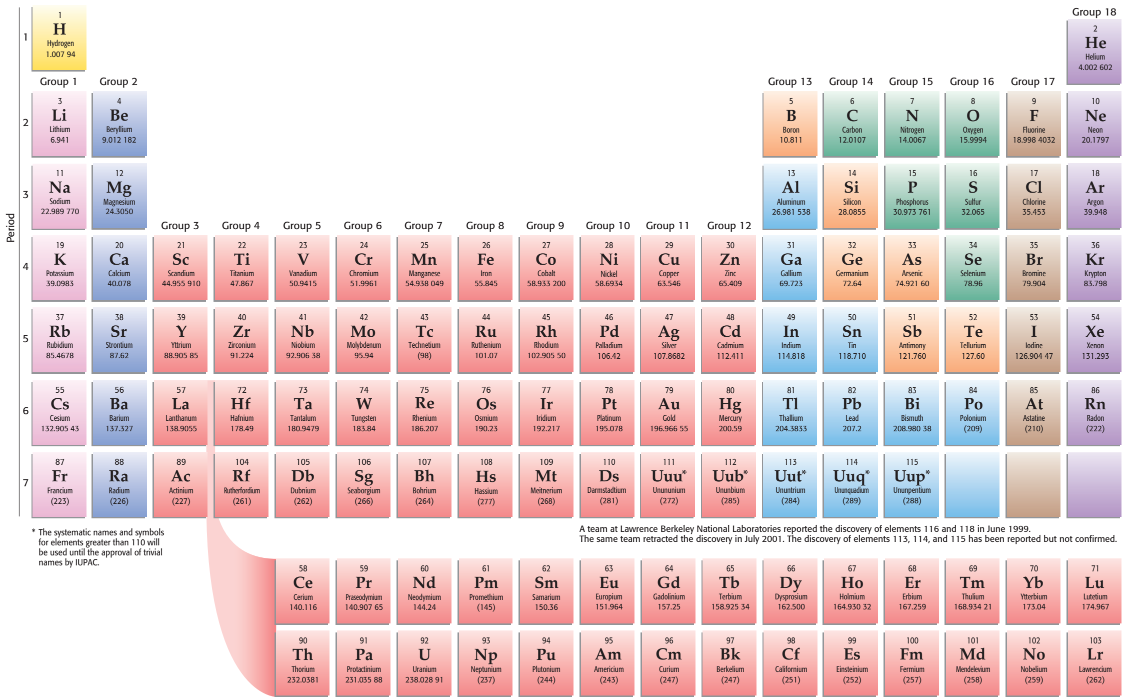
sampling the Brillouin zone: special points



$$
\begin{aligned}
\rho(\mathbf{r}) &= \sum_v \sum_{\mathbf{k}\in \mathrm{BZ}} |u_{v\mathbf{k}}(\mathbf{r})|^2 \\
&= \sum_v \sum_{S\in\mathcal{G}} \sum_{\mathbf{k}\in \mathrm{W}} |u_{vS\cdot\mathbf{k}}(\mathbf{r})|^2 \\
&= \sum_v \sum_{S\in\mathcal{G}} \sum_{\mathbf{k}\in \mathrm{W}} |u_{vS\mathbf{k}}(S^{-1}\cdot\mathbf{r})|^2 \\
&= \sum_{S\in\mathcal{G}} \rho_{\mathrm{W}}(S^{-1}\cdot\mathbf{r})
\end{aligned}
$$

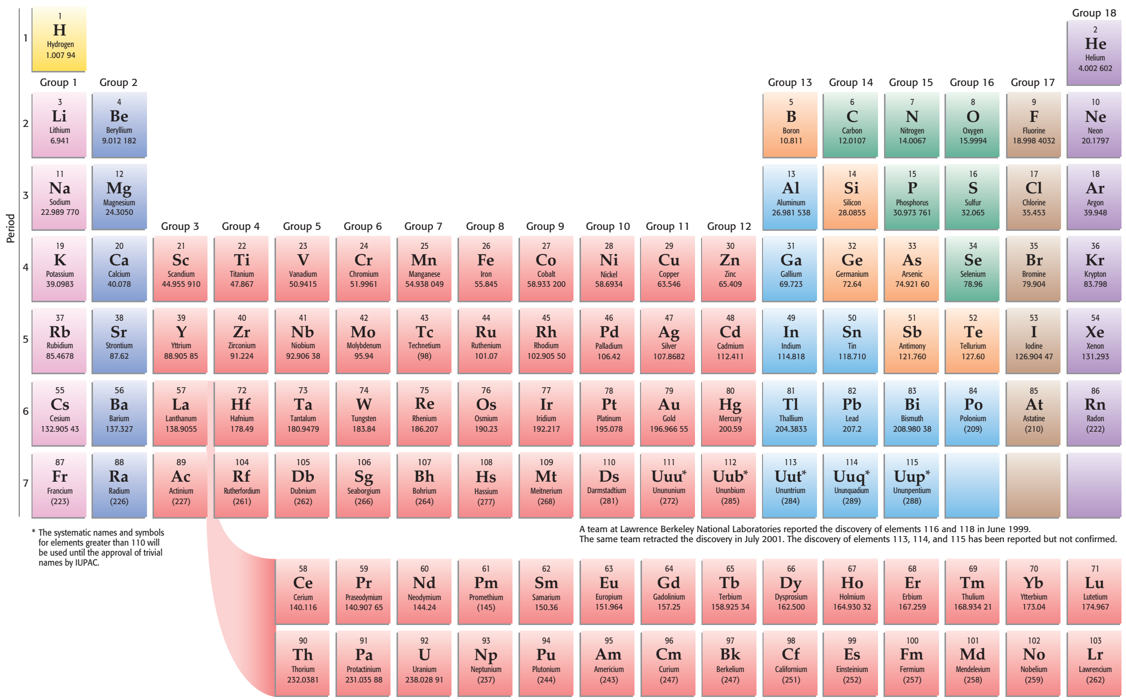
PWs: pros & cons

treating core states



$$\epsilon_{1s} \sim Z^2 \qquad a_{1s} \sim \frac{1}{Z}$$

treating core states



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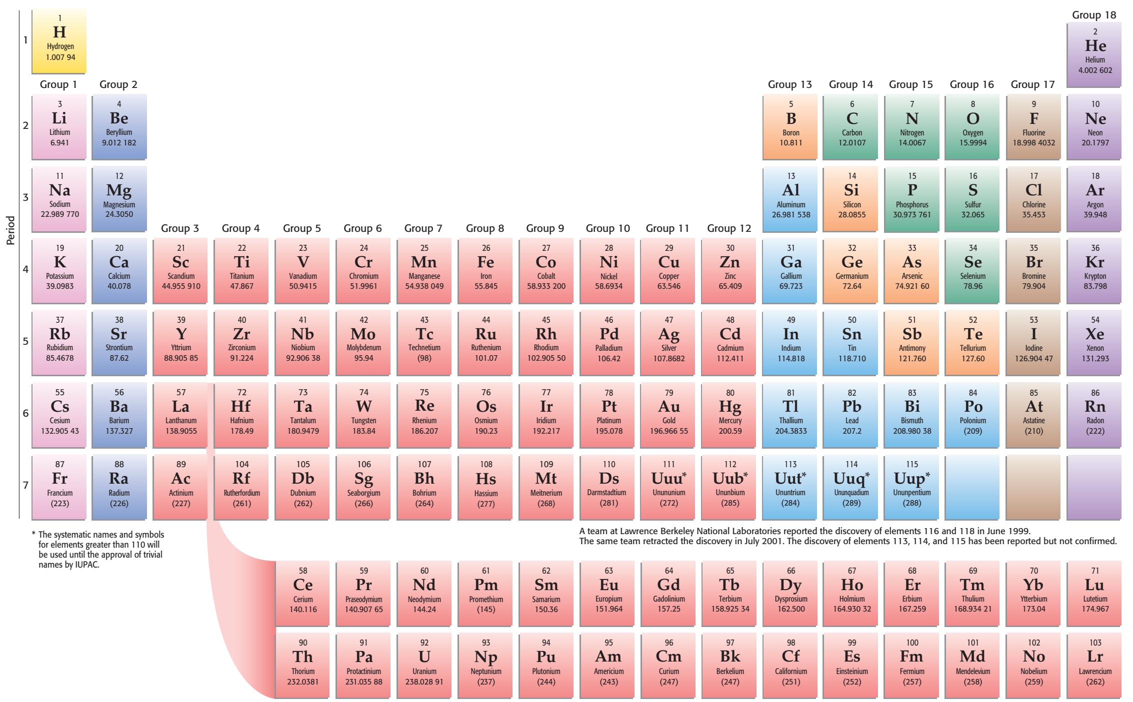
$$E_{cut} \sim Z^2$$

treating core states



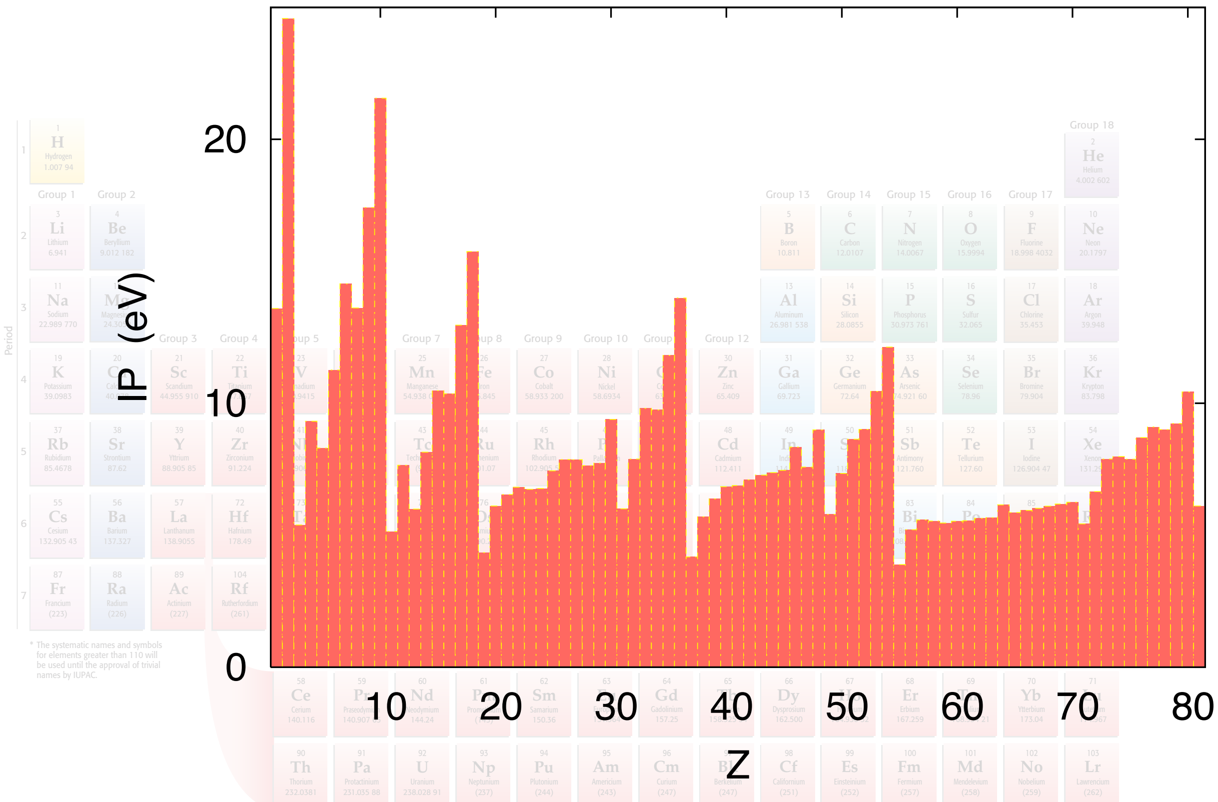
$$\epsilon_{1s} \sim Z^2 \qquad a_{1s} \sim \frac{1}{Z}$$

$$E_{cut} \sim Z^2$$

$$N_{PW} = \frac{4\pi}{3} k_{cut}^3 \frac{\Omega}{(2\pi)^3}$$

$$\sim Z^3$$

treating core states



$$\epsilon_{1s} \sim Z^2 \quad a_{1s} \sim \frac{1}{Z}$$

$$E_{cut} \sim Z^2$$

$$I_P \sim 1 \quad a \sim 1$$

$$N_{PW} = \frac{4\pi}{3} k_{cut}^3 \frac{\Omega}{(2\pi)^3}$$

$$\sim Z^3$$

trashing core states: pseudopotentials

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pseudo-atoms do not have core states: valence states of any given angular symmetry are the lowest-lying states of that symmetry:

