Continuum and bound states

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Great progress in ab initio approach to bound states starting from realistic interactions

Predictability

Problems involving continuum states are still difficult esp. with realistic interactions

Application of bound state technique to continuum problem
Reducing the continuum problem to a class of bound-state problems in which \( L^2 \) basis functions are employed

References:
Various problems including continuum states

- Decay of resonance
  \[ A^* \rightarrow B+b, \ C+d+e \]

- Strength (response) function due to perturbation \( W \)
  \[ A+W \rightarrow A^*, \ B+b, \ C+d+e \]

- Radiative capture reactions
  \[ A+a \rightarrow C+W(\gamma) \]
  (Inverse process: \( C+W \rightarrow A+a \))

- Two-body scattering and reactions
  \[ A+a \rightarrow B+b \]
1. Methods of strength function calculation

\[ S(E) = \sum_\nu |\langle \Psi_\nu |W|\Psi_0 \rangle|^2 \delta(E_\nu - E) \]

\[ = \langle \Psi_0 |W^\dagger \delta(H - E)W|\Psi_0 \rangle \]

\[ = -\frac{1}{\pi} \text{Im} \langle \Psi_0 |W^\dagger G(E + i\epsilon)W|\Psi_0 \rangle \]

This formulation is known for many years to include continuum effects

Shlomo & Bertsch, Recently Matsuo, Khan et al., others

It is limited to the case of single-particle in continuum, based on a mean field theory

Extension to more general case is desired
Double photoionization of two-electron atom
Exterior complex scaling
No application yet so far in nuclear physics

**Driven equation of motion method**

\[
S(E) = - \frac{1}{\pi} \text{Im} \langle \Psi_0 \vert W^\dagger \mathcal{G}(E + i\epsilon) W \vert \Psi_0 \rangle
\]

\[
\Psi = \mathcal{G}(E + i\epsilon) W \Psi_0
\]

\[
S(E) = \frac{1}{\pi} \text{Im} \langle \Psi \vert W \vert \Psi_0 \rangle
\]

\[
(H - E)\Psi = -W\Psi_0
\]

Outgoing-wave boundary condition
Continuum is made to damp asymptotically.

Complex scaling method

\[ U(\theta) \quad x \rightarrow e^{i\theta} x \]

\[
S(E) = -\frac{1}{\pi} \text{Im} \langle \Psi_0 | W^\dagger U^{-1}(\theta) R(\theta) U(\theta) W | \Psi_0 \rangle
\]

\[
R(\theta) = U(\theta) G(E + i\epsilon) U^{-1}(\theta) = 1/(E - H(\theta) + i\epsilon)
\]

\[
H(\theta) \Psi^\lambda(\theta) = E^\lambda(\theta) \Psi^\lambda(\theta)
\]

Non-Hermitian, but can be diagonalized in \(L^2\) basis.
Stability of \(S(E)\) wrt \(\theta\) is examined.
L(\(z\)) is finite, hence the norm of \(\Psi(\tau)\) is finite, so that \(\Psi(\tau)\) can be obtained in L\(^2\) basis

\[ L(\tau) = \int_{E_{\text{min}}}^{\infty} \frac{S(E)}{(E - \tau)(E - \tau^{*})} dE = \int_{E_{\text{min}}}^{\infty} \frac{S(E)}{(E - E_R)^2 + E_I^2} dE \]

\[ \tau = E_R + iE_I \]

\[ L(\tau) = \langle \Psi_0 | W^\dagger G(\tau^{*}) G(\tau) W | \Psi_0 \rangle \]

\[ = \langle \Psi(\tau) | \Psi(\tau) \rangle \quad \Psi(\tau) = G(\tau) W \Psi_0 \]

\[ (H - \tau) \Psi(\tau) = - W \Psi_0 \]

L(\(z\)) is finite, hence the norm of \(\Psi(\tau)\) is finite, so that \(\Psi(\tau)\) can be obtained in L\(^2\) basis

L(\(z\)) has to be computed for many \(\tau\) values (\(E_R\) varied, \(E_I\) fixed) to make the inversion possible

**The inversion from L(\(z\)) to S(\(E\)) demands professional skill**
Test in Solvable three-body problem

Hyperscalar potential \( V(\rho) = V_0 \exp(-\kappa \rho^2) \)

\[
\rho^2 = \sum_{i=1}^{3} A_i (r_i - x_3)^2 = \frac{1}{A} \sum_{i<j} A_i A_j (r_i - r_j)^2
\]

One charged particle, two neutral particles

(Numerically) Exactly solvable in Hyperspherical harmonics method

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<th>( V_0 )</th>
<th>( \kappa )</th>
<th>( E_0 )</th>
<th>( \sqrt{\langle \rho^2 \rangle} )</th>
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Electric dipole strength

CDS: calculated from continuum discretized states
CDA: calculated from CDS with tail corrected

Set 1 (Left upper), Set 2 (Left lower), Set 3 (Right upper), Set 4 (Right lower)
Electric dipole strength

Complex scaling method
For a fully-fledged application of complex scaling method
Next talk by W. Horiuchi

Strength functions of $^4\text{He}$
using realistic nuclear interaction
II. Scattering problem

