Elastic scattering using artificial confining potentials

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1. Structure of this poster

Want to extract scattering information from bound state programs with minimal extra work. First diagonalize Hamiltonian within artificial confining potential. Initially used stabilization to extract phase shifts, but something better came along.

1. Stabilization I and II

2. Stabilization results, Ps-H, Ps-Ps, Ps-He.

3. The confined variational method (CVM). The positive energy of a pseudo-state inside a confining potential can be easily related to the phase shift when confining potential is removed.
2. What is Stabilization?

Diagonalize the Hamiltonian with a basis of square-integrable $L^2$ functions.

\[
\left( -\frac{\nabla^2}{2} + V(r) \right) \Psi(r) = E \Psi(r)
\]

\[
\Psi(r) = \sum_i c_i \psi_i(r)
\]

The positive energy solutions with $E > 0$ give a reasonable approximation to the exact continuum wave function with $E$ over a finite range. (A.U. Hazi, Phys.Rev. A 1 1109 (1970))

Get phase shift from fitting the wave functions.
3. Stochastic variation method (SVM)

In the SVM, wave functions are expanded as a linear combination of explicitly correlated gaussians (ECG). All the integrals involved in determining the energy have simple analytic forms.

\[
\Psi = \sum_i c_i \exp \left( -\frac{1}{2} \sum_{j<k} A_{jk}^i \mathbf{r}_j \cdot \mathbf{r}_k \right) = \sum_i c_i \exp \left( -\sum_{j<k} B_{jk}^i (\mathbf{r}_j - \mathbf{r}_k)^2 \right)
\]

The gaussian form is not the best form to represent the inter-particle interactions. But it is possible to get a very good wave function if enough terms are included and the exponents are carefully chosen.

Exponents optimized by trial and error. Reasonably quick convergence of electron-positron correlations achieved. Dimension of basis \(\approx 100-2000\).
4. Stabilization version I and II

The basis functions ECGs are divided into two classes *inner* basis and *outer* basis. In stabilization II add confining potential

\[ V_{CP} = \lambda r^n \]

to localize ECGs near scattering center (\( \lambda = 10^{-19} \) and \( n = 12 \))

The *inner* basis is designed to represent the wave function in the interaction region, when all particles are close together. Basis generated by SVM.

The *outer* basis is designed to represent the wave function in the asymptotic region. Designed to give a description of \( \sin(kr) \) between receding particles at asymptotic distances. Constructed as linear combinations of ECGs.
5. Stabilization I, II: Scattering information

- Combine inner and outer basis set of ECGs
- Remove ECGs which cause the linear dependence (stabilization I only).
- Diagonalize wave function and keep low energy states with $E_n = k_n^2/2$.
- Compute the overlap of wave functions of target and the whole system. Example for $e^+\text{-H}$ system.

$$F_n(r_0) = \int d^3 r_1 \, \Psi_n(r_0, r_1) \phi_H(r_1)$$

- Perform a least squares fit of $A \sin(kr_0 + \delta)$ to $F_n(r_0)$ for a finite range outside of the interaction region.
6. Stabilization II: Test $e^+H$ scattering

The $s$-wave phase shift for positron scattering from atomic hydrogen is a good first test.

The scattering lengths were

$$A_{\text{exact}} = -2.104 \ a_0$$
$$A_{\text{stab}} = -2.094 \ a_0$$

Stabilization II fluctuations smaller than those of Stabilization I.

Line is fit to Bhatia et al.

- J.Y.Zhang and J.Mitroy, PRA under review.
7. Stabilization II: Ps-He scattering

The size of the inner basis was 1600.

The scattering lengths were

\[ A_{\text{stab}} = 1.566 \, a_0 \]
\[ A_{\text{QMC}} = 1.40 \, a_0 \]

Stabilization I with a model potential gave

\[ A = 1.57 \pm 0.08 \, a_0 \]

- QMC = quantum Monte Carlo (S. Chiesa *et al* 66 042502 (2002)).
- (5 experiments, with widely differing estimates of scattering length have been done)
8. Stabilization II: Ps-He Pick-off annihilation

The positron can undergo $2\gamma$ annihilation with electrons in the helium target. Experimental parameter is $^1Z_{\text{eff}}$.

The zero energy $^1Z_{\text{eff}}$ was

$$^1Z_{\text{eff}} = 0.1157$$

Experimentally, one has $0.125(2)$ (at $k \approx 0.07 \ a_0^{-1}$). Other experiments gave $0.118(16)$, $0.116(4)$ and $0.129(6)$.