ϕ_{val}^{ps} is nodeless and smooth

trashing core states: pseudopotentials

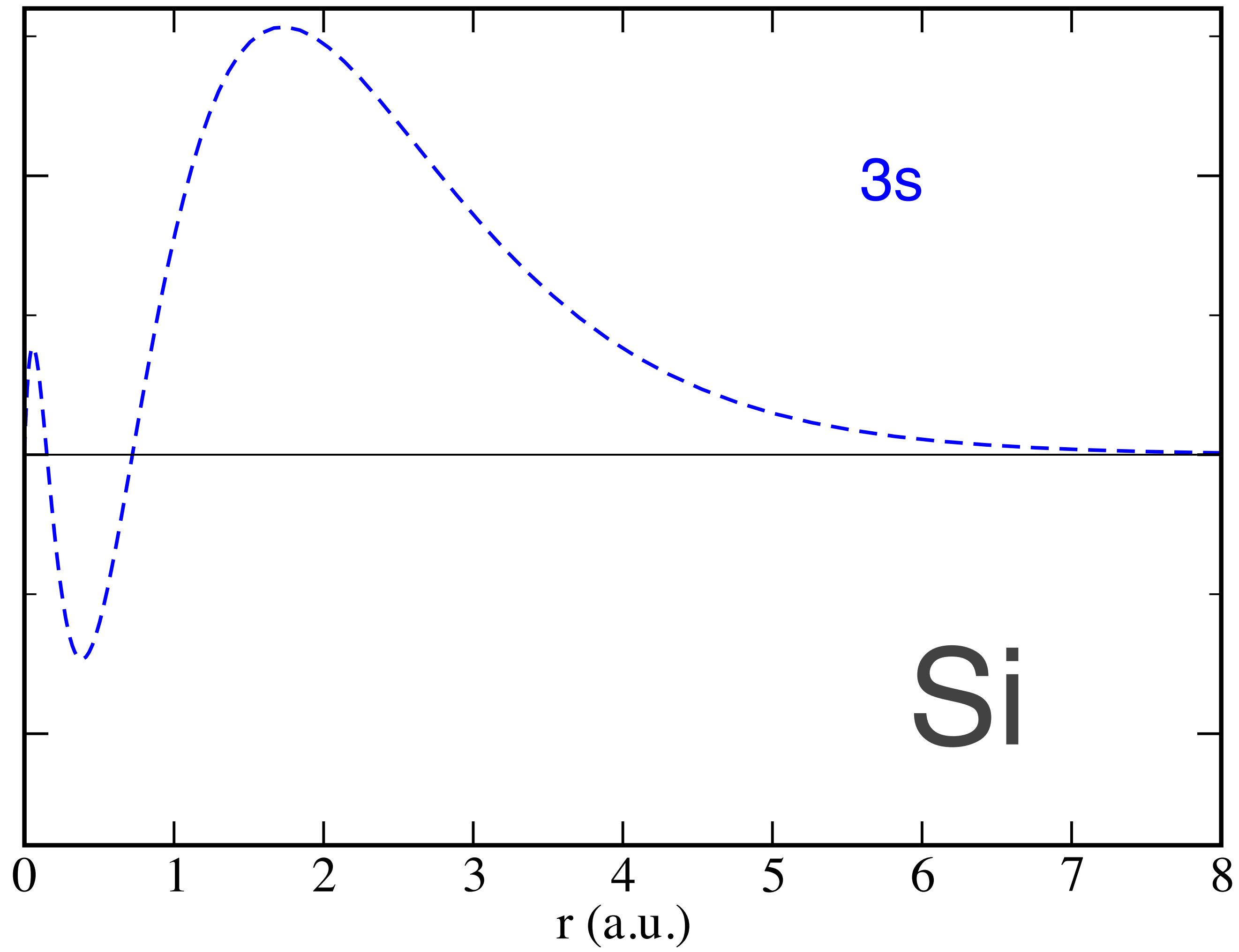
pseudo-atoms do not have core states: valence states of any given angular symmetry are the lowest-lying states of that symmetry:

ϕ_{val}^{ps} is nodeless and smooth

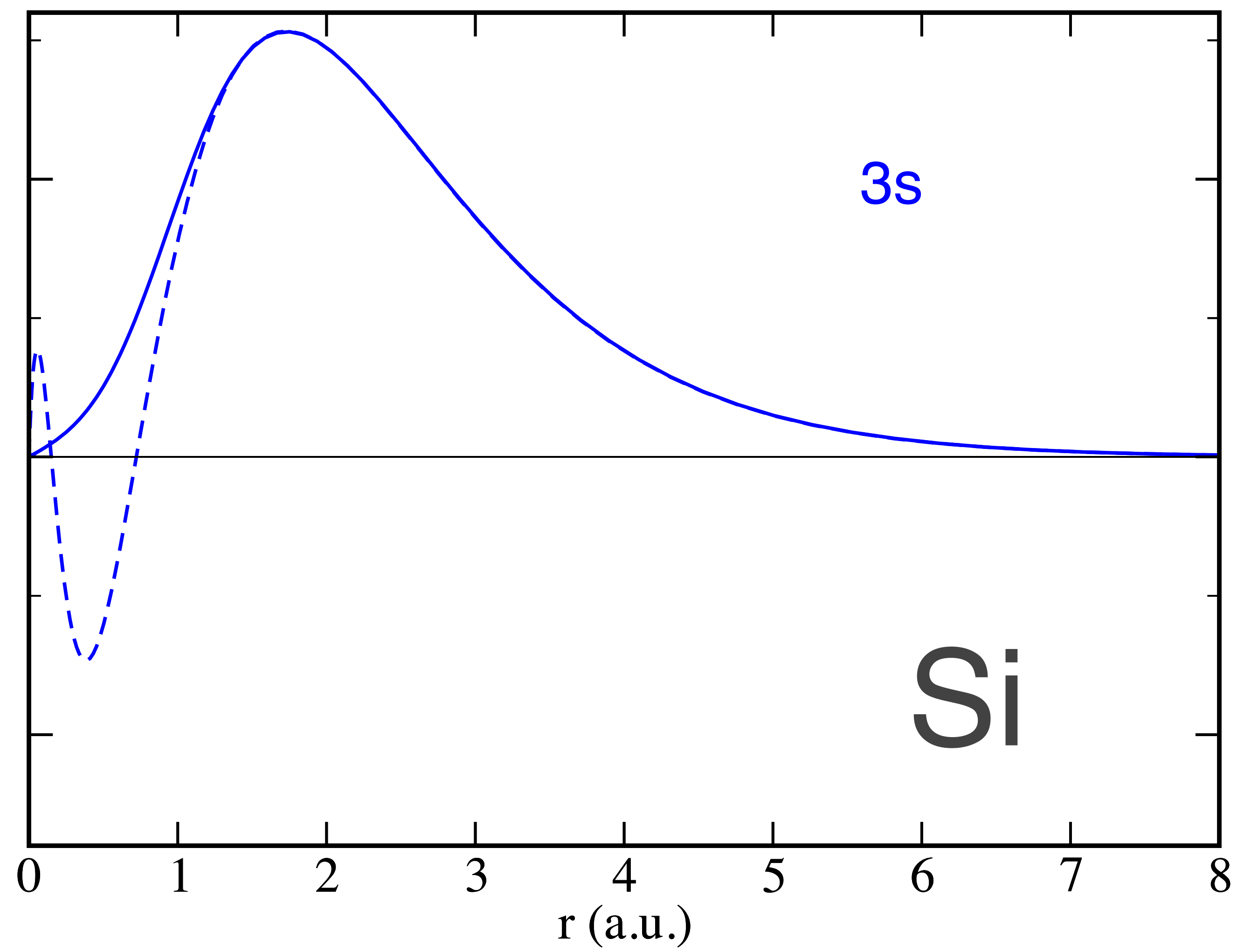
the chemical properties of the pseudo-atom are the same as those of the true atom:

$$\epsilon_{val}^{ps} = \epsilon_{val}^{ae}$$

$$\phi_{val}^{ps}(r) = \phi_{val}^{ae}(r) \quad \text{for} \quad r > r_c$$



3s
Si
0
1
2
3
4
5
6
7
8
r (a.u.)



