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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- Examples
  - Helium atom
  - $p-d$ & $p-{}^3$He Scattering

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- Notation
  $\Psi_0, \Psi_1, \ldots$ exact eigenvectors of a given H
  $E_0 < E_1 < \cdots$ exact eigenvalues

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- Notation
  $\Psi_0, \Psi_1, \ldots$ exact eigenvectors of a given H
  $E_0 < E_1 < \cdots$ 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 $\overline{\Psi}$, then

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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 $\overline{\Psi} \rightarrow \Psi + \delta\Psi$
- Search for the $\overline{\Psi}$ 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 $Z = 2$

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

Bohr radius

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- First order perturbation theory

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

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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) ortonormal basis of functions Φ_k

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  E =Lagrange multiplier

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

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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)

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

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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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  - very effective for strong repulsive *central* potentials
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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)

Variational methods for scattering states

- Elastic and inelastic many-particle scattering

$$
\begin{aligned}
p + d \quad &\longrightarrow p + d \quad && \text{elastic} \\
&\longrightarrow p + p + n && \text{breakup} \\
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  gives the "best" approximation of Ψ at a given E.

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

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

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

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- $\overline{\Psi}_a = \Psi_a$ stationary point of $[S_{\alpha,\alpha}]$
- In this case: $[S_{\alpha,\beta}] = S_{\alpha,\beta}$

Two-Body Scattering - central potential

- $\Psi = \frac{u(r)}{r} Y_{\ell m}(\hat{r})$, $E = \frac{\hbar^2 k^2}{2\mu}$, $\mu =$ 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 ($V \to 0$):

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

  behaviour for $r \to \infty$:

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

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

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- no Coulomb case:

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

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

Two-Body Scattering - central potential

- We have to regularize the function $G_\ell(\eta, kr)$

  $\widetilde{G}_\ell(\eta, kr) = G_\ell(\eta, kr)[1 - \exp(-\gamma r)]^{2\ell+1}$

  γ is a variational parameter

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- Let us introduce the *ingoing* and *outgoing* solutions

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- behaviour for $r \to \infty$:

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

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

Two-Body Scattering - central potential

- Trial wave function

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

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- Exact wave function

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

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

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

Two-Body Scattering - central potential

- Trial wave function

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

- Exact wave function

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

$f_i(r)$ complete basis, $\overline{a}_i$ linear variational parameters
$f_i(r \to \infty) \to 0$

- Exercize: show that

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

this is an *exact* relation

Two-Body Scattering - central potential

- If $\overline{\Psi} = \Psi + \varepsilon$ $\qquad [\Psi = \frac{u(r)}{r} Y_{\ell m}(\hat{r})]$

$$
\begin{aligned}
S &= \overline{S} + \int_0^\infty dr\, [\overline{u}(r)\mathcal{L}u(r) - u(r)\mathcal{L}\overline{u}(r)] \\
&\equiv \overline{S} + \langle\overline{\Psi}|H-E|\Psi\rangle - \langle\Psi|H-E|\overline{\Psi}\rangle \\
&= \overline{S} - \langle\Psi|H-E|\overline{\Psi}\rangle \\
&= \overline{S} - \langle\overline{\Psi}+\varepsilon|H-E|\overline{\Psi}\rangle \\
&\equiv \overline{S} - \langle\overline{\Psi}|H-E|\overline{\Psi}\rangle + \langle\varepsilon|H-E|\varepsilon\rangle \\
&\equiv [S] + \langle\varepsilon|H-E|\varepsilon\rangle
\end{aligned}
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- $\overline{\Psi} = \Psi$ stationary point of $[S]$
  in this case: $[S] = S$
  $[S] - S$ quadratic in ε

Applications

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  Example $(n + d) \to (n + d) + (n + n + p)$

$$\begin{aligned} \mathcal{O}_{1+1+1} &\to \frac{e^{\mathrm{i}Q\rho}}{\rho^{5/2}} && \text{region A} \\ \mathcal{O}_{1+1+1} &\to \psi_0(r_{12}) e^{\mathrm{i}Qy} && \text{region B} \end{aligned}$$

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

$\boldsymbol{y} = \boldsymbol{r}_3 - (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$

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- Three charged particles: asymptotic behaviour not completely known

  ionization $e + H \to e + e + p$

Linear Basis

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

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

$\Phi_k \rightarrow 0$ in the asymptotic regions

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- Minimization of $\overline{\mathcal{S}}_{\alpha,\alpha} - \langle \overline{\Psi}_\alpha | H - E | \overline{\Psi}_a \rangle$ with respect to a_k and $\overline{\mathcal{S}}_{\alpha,\alpha}$

$$\begin{pmatrix} \langle \Phi_1 | H - E | \Phi_1 \rangle & \langle \Phi_1 | H - E | \Phi_2 \rangle & \dots \\ \langle \Phi_2 | H - E | \Phi_1 \rangle & \langle \Phi_2 | H - E | \Phi_2 \rangle & \dots \\ \vdots & \vdots & \\ \langle \Phi_1 | H - E | \mathcal{O}_\alpha \rangle & \langle \Phi_2 | H - E | \mathcal{O}_\alpha \rangle & \dots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \overline{\mathcal{S}}_{\alpha,\alpha} \end{pmatrix} = \begin{pmatrix} \langle \Phi_1 | H - E | \mathcal{I}_\alpha \rangle \\ \langle \Phi_2 | H - E | \mathcal{I}_\alpha \rangle \\ \vdots \\ \langle \mathcal{I}_\alpha \rangle | H - E | \mathcal{O}_\alpha \rangle \end{pmatrix}$$

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- Linear system

  standard numerical methods LAPACK

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