- Coleman et al, JPB 8 L185 (1975).
- Canter et al PRA 12 375 (1975).
### 9. Stabilization Summary

<table>
<thead>
<tr>
<th>System</th>
<th>Quantity</th>
<th>Method</th>
<th>Value</th>
<th>Other</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e^+H$</td>
<td>$A$</td>
<td>Stabil. II</td>
<td>$-2.094$</td>
<td>$-2.104$ Kohn 1974</td>
</tr>
<tr>
<td>$e^+H$</td>
<td>$Z_{\text{eff}}(k = 0)$</td>
<td>Stabil. II</td>
<td>8.75</td>
<td>8.88 Kohn 1974</td>
</tr>
<tr>
<td>$e^+\text{He}$</td>
<td>$A$</td>
<td>Stabil. II</td>
<td>$-0.480$</td>
<td>$-0.50$ Kohn 1995</td>
</tr>
<tr>
<td>$e^+\text{He}$</td>
<td>$Z_{\text{eff}}(k = 0)$</td>
<td>Stabil. II</td>
<td>3.956</td>
<td>3.932 Kohn 1996</td>
</tr>
<tr>
<td>Ps – H Sing</td>
<td>$A$</td>
<td>Stabil. II</td>
<td>4.339</td>
<td>4.319 Kohn 2003</td>
</tr>
<tr>
<td>Ps – H Trip</td>
<td>$A$</td>
<td>Stabil. II</td>
<td>2.126</td>
<td>2.126 Kohn 2003</td>
</tr>
<tr>
<td>Ps – He</td>
<td>$A$</td>
<td>Stabil. II</td>
<td>1.566</td>
<td>1.40 QMC 2002</td>
</tr>
<tr>
<td>Ps – He</td>
<td>$Z_{\text{eff}}(k = 0)$</td>
<td>Stabil. II</td>
<td>0.1157</td>
<td>0.125(2) Exp. 1975</td>
</tr>
<tr>
<td>Ps – Ps Sing</td>
<td>$A$</td>
<td>Stabil. I</td>
<td>8.44</td>
<td>9.14 QMC 2001</td>
</tr>
<tr>
<td>Ps – Ps Trip</td>
<td>$A$</td>
<td>Stabil. I</td>
<td>3.00</td>
<td>3.02 QMC 2001</td>
</tr>
</tbody>
</table>
10. The box variational method

The energy shifts of a particle in an infinite sided box can be used to generate the phase shifts. (I.C. Percival, Proc.Phys.Soc A 70 494 (1957))

$$\left( -\frac{\nabla^2}{2} + V(r) \right) \Psi(r) = E\Psi(r)$$

Solution of unconfined positive energy Schrodinger at $E_n$ is the same for $r < R_0$.

For $V = 0$ one has

$$E_n = \frac{n^2 \pi^2}{2R_0^2}$$

$$\Psi_n(r = R_0) = 0$$

$$\Psi_n(r) = \sin(k_nR_0+\delta_n) = 0 ; r > R_0$$

$$k_nR + \delta = m\pi \Rightarrow \delta_n = m\pi - k_nR_0$$

The phase shift can be extracted from the shift of the energy. Foundation for scattering calculations using Quantum Monte Carlo.
11. The confined variational method (CVM)

Cannot use $V = \infty$ wall with SVM, use sloped wall. Will get phase shift from energy inside confining potential.

- Diagonalize the Hamiltonian in a finite region of space defined by a confining potential.
- $V_1(r)$ represents a general many body potential
- $\lambda V_2(r)$ is a simple model potential
- $V_1(R_0) \approx \lambda V_2(R_0) \approx 0$

- $W_{CP}(r) = A \Theta(r - R_0)g(r - R_0) = A \Theta(r - R_0)(r - R_0)^2$ is the confining potential. $\Theta(r)$ is the Heaviside function, so $W_{CP}(r - R_0) = 0$ for $r < R_0$.
- Matrix elements of $\Theta(r - R_0)(r - R_0)^2$ easy to calculate with ECGs. Essentially, one dimensional integral which is done numerically.
12. The CVM: Fundamental theorem