3s
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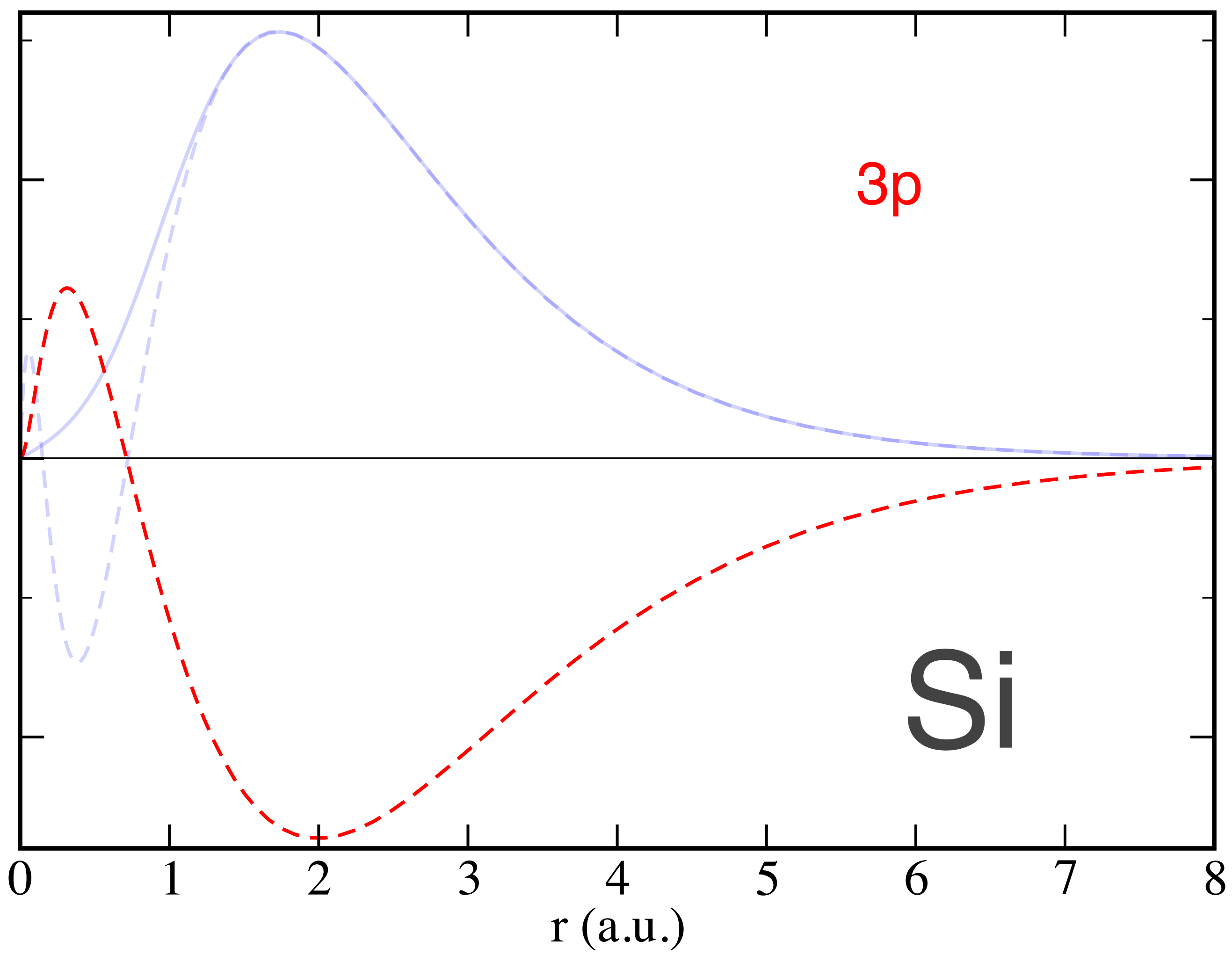
3p
Si
0
1
2
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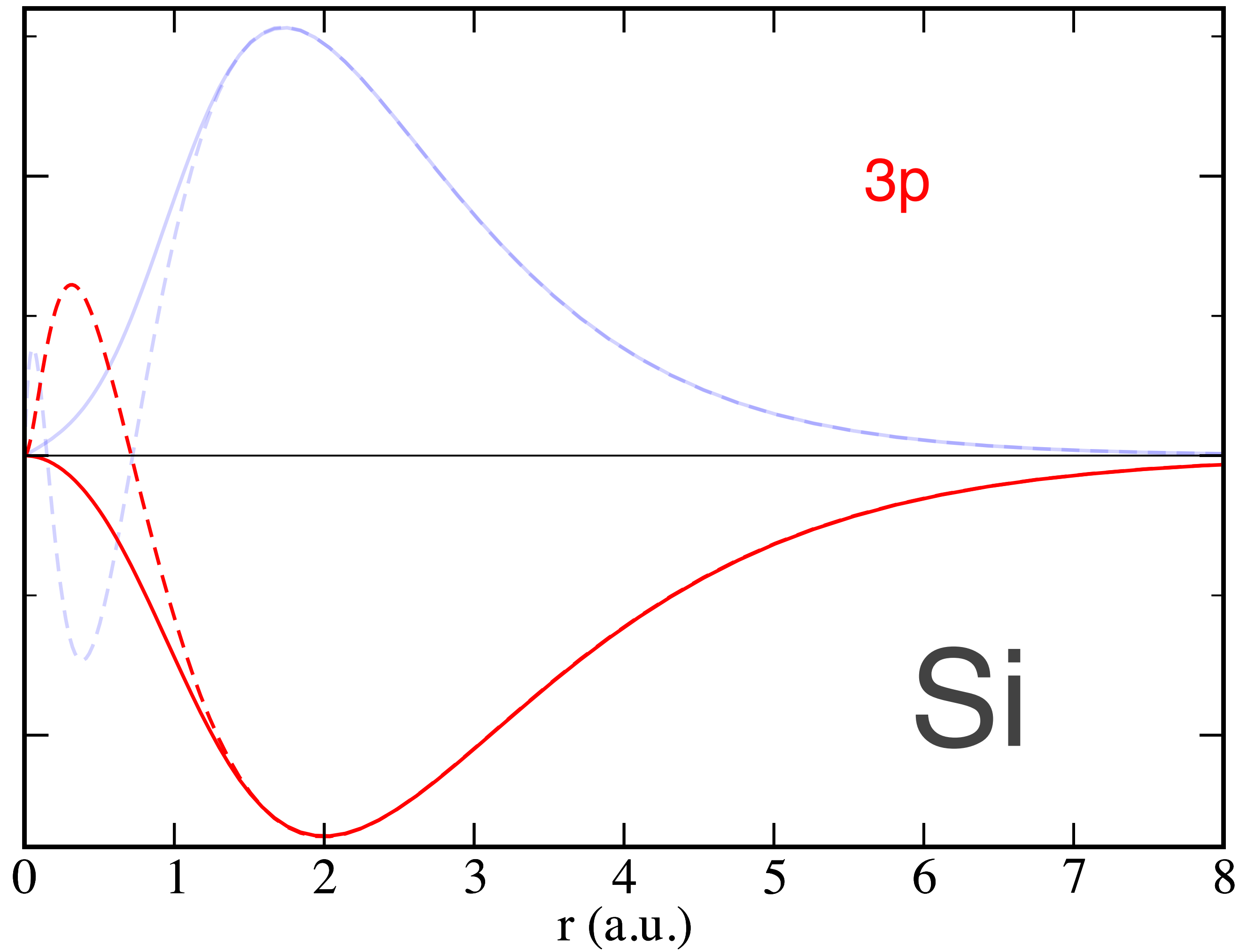
7
8
r (a.u.)


3p
Si
0
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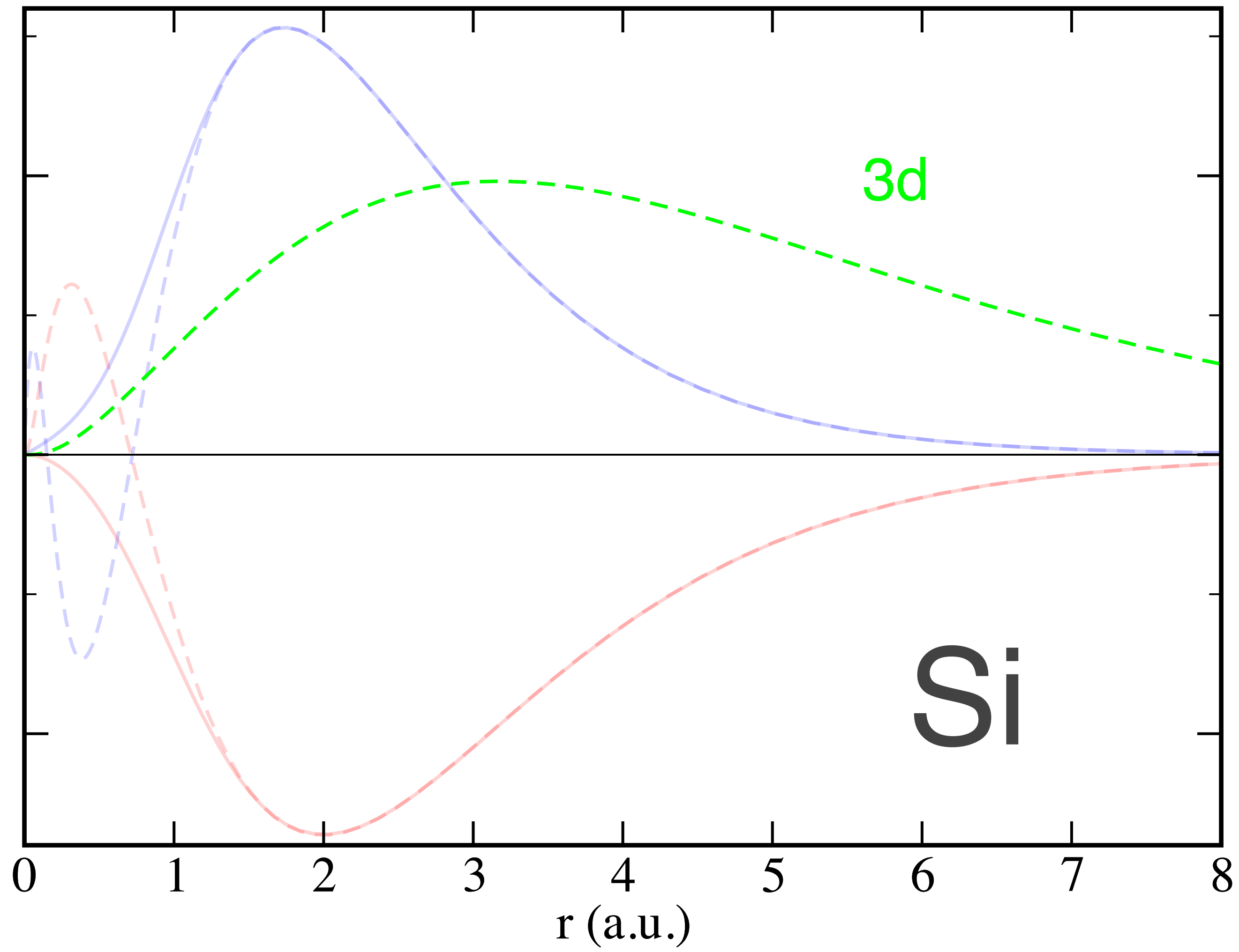
r (a.u.)