A single-channel case

\[ H \Psi_{JM} = E \Psi_{JM} \]

with appropriate boundary condition

To make use of bound-state technique, we define spectroscopic amplitude (SA)

\[
y(r) = \langle \Phi_{cJM}(r) | \Psi_{JM} \rangle
\]

\[
\Phi_{cJM}(r) = \left[ [\psi_{I1}(\alpha_1)\psi_{I2}(\alpha_2)]_I Y_\ell(\hat{r}_c) \right]_{JM} \frac{\delta(r_c - r)}{r_c r}
\]

Phase shift is determined from the asymptotics of SA
Equation of motion for $y(r)$

\[
\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell + 1)}{r^2} - \frac{2\mu}{\hbar^2} U(r) + k^2 \right] y(r) = \frac{2\mu}{\hbar^2} [z(r) + w(r)]
\]

$z(r) = \langle \Phi_{cJM}(r) \mid V_c - U \mid \Psi_{JM} \rangle$ 

$V_c = \sum_{i \in \alpha_1, j \in \alpha_2} v_{ij}$

$U(r)$: a local potential chosen to make $V_c - U$ vanish for large $r$

$w(r) = \langle \Phi_{cJM}(r) \mid H_{\alpha_1} - E_{\alpha_1} + H_{\alpha_2} - E_{\alpha_2} \mid \Psi_{JM} \rangle$

Formal solution for $y(r)$ with a proper asymptotics

\[
y(r) = \lambda v(r) + \frac{2\mu}{\hbar^2} \int_0^\infty G(r, r') [z(r') + w(r')] r'^2 \, dr'
\]

Exact!

Green’s function \( v(r) \) is a regular solution. \( \lambda \) is a constant to be determined

\[
\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell + 1)}{r^2} - \frac{2\mu}{\hbar^2} U(r) + k^2 \right] G(r, r') = \frac{1}{rr'} \delta(r - r')
\]
\[ H \Psi_{JM} = E \Psi_{JM} \]

Diagonalize in \( L^2 \) basis set to obtain discretized energies and approximate wave functions

\[
\Psi_k = \mathcal{A} \left\{ \left[ \psi_{I_1} (\alpha_1) \psi_{I_2} (\alpha_2) \right] Y_\ell(r) \right\}_{JM} u_k(r) \quad k = 1, 2, \ldots
\]

\[
\Psi_{JM} \sim \sum_k C_k \Psi_k \quad \sum_{k'} (H_{kk'} - EB_{kk'}) C_{k'} = 0
\]

These ‘CDCC’ solutions are expected to be good in the interaction region but have bad asymptotics. Phase shifts are calculated at the discretized energies

\[
z(r) = \langle \Phi_{cJM}(r) \mid V_c - U \mid \Psi_{JM} \rangle \quad y(r) = \langle \Phi_{cJM}(r) \mid \Psi_{JM} \rangle
\]

\( z(r) \) is short-ranged, hence the exact wave function can be replaced with the approximate one in evaluating \( z(r) \). \( \lambda \) is determined by comparing, at short distances, to the approximate \( y(r) \) calculated from this replacement.

Green’s function assures correct asymptotics (GFM)
α+n scattering in a single-channel calculation
microscopic, full antisymmetrization
use of elaborated α wave function
Comparison with R-matrix or empirical p.s.

Effective force (C+LS)

Realistic force (C+T+LS)
Discussion on $\alpha+n$ phase shifts

S-wave phase shifts are reasonable
P-wave phase shifts are too small
Understandable from Pauli principle

$\alpha$: S-wave dominant, D-wave ($< 15\%$)
P-wave neutron can penetrate into $\alpha$
S-wave neutron is repelled by Pauli exclusion

$\alpha$ can be distorted or excited by P-wave neutron particularly through tensor force
This effect cannot be accounted for in a single-channel RGM (Quaglioni & Navratil)

Improving the solution in the interaction region is needed esp. for realistic interactions

1. To add many more channels (standard approach)
2. To solve $A$-body Schroedinger eq. more accurately in a confined region

For detailed analysis for d+d scattering including many distorted channels (method 1)

Talk by S. Aoyama
Cluster breaking effects in four nucleons scattering
Two problems remain:

1. Phase shifts are obtained only at discretized energies. Scattering energy is not under control.
2. Discretized solution is not degenerate, so that coupled-channels problems cannot be solved.