If the positive energies of the two eigenstates of the Schrödinger equations

\[
\left(-\frac{\nabla^2}{2} + V_1(r) + W_{\text{CP}}(r)\right) \Psi_1(r) = E_1 \Psi_1(r)
\]
\[
\left(-\frac{\nabla^2}{2} + \lambda V_2(r) + W_{\text{CP}}(r)\right) \Psi_2(r) = E_2 \Psi_2(r)
\]

\[E_1 = E_2 \quad (E_1 > 0)\]

are the same, the phase shifts of the two continuum Schrödinger equations at that energy

\[
\left(-\frac{\nabla^2}{2} + V_1(r)\right) \Psi(r) = E_1 \Psi(r)
\]
\[
\left(-\frac{\nabla^2}{2} + \lambda V_2(r)\right) \Psi(r) = E_1 \Psi(r)
\]

must be the same.
13. **CVM: Energy → phase shift**

- SVM of many body problem under $W_{CP}(R)$ giving $E_1$.
- Solve for $\lambda V_2(r)$ under $W_{CP}(R)$ to give $E_2$.
- Tune $\lambda$ so that $E_2 = E_1$.
- Integrate $\lambda V_2(r)$ to get phase shift.

**Alternatives**

- Boundary Condition (BC) Method. $\cot(kR_0 + \delta) = \frac{1}{\Psi(R_0)} \left( \frac{d\Psi(r)}{dr} \right)_{r=R_0}$. Relies on local values of wave function being accurate at $r = R_0$. (Note: Guerout et al *JPB* 37 3043 (2004))

- Improved stabilization Method. Use $W_{CP}(R)$ instead of $\lambda r^{12}$ to generate the inner basis. The confining potential is now zero for $r < R_0$. 
14. CVM: Advantages and disadvantages

- Advantages:
  - Phase shift converges monotonically since energy converges monotonically.
  - Phase shift is accurate to $(\delta \psi)^2$ due to the use of variational energy.
  - Only need to solve the bound-state problem for the full many body interaction.
  - Polarization effects: $-\frac{\alpha d}{2r^4}$ can be added to $\lambda V_2(r)$.

- Disadvantages:
  - Cannot always predetermine the energy at which the phase shift will be generated.
  - Only useful for low energy elastic scattering.
15. Validation for simple potentials

- Let \( V_1(r) = -\exp(-1.4r) \)
- Confining potential \( W_{CP}(r) = 3 \times 10^{-4}(r - 16)^2 \)
- Choose \( \lambda V_2(r) = \lambda(\exp(-r^2) + r \exp(-2r)) \)
- Energy of \( V_1 \) given in LTO basis. Tune \( \lambda \) until \( \lambda V_2 \) has same energy.
- Get \( \delta_{CVM} \) by integrating \( \lambda V_2 \)
- \( \delta_{exact} \) generated by using Numerov method for \( V_1 \) at \( E_N(V_1) \).

Table 1: Convergence of energy and phase shift. \( BC \) = boundary condition, \( CVM \) is \( E \to \delta \) conversion.

<table>
<thead>
<tr>
<th>( N )</th>
<th>( E_N(V_1) )</th>
<th>( \delta_{exact,E} )</th>
<th>( \delta_{BC,N} )</th>
<th>( \delta_{CVM,N} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 1.12819841263 \times 10^{-2} )</td>
<td>0.4773965</td>
<td>0.5309627</td>
<td>0.4773945</td>
</tr>
<tr>
<td>30</td>
<td>( 7.45477054765 \times 10^{-3} )</td>
<td>0.4199395</td>
<td>0.4147941</td>
<td>0.4199395</td>
</tr>
<tr>
<td>40</td>
<td>( 7.41813844495 \times 10^{-3} )</td>
<td>0.4193230</td>
<td>0.4194748</td>
<td>0.4193230</td>
</tr>
<tr>
<td>50</td>
<td>( 7.41813787171 \times 10^{-3} )</td>
<td>0.4193230</td>
<td>0.4193572</td>
<td>0.4193230</td>
</tr>
</tbody>
</table>
16. Electron-Hydrogen scattering, $^1S^e$ channel

- $A = 6.3790665 \times 10^{-5}$, $R_0 = 19 \ a_0$, $N$ = number of ECGs

- Energies of three lowest states optimized.