3d
Si
0
1
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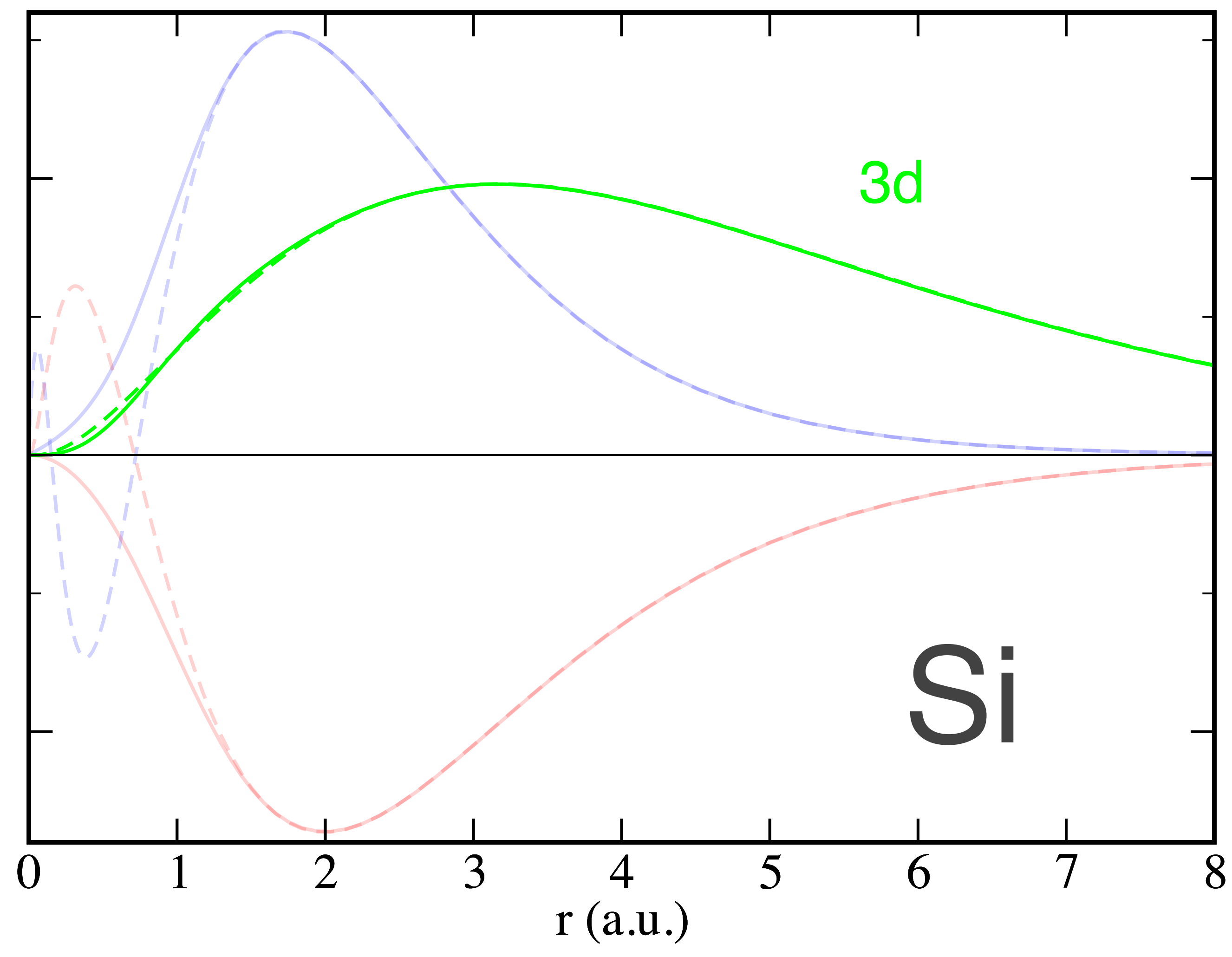
8
r (a.u.)


3d
Si
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8
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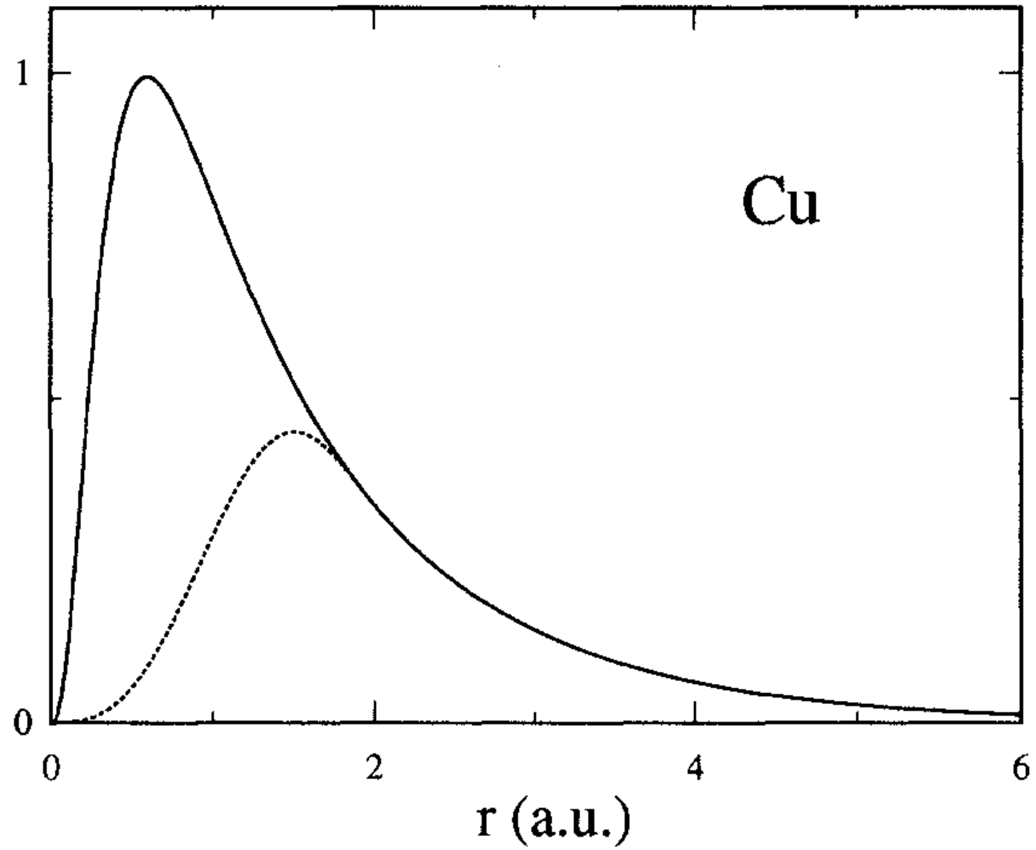
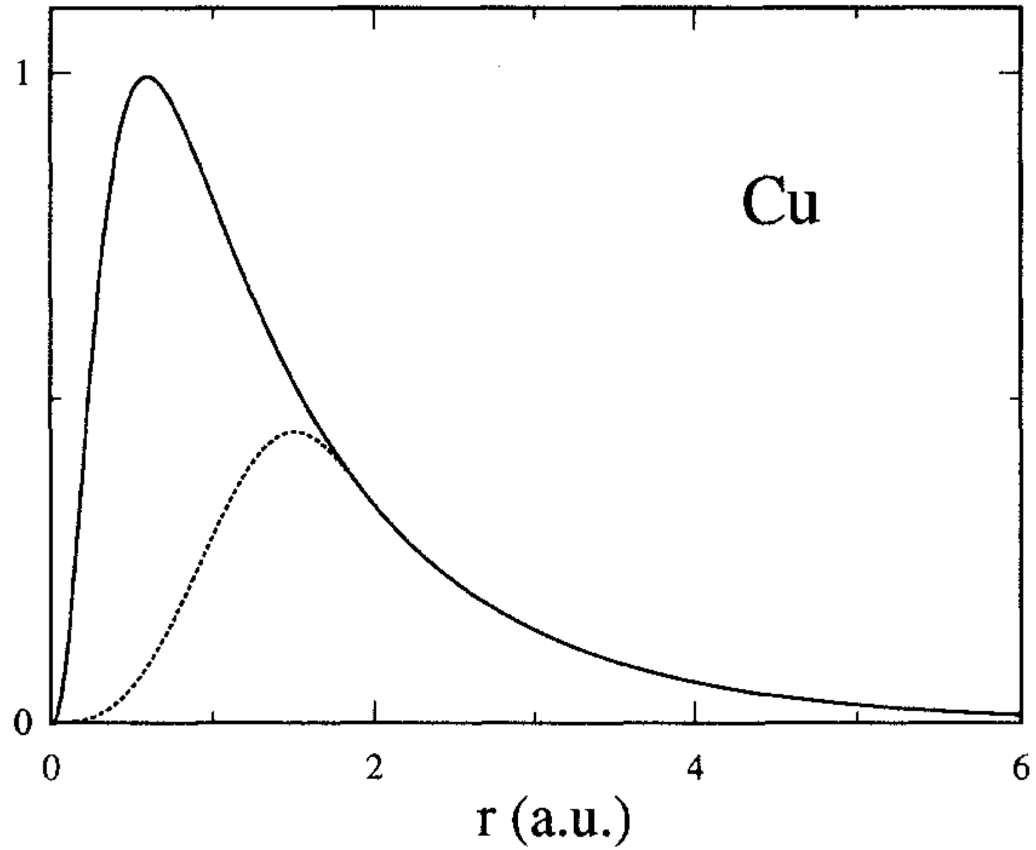
US pseudopotentials



US pseudopotentials



$$H_{US}\phi_n = \epsilon_n S\phi_n \qquad \langle\phi_n|S|\phi_m\rangle = \delta_{nm}$$

watching the sound of waves

a short digression on signal analysis & Fourier transforms

watching the sound of waves

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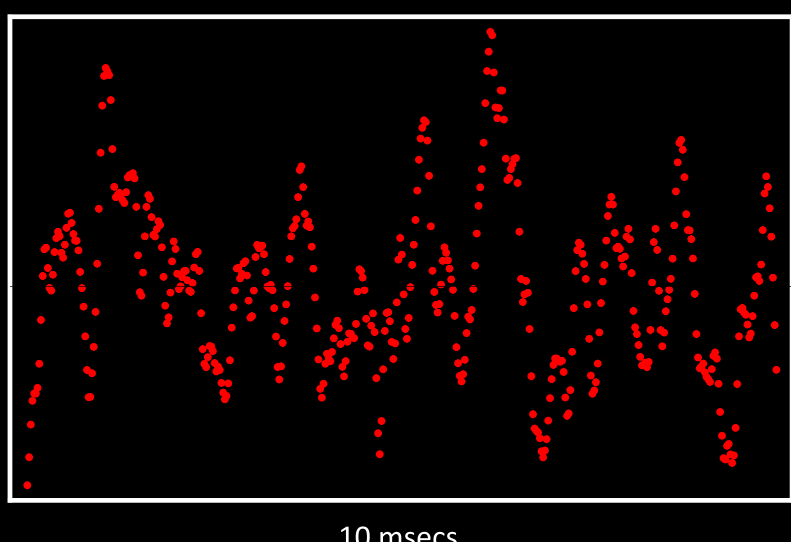
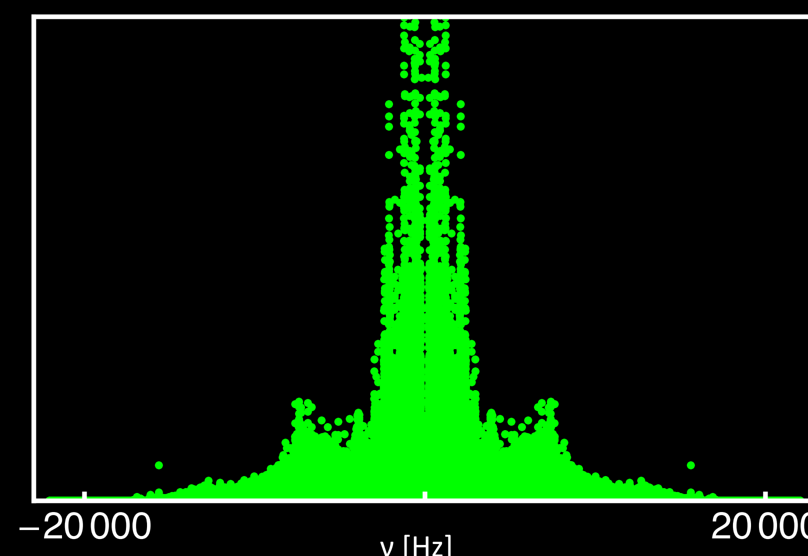
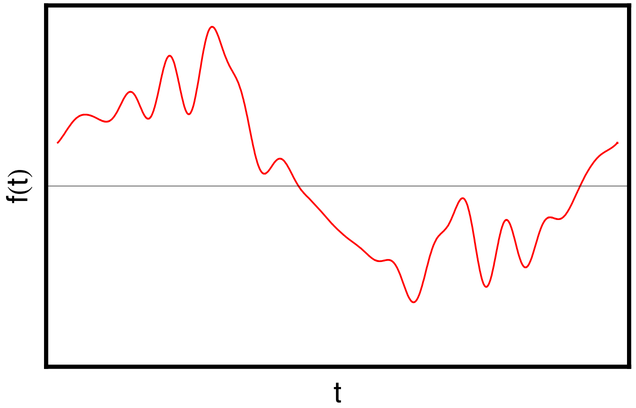
a short digression on signal analysis & Fourier transforms





