

Variational Methods

Introduzione

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- Variational Methods for Bound States

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- Variational Methods for Scattering States

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 - Ψ_0, Ψ_1, \dots exact eigenvectors of a given H
 - $E_0 < E_1 < \dots$ exact eigenvalues

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- Notation
 - Ψ_0, Ψ_1, \dots exact eigenvectors of a given H
 - $E_0 < E_1 < \dots$ exact eigenvalues
- Framework: non-relativistic quantum mechanics
 - “standard nuclear model”: nucleons interacting via static potentials
 - how well the properties of nuclei are described in this model?

The Variational Method for the Ground State

- Theorem: given a “trial” wave function $\bar{\Psi}$, then

$$\langle H \rangle = \frac{\langle \bar{\Psi} | H | \bar{\Psi} \rangle}{\langle \bar{\Psi} | \bar{\Psi} \rangle} \geq E_0$$

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- Relatively poor $\overline{\Psi}$ can give fairly good estimates of E_0

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- $\langle H \rangle$ is stationary with respect to the variation $\bar{\Psi} \rightarrow \bar{\Psi} + \delta \bar{\Psi}$
- Search for the $\bar{\Psi}$ giving $\delta \langle H \rangle = 0$

Example: the Helium atom - 1

- Basic Hamiltonian

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

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- Neglecting the last term:

nucleus charge $Z = 2$

$$\bar{\Psi} = \frac{Z^3}{\pi a_0^3} e^{\frac{-Z(r_1+r_2)}{a_0}} \chi_{\text{singlet}}$$

Bohr radius

Example: the Helium atom - 1

- First order perturbation theory

$$\langle \bar{\Psi} | H | \bar{\Psi} \rangle = \left(Z^2 - \frac{27}{8} Z \right) \left(\frac{e^2}{a_0} \right) \approx -74.8 \text{ eV}$$

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- Each electron feels a screened nucleus charge $Z < 2$ by the other electron

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- E_1 energy of the first excited state
- Usually not very useful

Linear Basis

- Expansion on a (truncated) orthonormal basis of functions Φ_k

$$\bar{\Psi}_N = \sum_{k=1}^N a_k \Phi_k \quad a_k \text{ variational parameters}$$

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 $E = \text{Lagrange multiplier}$

$$\begin{pmatrix} \langle \Phi_1 | H | \Phi_1 \rangle & \langle \Phi_1 | H | \Phi_2 \rangle & \dots \\ \langle \Phi_2 | H | \Phi_1 \rangle & \langle \Phi_2 | H | \Phi_2 \rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

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- Algebraic eigenvalue problem
standard numerical methods LAPACK
special methods for big matrices (Lanczos, ...)

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- $E_k^{(N)} \rightarrow E_k$ smoothly as $N \rightarrow \infty$

Example: the Helium atom - 2

- Drake and coworkers, PRL **59**, 1549 (1987)

$$\bar{\Psi} \sim \sum_{i,j,k} a_{i,j,k} r_1^i r_2^j r_{12}^k \exp(-\alpha r_1 - \beta r_2) \left[Y_{\ell_1}(\hat{r}_1) Y_{\ell_2}(\hat{r}_2) \right]_{LM} \chi_S$$

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- Converged digits for the ground and several excited state energies: 25

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	$1/\alpha$
Electron $g - 2$	137.035 999 6(5)
He 2^3P	137.035 986 4(31)

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- One has to check *always* the convergence of $\langle \mathcal{O} \rangle_N$
- In some cases (HH basis) the convergence properties are **known analytically**
Schneider, Phys. Lett. **40B**, 439 (1972)

Variational calculations in Nuclear Physics

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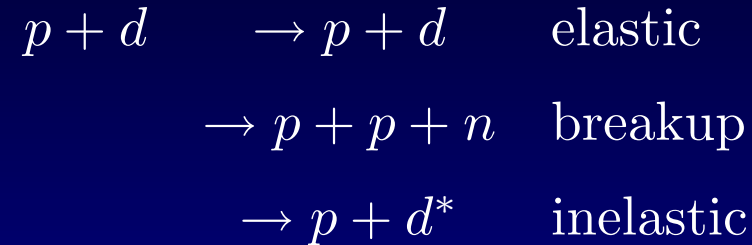
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- In the last years, accurate variational calculations have been obtained for $A = 3, 4$
 - gaussian basis (Kamimura, Varga)
 - hyperspherical harmonic basis (Pisa, Trento)