- CK = Complex Kohn (Bhatia and Temkin 2001 *Phys. Rev. A* 64 032709)

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E_{1,N}$</th>
<th>$E_{3,N}$</th>
<th>$k_{3,N}$</th>
<th>$\delta_{\text{CVM},3,N}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>125</td>
<td>$-0.52774883$</td>
<td>$-0.47999857$</td>
<td>0.2000072</td>
<td>2.06663</td>
</tr>
<tr>
<td>175</td>
<td>$-0.52775029$</td>
<td>$-0.47999983$</td>
<td>0.2000009</td>
<td>2.06692</td>
</tr>
<tr>
<td>225</td>
<td>$-0.52775070$</td>
<td>$-0.48000000$</td>
<td>0.2000000</td>
<td>2.06697</td>
</tr>
<tr>
<td>265</td>
<td>$-0.52775072$</td>
<td>$-0.48000006$</td>
<td>0.1999997</td>
<td><strong>2.06698</strong></td>
</tr>
<tr>
<td>Exact $H^-$ , CK</td>
<td>$-0.52775102$</td>
<td></td>
<td></td>
<td>2.06678(20)</td>
</tr>
<tr>
<td>Kohn</td>
<td></td>
<td></td>
<td></td>
<td>2.0673(9)</td>
</tr>
</tbody>
</table>
17. Electron-Hydrogen scattering, $^3S^e$ channel

- $A = 9.1599714 \times 10^{-5}$, $R_0 = 18.0 \ a_0$, $N =$ number of ECGs

- Energies of two states optimized.


<table>
<thead>
<tr>
<th>$N$</th>
<th>$E_{2,N}$</th>
<th>$k_{2,N}$</th>
<th>$\delta_{\text{CVM},2,N}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>-0.479999738</td>
<td>0.2000131</td>
<td>-0.42463</td>
</tr>
<tr>
<td>125</td>
<td>-0.479999913</td>
<td>0.2000043</td>
<td>-0.42427</td>
</tr>
<tr>
<td>150</td>
<td>-0.479999970</td>
<td>0.2000015</td>
<td>-0.42416</td>
</tr>
<tr>
<td>175</td>
<td>-0.479999994</td>
<td>0.2000003</td>
<td>-0.42411</td>
</tr>
<tr>
<td>200</td>
<td>-0.48000000</td>
<td>0.2000000</td>
<td>-0.42410</td>
</tr>
<tr>
<td>240</td>
<td>-0.48000002</td>
<td>0.1999999</td>
<td><strong>-0.42409</strong></td>
</tr>
</tbody>
</table>

CK                  -0.42418(20)

Kohn                -0.4245(5)
18. Positron-Hydrogen scattering

- $A = 1.35898799 \times 10^{-4}$, $R_0 = 18 \ a_0$, $N =$ number of ECGs

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E_{1,N}$</th>
<th>$k_{1,N}$</th>
<th>$\delta_{\text{CVM},1,N}$</th>
<th>$Z_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>-0.49499792</td>
<td>0.1000208</td>
<td>0.14749</td>
<td>7.174</td>
</tr>
<tr>
<td>150</td>
<td>-0.49499969</td>
<td>0.1000031</td>
<td>0.14803</td>
<td>7.304</td>
</tr>
<tr>
<td>200</td>
<td>-0.49499986</td>
<td>0.1000014</td>
<td>0.14809</td>
<td>7.364</td>
</tr>
<tr>
<td>250</td>
<td>-0.49499993</td>
<td>0.1000007</td>
<td>0.14811</td>
<td>7.342</td>
</tr>
<tr>
<td>300</td>
<td>-0.49499998</td>
<td>0.1000002</td>
<td>0.14812</td>
<td>7.370</td>
</tr>
<tr>
<td>350</td>
<td>-0.49499999</td>
<td>0.1000001</td>
<td>0.14813</td>
<td>7.390</td>
</tr>
<tr>
<td>400</td>
<td>-0.49500000</td>
<td>0.1000000</td>
<td><strong>0.14813</strong></td>
<td><strong>7.392</strong></td>
</tr>
<tr>
<td>COP</td>
<td></td>
<td></td>
<td>0.1483(2)</td>
<td>7.363</td>
</tr>
<tr>
<td>Kohn</td>
<td></td>
<td></td>
<td>0.1479</td>
<td>7.568</td>
</tr>
</tbody>
</table>
19. $e^{-}\text{He}$ scattering

- $A = 1.05996 \times 10^{-4}$, $R_0 = 18\ a_0$, $N =$ number of ECGs
- Kohn = Kohn variational, CI type basis (Nesbet 1979 *PRA* 20 58)
- MCHF = Multi Configuration Hartree-Fock (Saha 1993 *PRA* 48 1163)