sampling signals



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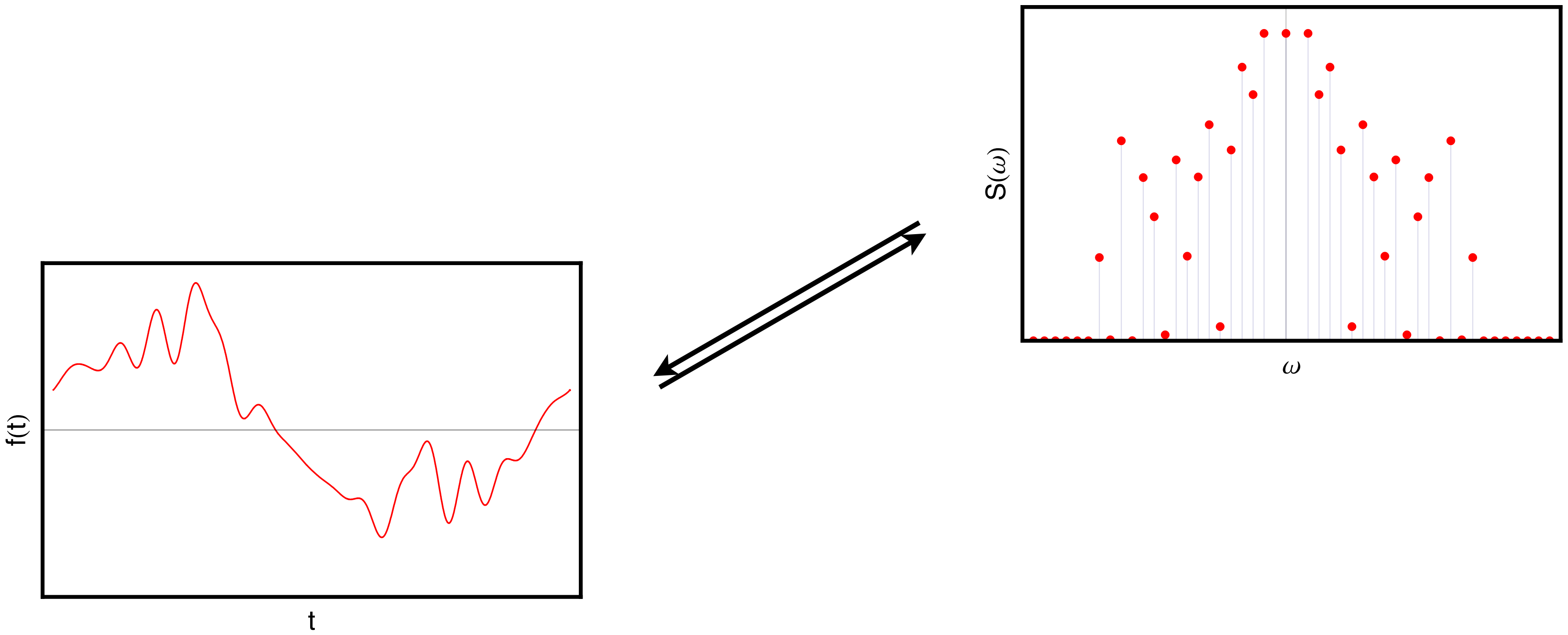

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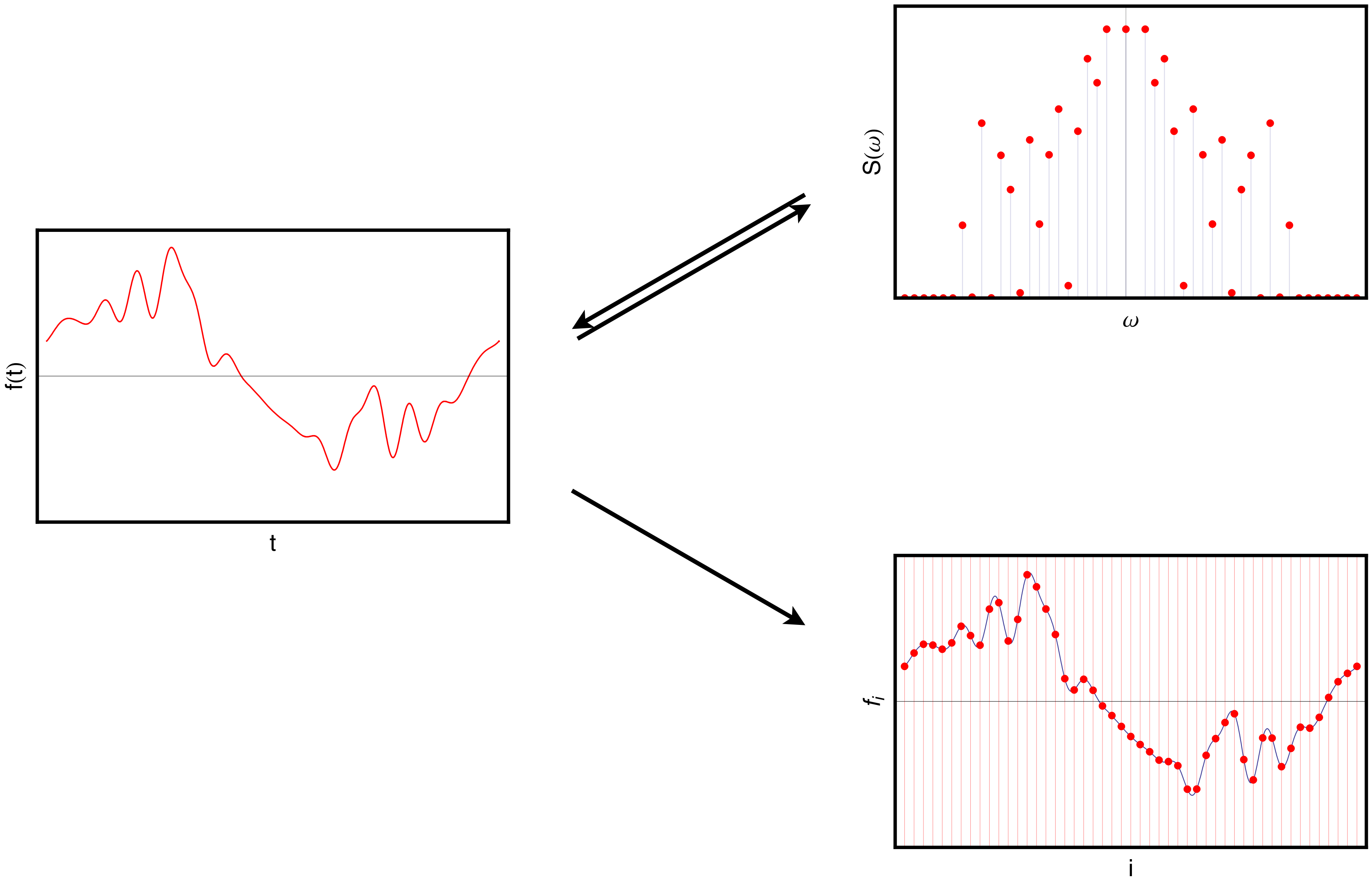

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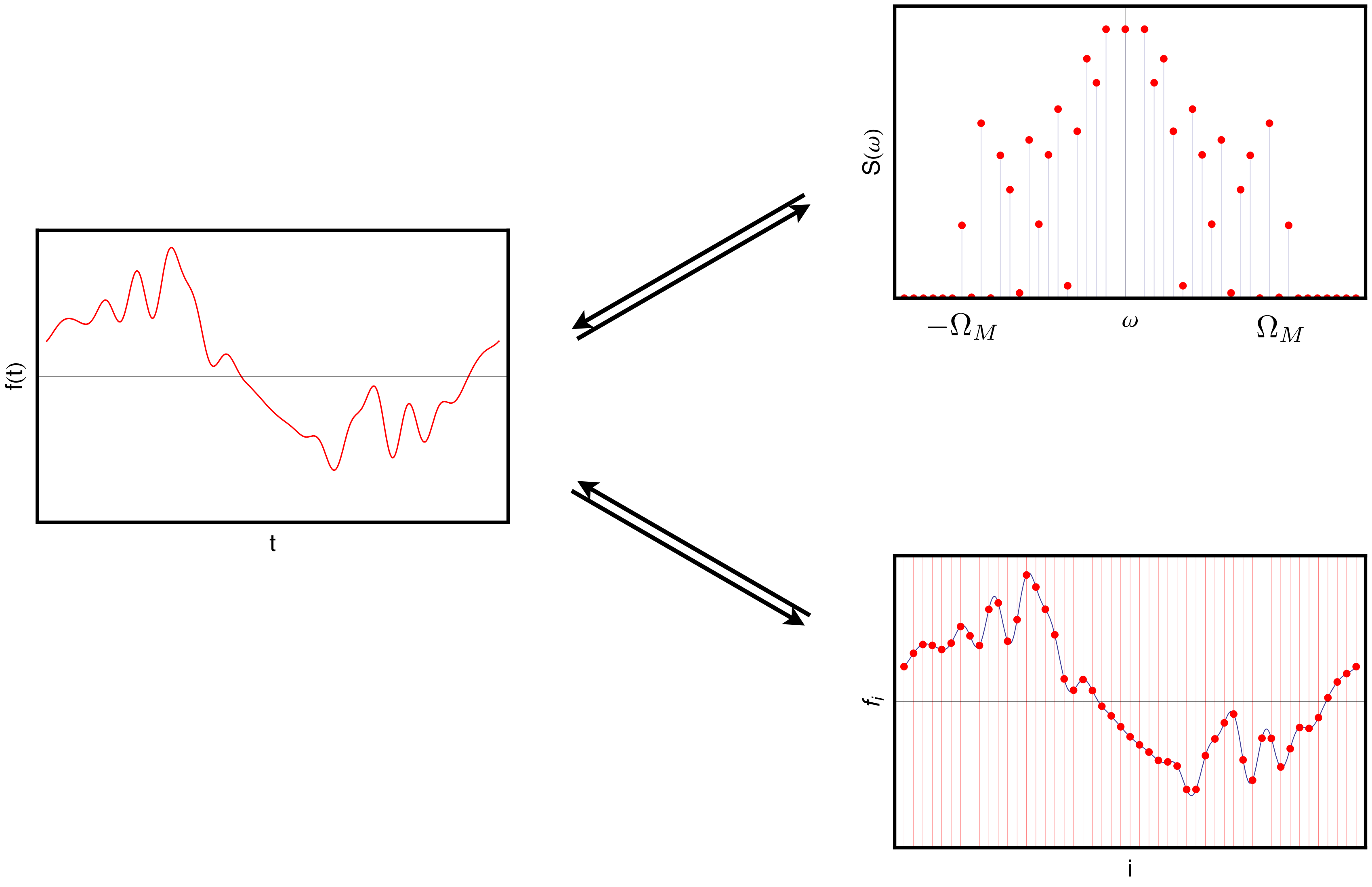

