Feshbach-Fano-R-matrix (FFR) method

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Outline

- Feshbach-Fano partitioning
- Motivation for the FFR method
- FFR – construction of the discrete state
- FFR – resonance position and width, cross section
- Application to potential scattering
- Application to low-energy electron-molecule scattering
- Conclusions
**Feshbach-Fano projection approach**

- Main idea – decomposition of the T-matrix into the resonant and background part

$$T(\epsilon, \epsilon') = T_{res}(\epsilon, \epsilon') + T_{bg}(\epsilon, \epsilon')$$

- Resonant term $T_{res}$ – corresponds to all rapid variations in the cross section

- Background term $T_{bg}$ – smooth quantity in the energy region of interest, allows for the use of different approximations

- Corresponding separation of the Hilbert space:

$$\mathcal{H} = Q \oplus \mathcal{P}$$

- Projection operator onto the resonant subspace $Q$:

$$Q = |\varphi_d\rangle\langle \varphi_d|$$
**Feshbach-Fano projection approach**

- **Discrete state** \( |\varphi_d\rangle - \) square integrable function, \( \epsilon_d = \langle \varphi_d | H^\Omega | \varphi_d \rangle \)

- **Resonance parameters** \( \Gamma(\epsilon) \) and \( \Delta(\epsilon) \) are determined by the discrete state – continuum coupling

\[
V_{d\epsilon} = \langle \varphi_d | H | \text{bg} \varphi_{\epsilon}^{(+)} \rangle
\]

- **Energy-dependent resonance width and level shift function**

\[
\Gamma(\epsilon) = 2\pi |V_{d\epsilon}|^2
\]

\[
\Delta(\epsilon) = \frac{1}{2\pi} \int \frac{\Gamma(\epsilon')}{\epsilon - \epsilon'} d\epsilon'
\]

- **Resonant part of the T-matrix**

\[
T_{res}(\epsilon) = \frac{1}{2\pi} \frac{\Gamma(\epsilon)}{\epsilon - \epsilon_d - \Delta(\epsilon) + i\Gamma(\epsilon)}
\]
Motivation for the FFR method

- Major drawback of the FF approach – definition of the discrete state is ambiguous

- Calculation of the coupling $V_{d\epsilon}$ is a very difficult task.

- Complex absorbing potential, stabilization methods

- The coupling can be easily extracted from the R-matrix results provided $\varphi_d(r)$ can be expanded in terms of R-matrix basis

- FFR method – general procedure that defines the discrete state and determines its coupling with background continuum.
Expand the discrete state in terms of the R-matrix basis

\[ H^\Omega(r) \phi_k^\Omega(r) = (T + V_{\text{eff}} + L) \phi_k^\Omega = E_k^\Omega \phi_k^\Omega(r) \]

To make it possible we have to restrict \( \varphi_d(r) \) to be not only square integrable but completely contained within the internal region:

\[ \varphi_d(r) = 0 \text{ for } r \geq r_\Omega. \]

\[ \Rightarrow \quad \varphi_d(r) = \sum c_k \phi_k^\Omega(r), \quad \varphi_d(r_\Omega) = \sum c_k \phi_k^\Omega(r_\Omega) = 0 \]

The derivative of \( \varphi_d(r) \) vanish automatically at \( r_\Omega \) because of the properties of the basis:

\[ \frac{d}{dr} \phi_k^\Omega(r) \bigg|_{r=r_\Omega} = 0 \]
Spectra comparison

Energy

V

cross section

R

$E_6^\alpha$

$E_5^\alpha$

$E_4^\alpha$

$E_3^\alpha$

$E_2^\alpha$

$E_1^\alpha$

$E_0^\alpha$
Spectra comparison

Energy

\[ V \]

\[ \Sigma_{\text{res}} \]

\[ \text{cross section} \]

\[ R \]

\[ E_6^\alpha \rightarrow E_5^\alpha \]

\[ E_5^\alpha \rightarrow E_4^\alpha \]

\[ E_4^\alpha \rightarrow E_3^\alpha \]

\[ E_3^\alpha \rightarrow E_2^\alpha \]

\[ E_2^\alpha \rightarrow E_1^\alpha \]

\[ E_1^\alpha \rightarrow E_0^\alpha \]
Construction of the projector onto the background subspace

- $\Sigma_{res}$ – energy region where cross section shows resonance structure.