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E_{2,N}$</th>
<th>$k_{2,N}$</th>
<th>$\delta_{\text{CVM,2,N}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>$-2.88371629$</td>
<td>0.2000404</td>
<td>$-0.26658$</td>
</tr>
<tr>
<td>800</td>
<td>$-2.88372079$</td>
<td>0.2000179</td>
<td>$-0.26570$</td>
</tr>
<tr>
<td>1000</td>
<td>$-2.88372241$</td>
<td>0.2000098</td>
<td>$-0.26540$</td>
</tr>
<tr>
<td>1200</td>
<td>$-2.88372284$</td>
<td>0.2000077</td>
<td>$-0.26532$</td>
</tr>
<tr>
<td>1240</td>
<td>$-2.88372410$</td>
<td>0.2000014</td>
<td>$\mathbf{-0.26507}$</td>
</tr>
<tr>
<td>Kohn</td>
<td>0.200</td>
<td>$-0.2655(6)$</td>
<td></td>
</tr>
<tr>
<td>MCHF</td>
<td>0.200</td>
<td>$-0.2630$</td>
<td></td>
</tr>
</tbody>
</table>
\textbf{20. }$e^+\text{He}$ scattering

- $A = 1.17558 \times 10^{-4}$ , $R_0 = 17 \ a_0$ , $N =$ number of ECGs

- Kohn = Kohn variational (Campeanu and Humberston, 1977 \textit{JPB} 20 L153, van Reeth and Humberston, 1996 \textit{JPB} 29 L465). Note $Z_{\text{eff}}$ is taken from a fitted curve which has an incorrect functional form.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E_{2,N}$</th>
<th>$k_{2,N}$</th>
<th>$\delta_{\text{CVM,2},N}$</th>
<th>$Z_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>$-2.88371387$</td>
<td>0.2000525</td>
<td>0.03868</td>
<td>3.441</td>
</tr>
<tr>
<td>800</td>
<td>$-2.88372000$</td>
<td>0.2000219</td>
<td>0.03981</td>
<td>3.481</td>
</tr>
<tr>
<td>1000</td>
<td>$-2.88372182$</td>
<td>0.2000128</td>
<td>0.04015</td>
<td>3.484</td>
</tr>
<tr>
<td>1200</td>
<td>$-2.88372245$</td>
<td>0.2000096</td>
<td>0.04026</td>
<td>3.487</td>
</tr>
<tr>
<td>1240</td>
<td>$-2.88372389$</td>
<td>0.2000024</td>
<td>\textbf{0.04053}</td>
<td>\textbf{3.485}</td>
</tr>
<tr>
<td>Kohn</td>
<td>0.20</td>
<td>0.041</td>
<td>3.499</td>
<td></td>
</tr>
</tbody>
</table>
21. Summary

- Bound state calculations give a good description of wave functions in the interaction region.
- Stabilization II. Good to \( \sim 1-2\% \) accuracy. First realistic \textit{ab-initio} calculation of pick-off annihilation for \( \text{Ps-He} \) system.
- Confined Variational Method (CVM) superior to Stabilization II. Use the correspondence between the energy of a confined system and the phase shift of the unconfined system.
- Benchmark numbers for \( e^{\pm}\text{H} \) and and \( e^{\pm}\text{He} \) scattering. Present phase shifts are about an order of magnitude more precise.
- The basic numerical calculations for CVM use a bound state program with a minor modification.
- Dealing with a target that is a many body system is not an issue.
22. The future?

- The CVM is a good tool for studying scattering by composite systems since ECG basis permits all integrals to be done easily. Currently energy range is $E \leq 1 \text{ eV}$. 
- Practically any method of doing bound state calculations can be exploited to give elastic cross section at close to zero energy.
- The SVM has been used to describe electronic structure of small molecules. Accurate calculations for $e^{\pm\text{Molecule}}$ scattering are now possible. No definitive calculation (e.g. 1% accuracy) of $e^{\pm\text{Molecule}}$ scattering, even for the $\text{H}_2$ system in the fixed nucleus approximation.
- Able to do scattering calculations at similar scope and scale to the biggest bound state calculations. CVM is useful for scattering systems that were previously inaccessible.
- Adaption of Quantum chemistry codes to give phase shifts in the elastic scattering region?