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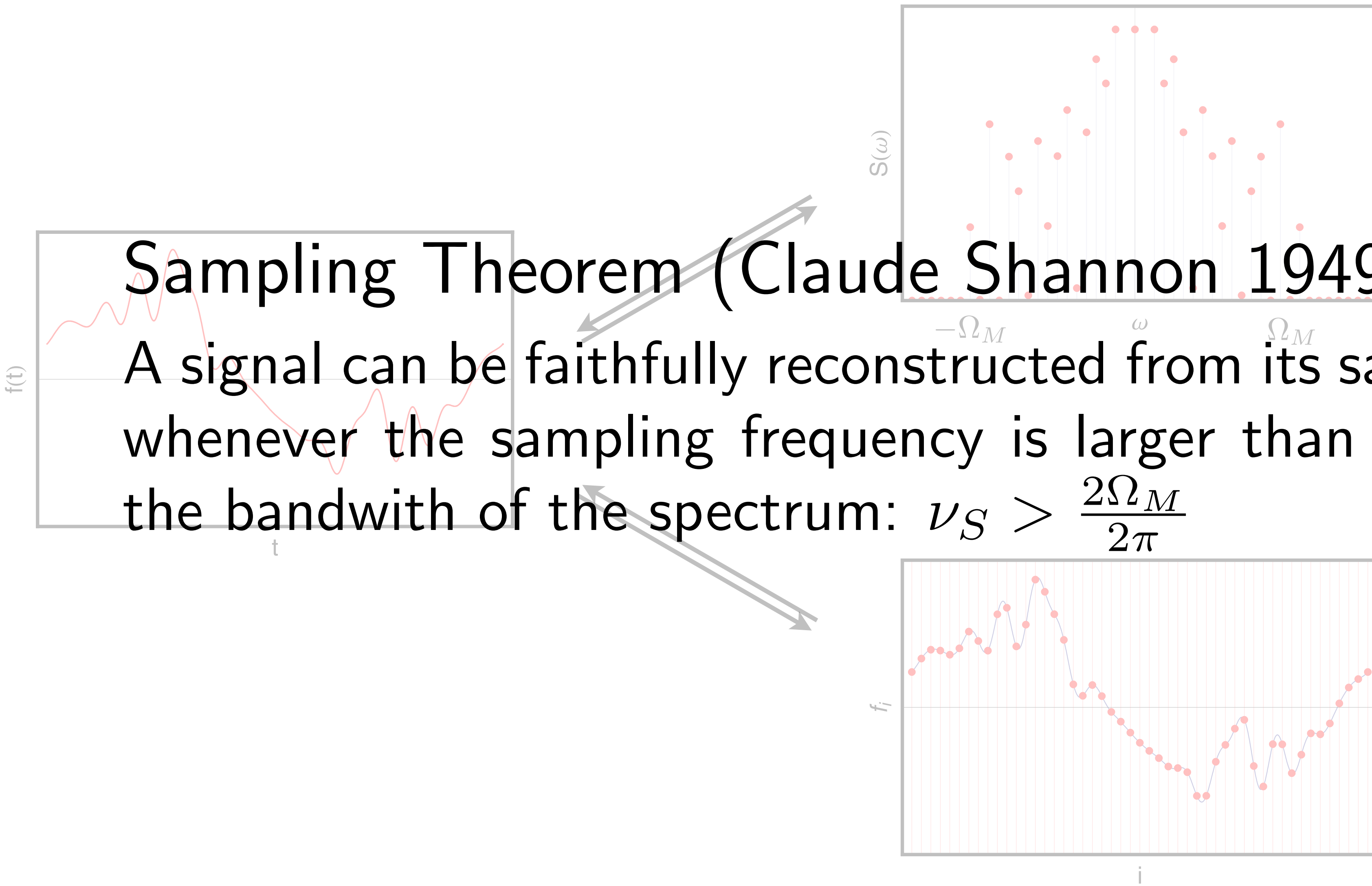


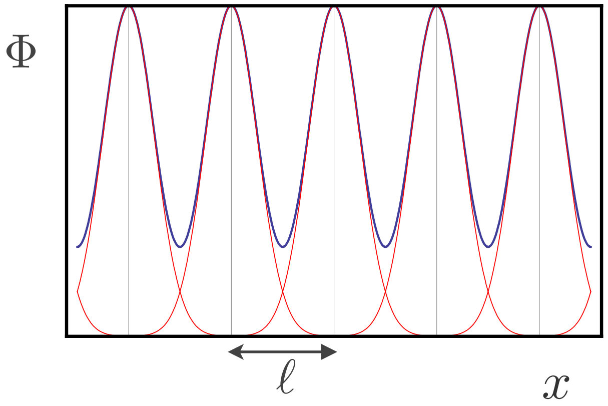
Sampling Theorem (Claude Shannon 1949)

A signal can be faithfully reconstructed from its sample whenever the sampling frequency is larger than twice the bandwith of the spectrum: $\nu_S > \frac{2\Omega_M}{2\pi}$

Fourier analysis

$$\Phi(x) = \sum_n \varphi(x - n\ell)$$

$$\Phi(x + \ell) = \Phi(x)$$



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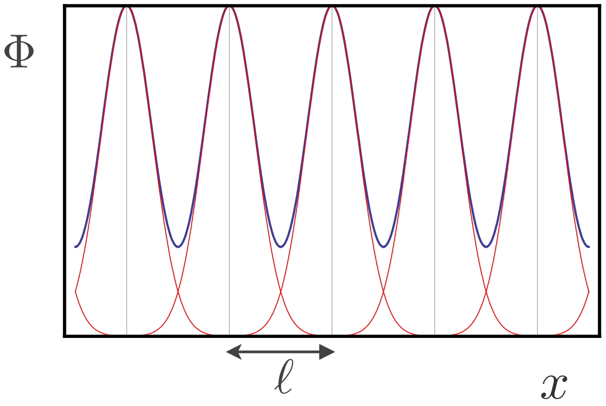

$$\Phi(x) = \sum_q \tilde{\Phi}(q) \mathrm{e}^{iqx} \qquad q_k = k\frac{2\pi}{\ell}$$

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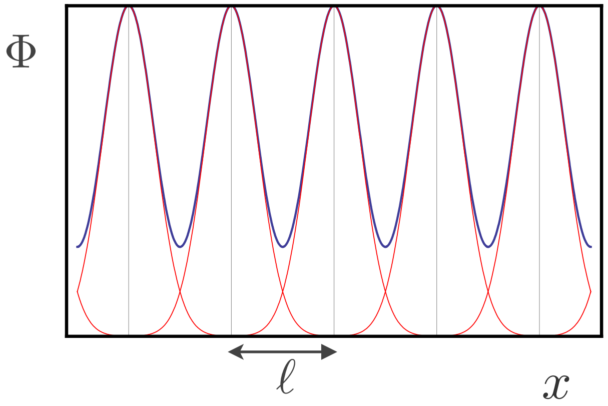

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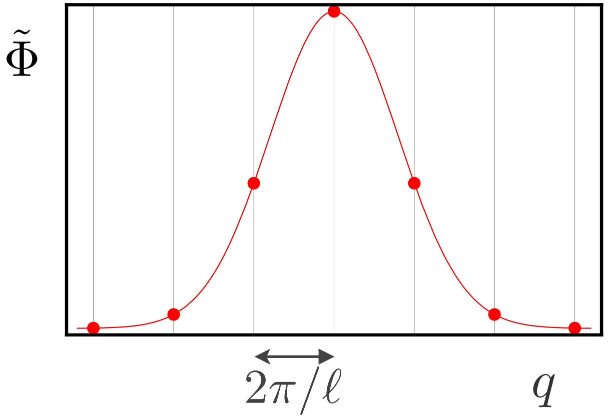
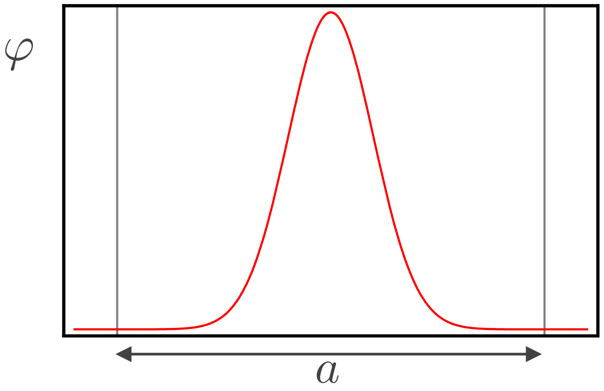


$$\begin{aligned} \tilde{\Phi}(q) &= \frac{1}{\ell}\int_0^\ell \Phi(x)\mathrm{e}^{-iqx}dx \\ &= \frac{1}{\ell}\int_{-\infty}^{\infty} \varphi(x)\mathrm{e}^{-iqx}dx \\ &= \frac{1}{\ell}\tilde{\varphi}(q) \end{aligned}$$

sampling theorem

$$\varphi(x) = 0 \quad \text{for} \quad |x| > \frac{a}{2}$$



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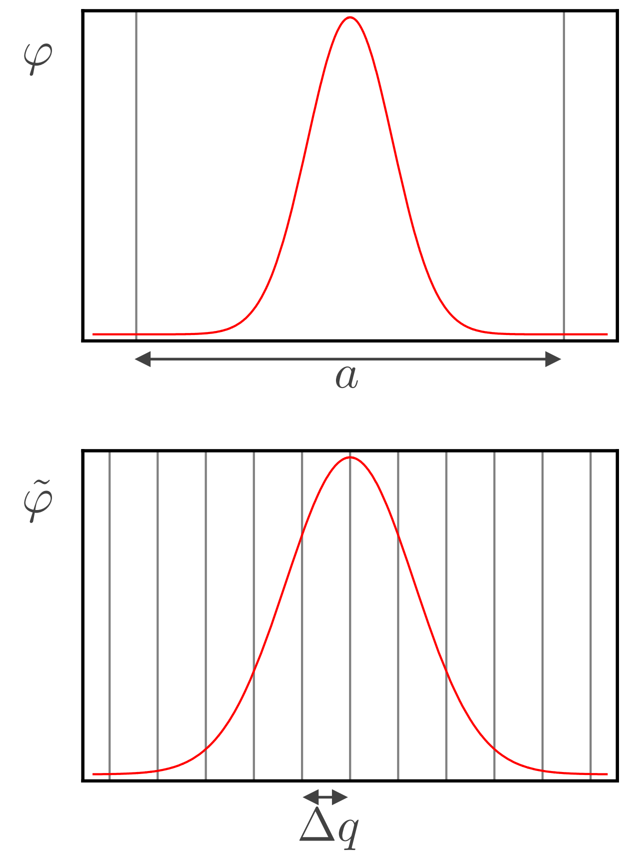

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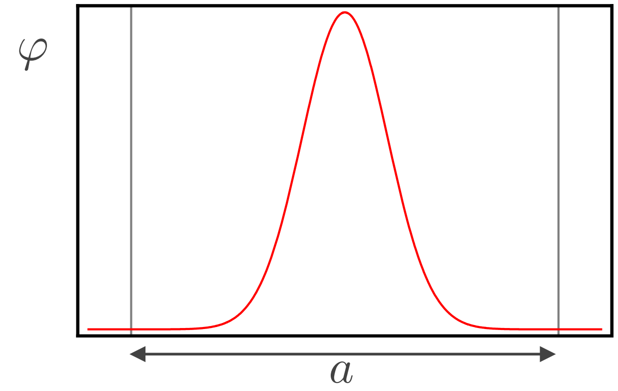