To fix the problems:

Enclose the system within a set of walls and adjust their strength to scattering energy. Only bound state solutions are needed.
Coupled-channels case

\[-\frac{\hbar^2}{2\mu_c} \left( \frac{d^2}{dr^2} - \frac{\ell_c(\ell_c + 1)}{r^2} + k_c^2 \right) u_c(r) + \sum_{c'} \int_0^\infty V_{cc'}(r, r') u_{c'}(r') \, dr' = 0\]

\[V_{cc'}(r, r') = V_{c'c}(r', r)\]

\[V_{cc'}(r, r') = 0 \quad \text{for} \quad r \geq a_c \quad \text{or} \quad r' \geq a_{c'}\]

\[u_c(r) \rightarrow h_c^-(r) \delta_{c,c_0} - S_{cc_0} h_c^+(r)\]

\[\left( \frac{d^2}{dr^2} - \frac{\ell_c(\ell_c + 1)}{r^2} + k_c^2 \right) u_c(r) = \frac{2\mu_c}{\hbar^2} F_c(r)\]

\[F_c(r) = \sum_{c'} \int_0^\infty V_{cc'}(r, r') u_{c'}(r') \, dr'\]
\[ u_c^k(r) = \lambda_c^k v_c(r) + \frac{2\mu_c}{\hbar^2} \int_0^\infty G_c(r, r') F_c^k(r') \, dr' \]

\( \lambda_c^k \) has to be determined \( F_c^k \) has to be given

To reduce to a bound-state problem, add a confining potential

\[ W_c(r) = 0 \quad \text{for } r \leq d_c \quad \quad W_c(r) \to \infty \quad \text{for } r \to \infty \]

\( a_c \leq d_c \)

Solution in the confining potential

\[-\frac{\hbar^2}{2\mu_c} \left( \frac{d^2}{dr^2} - \frac{\ell_c(\ell_c + 1)}{r^2} + k_c^2 \right) w_c(r) + \sum_{c'} \int_0^\infty V_{cc'}(r, r') w_{c'}(r') \, dr' + W_c(r) w_c(r) = 0 \]

- All the solutions become discrete bound states
- Both \( w_c \) and \( u_c \) satisfy the same eq. in the interaction region
- Tuning the strength of the confining potential in each channel generates the needed number of solutions with the same energy
- \( V_{cc'} \) is short-ranged, \( u_c \) can be replaced with \( w_c \) in evaluating \( F_c \)
S-matrix calculation

\[ u_c^k(r) = \lambda_c^k v_c(r) + \frac{2 \mu_c}{\hbar^2} \int_0^\infty G_c(r, r') F_c^k(r') \, dr' \]

\[ \lambda_c^k \] can be determined in the same way as before

A combination of \( u_c^k(r) \) is a desired scattering solution

\[ \sum_k X_{kc_0} u_c^k(r) \to h_c^+(r) \delta_{c, c_0} - S_{cc_0} h_c^+(r) \]

An example of the confining potential

\[ W_c(r) = V_c (r - d_c)^2 \, H(r - d_c) \]

Adjust \( V_c \) to obtain the required energy
Exactly solvable 2-channel model with a Feshbach resonance


\[ \tilde{V} = \frac{2(\kappa_2 - \kappa_1)}{\cosh^2 y} \begin{pmatrix} \kappa_1 & \sqrt{\kappa_1 \kappa_2} \sinh y \\ \sqrt{\kappa_1 \kappa_2} \sinh y & -\kappa_2 \end{pmatrix} \]

\[ y = (\kappa_2 - \kappa_1) r - \arccosh \sqrt{\kappa_1 \kappa_2 / \beta^2} \]

\( \Delta = 10 \)
\( E_R = 7 \)
\( \Gamma = 1 \)
Comparison between the exact and GFM wave functions

\[ w_c(r) = \sum_{i=1}^{N_B} C_i^{(c)} \phi_{\ell c}(a_i^{(c)}, r) \]
Eigenphase rep.

\[ S = \begin{pmatrix} \cos \varepsilon & -\sin \varepsilon \\ \sin \varepsilon & \cos \varepsilon \end{pmatrix} \begin{pmatrix} \exp(2i\delta_1) & 0 \\ 0 & \exp(2i\delta_2) \end{pmatrix} \begin{pmatrix} \cos \varepsilon & \sin \varepsilon \\ -\sin \varepsilon & \cos \varepsilon \end{pmatrix} \]
Conclusion

- Reducing continuum problems to a type of bound-state problems is discussed.

- Complex scaling method appears versatile.

- Both wave functions and S-matrix for coupled-channels scattering problems can be obtained using bound-state codes acting only in external region.

- Correct tail behavior is ensured with Green’s function.

- Application to real problems.
P-wave (K=1) phase shifts
Numerov vs CDA
(continuum-discretized approximation)

Asymptotics corrected with Green’s function
Nucleon-nucleon scattering

$^3S_1 + ^3D_1$ pn scattering

\[
S = \begin{pmatrix}
\exp(i \bar{\delta}_1) & 0 \\ 0 & \exp(i \bar{\delta}_2)
\end{pmatrix}
\begin{pmatrix}
\cos 2\bar{\varepsilon}_J & i \sin 2\bar{\varepsilon}_J \\ i \sin 2\bar{\varepsilon}_J & \cos 2\bar{\varepsilon}_J
\end{pmatrix}
\begin{pmatrix}
\exp(i \bar{\delta}_1) & 0 \\ 0 & \exp(i \bar{\delta}_2)
\end{pmatrix}
\]

Good agreement in wide energy region
$^{3}\text{P}_2 + ^{3}\text{F}_2$ pp scattering

G3RS potential with Coulomb potential

Phase shifts [deg]

$^{3}\text{P}_2$

$^{3}\text{F}_2$

$\bar{\varepsilon}_2$

$E$ [MeV]