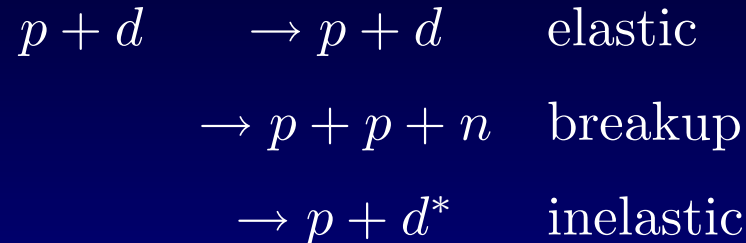
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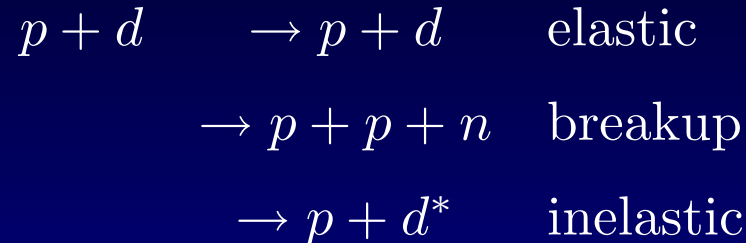
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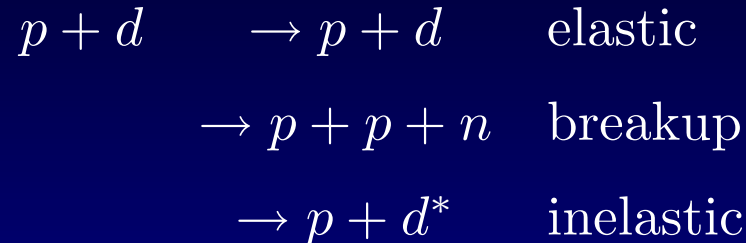
$$[S_{\alpha,\beta}] = \bar{S}_{\alpha,\beta} - \langle \bar{\Psi}_\beta | H - E | \bar{\Psi}_\alpha \rangle$$

gives the “best” approximation of Ψ at a given E .

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- $\bar{\Psi}_\alpha$ must have the appropriate asymptotic behaviour

Variational methods for scattering states

- If $\bar{\Psi}_\alpha = \Psi_\alpha + \varepsilon$, then

Ψ_α exact solution $H\Psi_\alpha = E\Psi_\alpha$

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- $\bar{\Psi}_\alpha = \Psi_\alpha$ stationary point of $[S_{\alpha,\alpha}]$
- In this case: $[S_{\alpha,\beta}] = S_{\alpha,\beta}$

Two-Body Scattering - central potential

- $\Psi = \frac{u(r)}{r} Y_{\ell m}(\hat{r})$, $E = \frac{\hbar^2 k^2}{2\mu}$, $\mu = \text{reduced mass}$, $\eta = (2\mu/\hbar^2)(e^2/2k)$

$$\mathcal{L} = -\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \right] + V(r) + \frac{e^2}{r} - \frac{\hbar^2 k^2}{2\mu}$$

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- Asymptotic solutions ($V \rightarrow 0$):

regular $F_\ell(\eta, kr)$ and the irregular $G_\ell(\eta, kr)$ Coulomb functions

behaviour for $r \rightarrow \infty$:

$$F_\ell(\eta, x) \rightarrow \sin\left(x - \eta \ln(2x) - \frac{\ell\pi}{2} + \sigma_\ell\right)$$

$$G_\ell(\eta, x) \rightarrow \cos\left(x - \eta \ln(2x) - \frac{\ell\pi}{2} + \sigma_\ell\right)$$

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- no Coulomb case:

$$F_\ell(\eta = 0, x) \rightarrow x j_\ell(x)$$

$$G_\ell(\eta = 0, x) \rightarrow -x y_\ell(x)$$

Two-Body Scattering - central potential

- We have to regularize the function $G_\ell(\eta, kr)$
$$\tilde{G}_\ell(\eta, kr) = G_\ell(\eta, kr)[1 - \exp(-\gamma r)]^{2\ell+1}$$

 γ is a variational parameter

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$$\mathcal{O}_\ell = \tilde{G}_\ell + iF_\ell$$