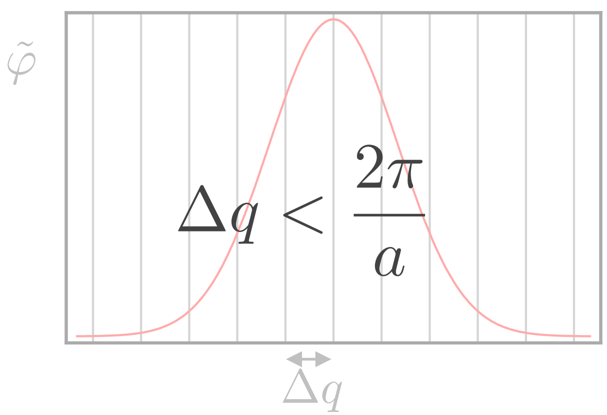

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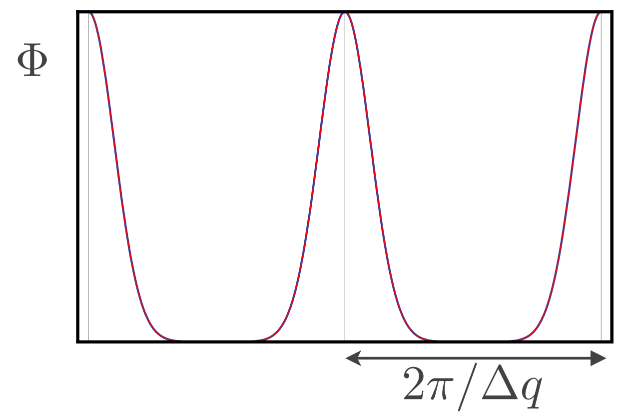

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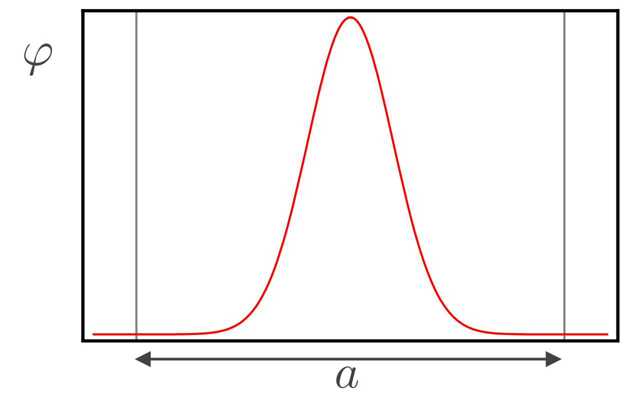

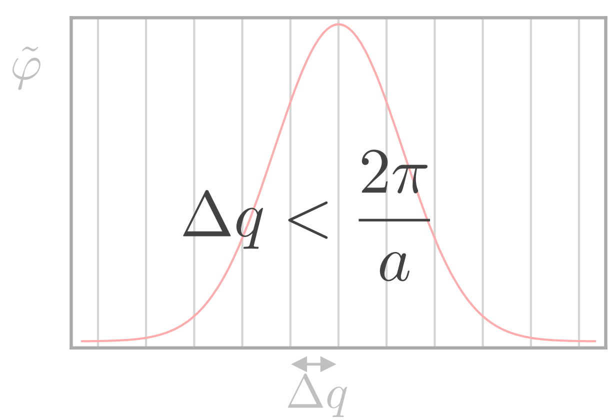

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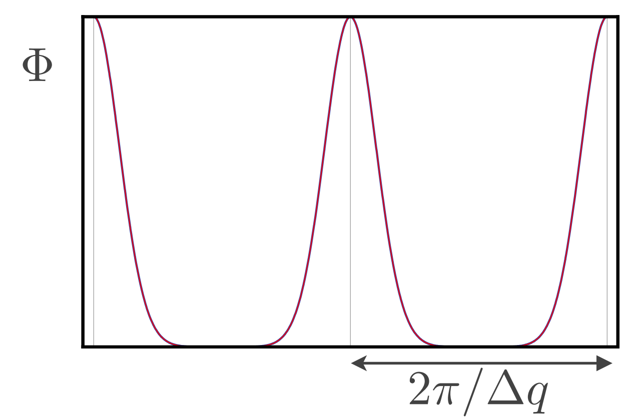

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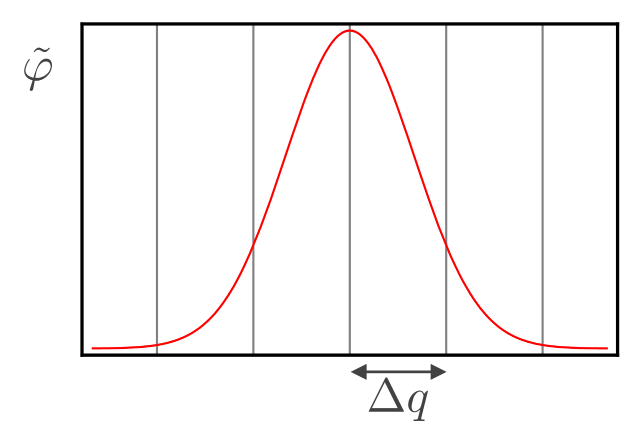

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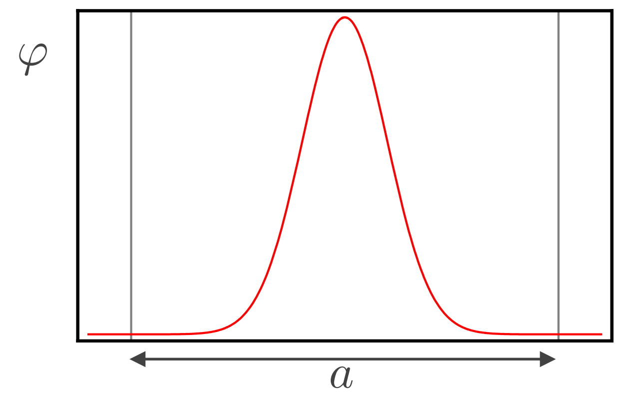

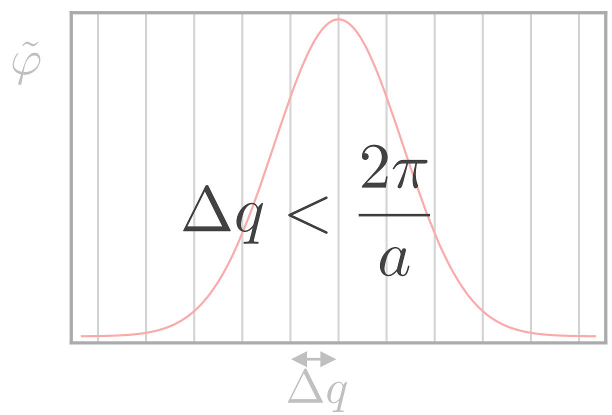

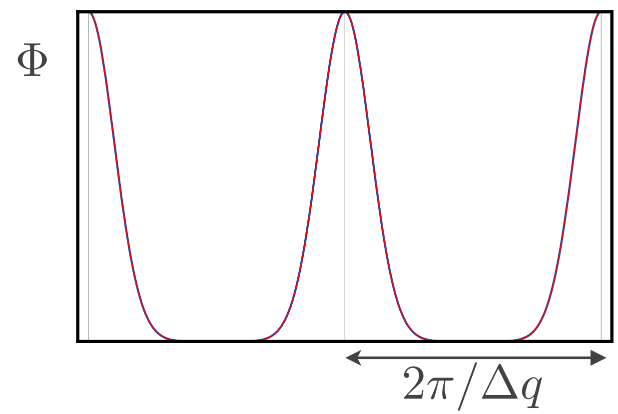

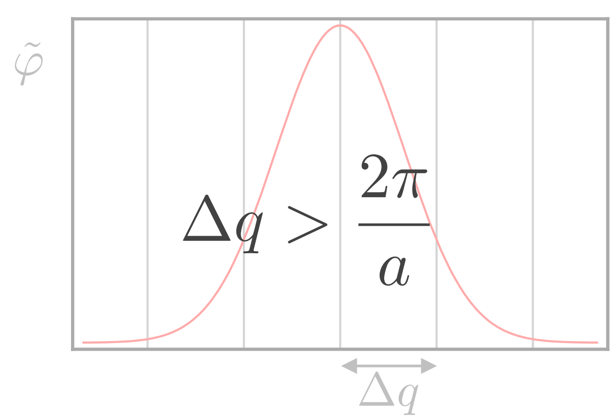

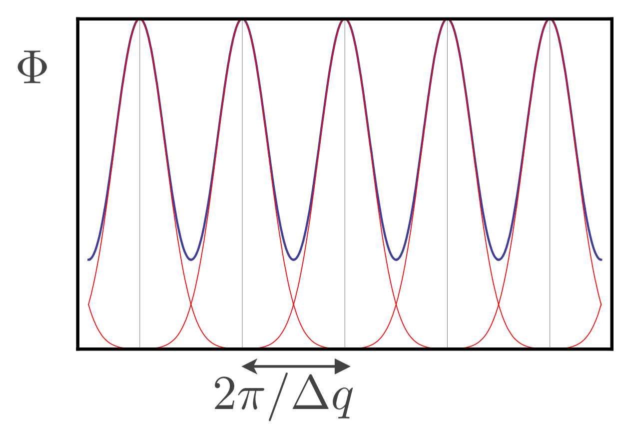

discrete Fourier transforms

$$f(t) = 0 \qquad \text{for } t \notin [0, T] \quad \rightarrow \quad \Delta\omega = \frac{2\pi}{T}$$

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dFt

properties of the dFt

$$
\begin{aligned}
f_{i+N} &= f_i \\
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discreteness in dual space

$\Downarrow$

periodicity in the primary space

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discreteness in dual space

$\Downarrow$

periodicity in the primary space

$$f_i \in \mathbb{R} \longrightarrow \begin{aligned} \tilde{f}_k &= \tilde{f}^*_{-k} \\ &= \tilde{f}^*_{N-k} \end{aligned}$$

the fast Fourier transform

$$\tilde{f}_k = \sum_{l=0}^{N-1} f_l \mathrm{e}^{-2\pi i \frac{lk}{N}}$$

$$\mathcal{O}\left(N^2\right) \text{ ops}$$

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for k≥N/2, use:

$$\begin{aligned} {}^{\frac{N}{2}}\tilde{f}_{k+\frac{N}{2}} &= {}^{\frac{N}{2}}\tilde{f}_k \\ \mathrm{e}^{-2\pi i \frac{k+N/2}{N}} &= -\mathrm{e}^{-2\pi i \frac{k}{N}} \end{aligned}$$

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$$\mathcal{O}\left(N^2\right) \longrightarrow \mathcal{O}(N\log(N))$$

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$$\begin{aligned} F_l &= f_l + i g_l \\ \tilde{f}_k &= \frac{1}{2}(\tilde{F}_k + \tilde{F}_{N-k}^*) \\ \tilde{g}_k &= \frac{1}{2i}(\tilde{F}_k - \tilde{F}_{N-k}^*) \end{aligned}$$

get two, pay one!

FFT of real data sets (II)

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get one, pay half!

multivariate FFTs

$$F(\mathbf{r}) = F(\mathbf{r}+\mathbf{R}) \to \begin{cases} F(\mathbf{r}) = \sum_{\mathbf{G}} \mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}} F(\mathbf{G}) \\ \tilde{F}(\mathbf{G}) = \frac{1}{\Omega} \int_{\Omega} \mathrm{e}^{-i\mathbf{G}\cdot\mathbf{r}} F(\mathbf{r}) d\mathbf{r} \end{cases} \qquad \mathbf{G}\cdot\mathbf{R} = 0 \mod (2\pi)$$

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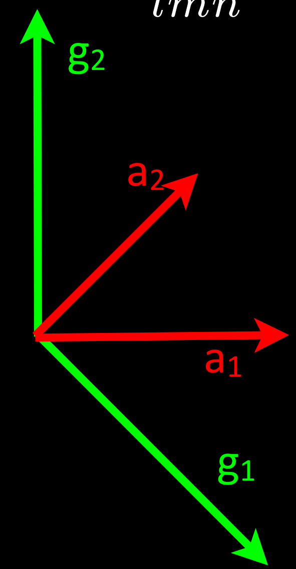
$$\mathbf{G}_{pqs} = p\mathbf{g}_1 + q\mathbf{g}_2 + s\mathbf{g}_3$$

$$\mathbf{r}_{lmn} = \frac{l}{N}\mathbf{a}_1 + \frac{m}{N}\mathbf{a}_2 + \frac{n}{N}\mathbf{a}_3$$

$$\mathbf{g}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$



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$$\mathbf{g}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij} \rightarrow$$

$$\mathbf{G}_{pqs} \cdot \mathbf{r}_{lmn} = \frac{2\pi}{N}(pl + qm + sn)$$

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$$\mathbf{r}_{lmn} = \frac{l}{N}\mathbf{a}_1 + \frac{m}{N}\mathbf{a}_2 + \frac{n}{N}\mathbf{a}_3$$

$$\mathbf{g}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij} \rightarrow$$

$$\mathbf{G}_{pqs} \cdot \mathbf{r}_{lmn} = \frac{2\pi}{N}(pl + qm + sn)$$

FFT

$$\tilde{F}(p\mathbf{g}_1, q\mathbf{g}_2, s\mathbf{g}_3) = \frac{1}{N^3}\sum_{klm} \mathrm{e}^{-i2\pi\frac{pk+ql+sm}{N}} F\left(\tfrac{k}{N}\mathbf{a}_1, \tfrac{l}{N}\mathbf{a}_2, \tfrac{m}{N}\mathbf{a}_3\right)$$

$$F\left(\tfrac{k}{N}\mathbf{a}_1, \tfrac{l}{N}\mathbf{a}_2, \tfrac{m}{N}\mathbf{a}_3\right) = \sum_{pqs} \mathrm{e}^{i2\pi\frac{pk+ql+sm}{N}} \tilde{F}(p\mathbf{g}_1, q\mathbf{g}_2, s\mathbf{g}_3)$$

FFT^{-1}

multivariate FFTs (II)

$$F(k,l,m) = \sum_{pqs} \mathrm{e}^{i2\pi\,\frac{pk+ql+sm}{N}}\,\tilde{F}(p,q,s)$$

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$$3N^2 \times N \log N = N^3 \log\left(N^3\right)$$

correlation functions, convolutions, power spectra

$$C_A(t) = \langle A(t + t')A(t') \rangle$$

correlation functions, convolutions, power spectra

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correlation functions, convolutions, power spectra

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$\mathcal{O}\left(N^2\right)$ ops

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\end{aligned}
$$

$\mathcal{O}\left(N^2\right)$ ops

$$\frac{1}{N}\sum_k \mathrm{e}^{-i2\pi\frac{k(q-p)}{N}} = \delta_{qp}$$

correlation functions, convolutions, power spectra

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$$A\otimes A(l) = \frac{1}{N}\sum_k A(k+l)A(k) \qquad \mathcal{O}\left(N^2\right) \text{ ops}$$

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$$= \sum_k |\tilde{A}(p)|^2 \mathrm{e}^{i2\pi\frac{lp}{N}} \qquad \mathcal{O}\big(N\log N\big) \text{ ops}$$

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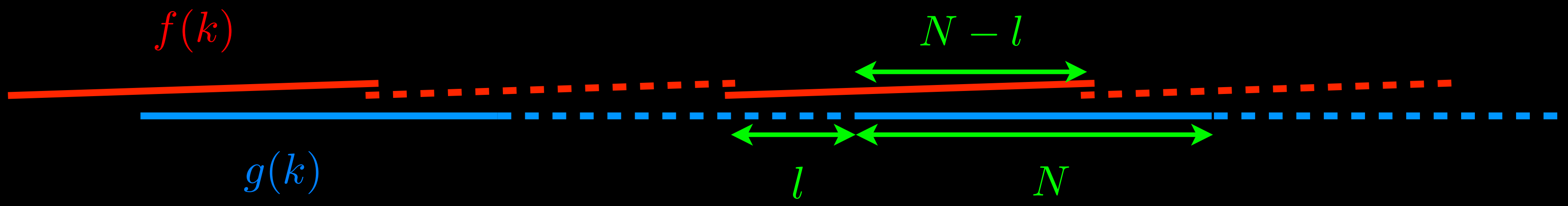

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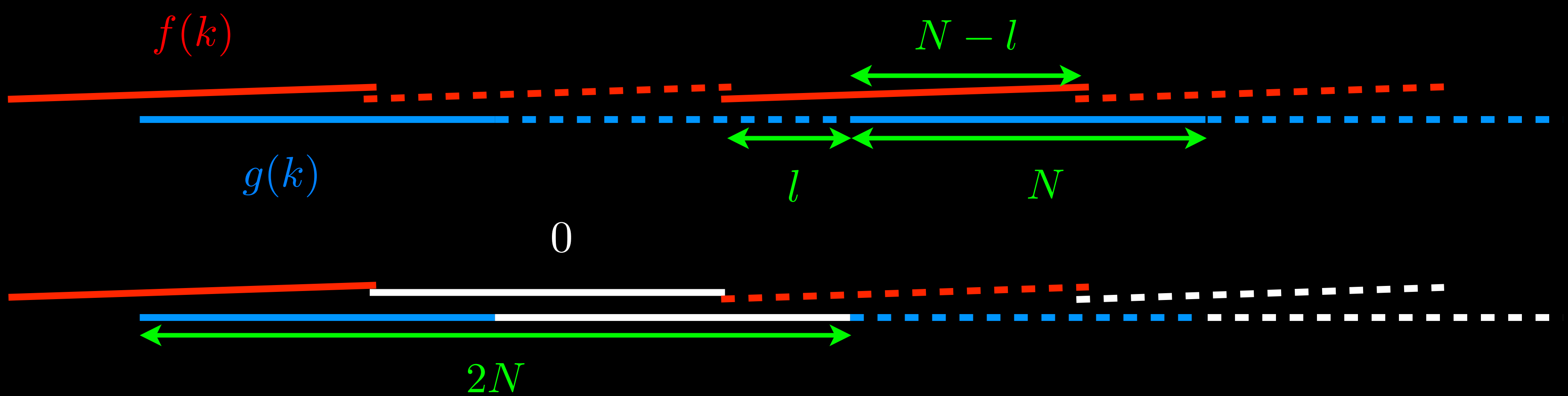

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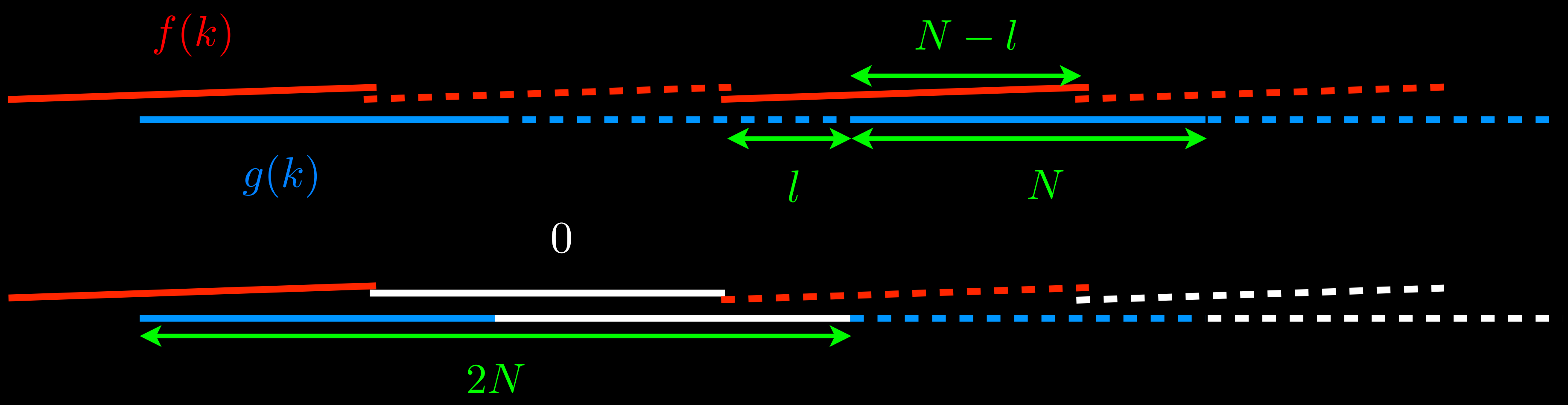

$$h(l) = \frac{1}{2N} \sum_{k=0}^{2N-1} f(k+l) g(k)$$

solving the Poisson equation

$$\Delta V(\mathbf{r}) = 4\pi\rho(\mathbf{r})$$

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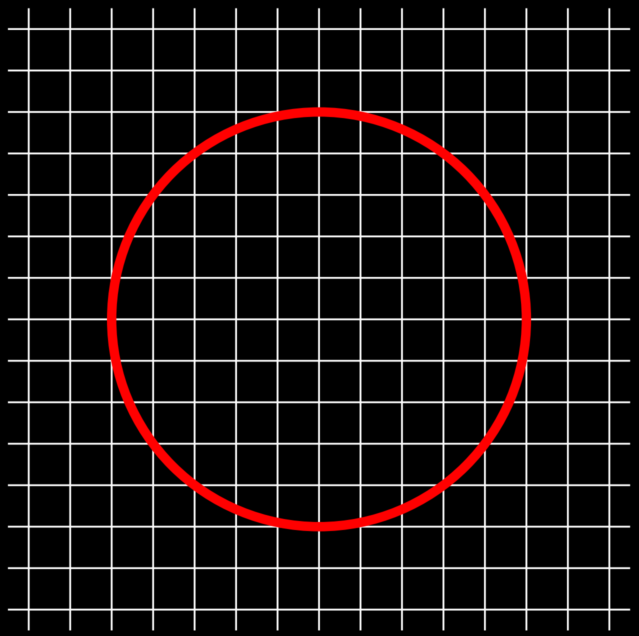

$$\rho(\mathbf{r}) \rightarrow \tilde{\rho}(\mathbf{G})$$

$$\mathbf{G}_{max} \sim \frac{2\pi}{h}$$

$$h \lesssim \frac{2\pi}{G_{max}}$$

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these slides at
http://talks.baroni.me