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- behaviour for $r \rightarrow \infty$:

$$\mathcal{O}_\ell(\eta, x) \rightarrow \exp[i(x - \eta \ln(2x) - \frac{\ell\pi}{2} + \sigma_\ell)]$$

$$\mathcal{I}_\ell(\eta, x) \rightarrow \exp[-i(x - \eta \ln(2x) - \frac{\ell\pi}{2} + \sigma_\ell)]$$

Two-Body Scattering - central potential

- Trial wave function

$$\bar{u}(r) = \sqrt{\frac{2\mu}{\hbar^2} \frac{1}{2ik}} \left[\sum_{i=1}^N \bar{a}_i f_i(r) + \bar{S} \mathcal{O}_\ell(\eta, kr) - \mathcal{I}_\ell(\eta, kr) \right]$$

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- Exact wave function

$$\bar{u}(r) = \sqrt{\frac{2\mu}{\hbar^2} \frac{1}{2ik}} \left[\sum_{i=1}^{\infty} a_i r f_i(r) + S \mathcal{O}_\ell(\eta, kr) - \mathcal{I}_\ell(\eta, kr) \right]$$

$f_i(r)$ complete basis, \bar{a}_i linear variational parameters

$$f_i(r \rightarrow \infty) \rightarrow 0$$

Two-Body Scattering - central potential

- Trial wave function

$$\bar{u}(r) = \sqrt{\frac{2\mu}{\hbar^2} \frac{1}{2ik}} \left[\sum_{i=1}^N \bar{a}_i r f_i(r) + \bar{S} \mathcal{O}_\ell(\eta, kr) - \mathcal{I}_\ell(\eta, kr) \right]$$

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- Exercise: show that

$$\int_0^\infty dr [\bar{u}(r) \mathcal{L}u(r) - u(r) \mathcal{L}\bar{u}(r)] = S - \bar{S}$$

this is an *exact* relation

Two-Body Scattering - central potential

- If $\bar{\Psi} = \Psi + \varepsilon$

$$[\Psi = \frac{u(r)}{r} Y_{\ell m}(\hat{r})]$$

$$\begin{aligned} S &= \bar{S} + \int_0^\infty dr [\bar{u}(r) \mathcal{L} u(r) - u(r) \mathcal{L} \bar{u}(r)] \\ &\equiv \bar{S} + \langle \bar{\Psi} | H - E | \Psi \rangle - \langle \Psi | H - E | \bar{\Psi} \rangle \\ &= \bar{S} - \langle \Psi | H - E | \bar{\Psi} \rangle \\ &= \bar{S} - \langle \bar{\Psi} + \varepsilon | H - E | \bar{\Psi} \rangle \\ &\equiv \bar{S} - \langle \bar{\Psi} | H - E | \bar{\Psi} \rangle + \langle \varepsilon | H - E | \varepsilon \rangle \\ &\equiv [S] + \langle \varepsilon | H - E | \varepsilon \rangle \end{aligned}$$

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- $\bar{\Psi} = \Psi$ stationary point of $[S]$
in this case: $[S] = S$
 $[S] - S$ quadratic in ε

Applications

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$$\mathcal{O}_{1+1+1} \rightarrow \frac{e^{iQ\rho}}{\rho^{5/2}} \quad \text{region A}$$

$$\mathcal{O}_{1+1+1} \rightarrow \psi_0(r_{12})e^{iQy} \quad \text{region B}$$

$\rho \sim \sqrt{r_1^2 + r_2^2 + r_3^2}$, $\hbar^2 Q^2 / m \sim$ total kinetic energy of the system

$$y = r_3 - (r_1 + r_2)/2$$

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- ψ_0 zero-energy scattering two-body wave function
(nn scattering length)
- Three charged particles: asymptotic behaviour not completely known
ionization $e + H \rightarrow e + e + p$

Linear Basis

- Expansion on a (truncated) orthonormal basis of functions Φ_k

$$\bar{\Psi}_\alpha = \sum_{k=1}^N a_k \Phi_k + \sum_{\beta} \bar{\mathcal{S}}_{\alpha,\beta} \mathcal{O}_\beta - \mathcal{I}_\alpha$$

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- Linear system

standard numerical methods LAPACK

special methods for big matrices (Lanczos, ...)