- Basic idea of the FFR method – similarity of the background Hamiltonian $PHP$ and the model Hamiltonian $^\circ H$

- Existence of the unitary mapping within $\Sigma_{res}$ ($^{bg}E_j^\Omega \in \Sigma_{res}$)

$$^{bg}\phi_j^\Omega (r) = \sum_{^\circ E_l \in \Sigma_{res}} a_{jl} \, ^\circ \phi_l^\Omega (r), \quad \sum_l a_{jl}^* a_{lj} = \delta_{ij}$$

- Outside $\Sigma_{res}$, the R-matrix spectrum is not affected by the presence of the resonance

$$^{bg}\phi_j^\Omega (r) = \phi_j^\Omega (r), \quad E_j^\Omega \notin \Sigma_{res}$$

Feshbach-Fano-R-matrix (FFR) method – p.7/26
Discrete state expansion

- Restricted projector onto the $\mathcal{P}$-subspace

$$P^\Omega = \sum_{^\circ E_j^\Omega \in \Sigma_{res}} |^\circ \phi_j^\Omega \rangle \langle ^\circ \phi_j^\Omega | + \sum_{^\circ E_j^\Omega \notin \Sigma_{res}} |\phi_j^\Omega \rangle \langle \phi_j^\Omega |$$

- Projector onto the resonant subspace $Q = |\varphi_d \rangle \langle \varphi_d |$

$$\varphi_d (r) = \sum_{^\circ E_k^\Omega \in \Sigma_{res}} c_k \phi_k^\Omega (r)$$

- Mutual orthogonality of the $\mathcal{P}$ and $Q$ subspaces: $PQ = 0$

$$\sum_{^\circ E_k^\Omega \in \Sigma_{res}} c_k \langle \phi_k^\Omega | \phi_j^\Omega \rangle = 0 \text{ for } ^\circ E_j^\Omega \in \Sigma_{res}$$
Discrete state expansion

- **Restricted projector onto the P-subspace**

\[
P^\Omega = \sum_{\Omega j \in \Sigma_{\text{res}}} |\phi_j^\Omega\rangle\langle\phi_j^\Omega| + \sum_{\Omega j \notin \Sigma_{\text{res}}} |\phi_j^\Omega\rangle\langle\phi_j^\Omega|
\]

- **Projector onto the resonant subspace** \( Q = |\varphi_d\rangle\langle\varphi_d| \)

\[
\varphi_d(r) = \sum_{\Omega k \in \Sigma_{\text{res}}} c_k \phi_k^\Omega(r)
\]

- **Mutual orthogonality** of the \( P \) and \( Q \) subspaces: \( PQ = 0 \)

\[
\sum_{\Omega k \in \Sigma_{\text{res}}} c_k \langle\phi_j^\Omega|\phi_k^\Omega\rangle = 0 \quad \text{for} \quad \Omega j \in \Sigma_{\text{res}}
\]

\[
\sum_{\Omega k \in \Sigma_{\text{res}}} c_k \phi_k^\Omega(r_{\Omega}) = 0
\]
Equations for the expansion coefficients

- Number of R-matrix levels within $\Sigma_{res}$:
  
  $$\#(E_k^\Omega \in \Sigma_{res}) : \ N$$
  $$\#(^\circ E_j^\Omega \in \Sigma_{res}) : \ N - 1$$

- Homogeneous system of $N$ equations for $N$ coefficients:

  $$\sum_{k=1}^{N} c_k \langle ^\circ \phi_j^\Omega | \phi_k^\Omega \rangle = 0 \quad \text{for} \quad j = 1, \ldots, N - 1$$

  $$\sum_{k=1}^{N} c_k \phi_k^\Omega (r^\Omega) = 0$$

- Non-trivial solution exists only if determinant of the system is zero. This is very restrictive condition for the model system $^\circ H$. 

Feshbach-Fano-R-matrix (FFR) method – p.9/26
Equations for the expansion coefficients

- Number of R-matrix levels within $\Sigma_{res}$:
  \[
  \#(E_k^{\Omega} \in \Sigma_{res}) : N \\
  \#(\phi_j^{\Omega} \in \Sigma_{res}) : N - 1
  \]

- Homogeneous system of $N$ equations for $N$ coefficients:
  \[
  \sum_{k=1}^{N} c_k \langle \phi_j^{\Omega} | \phi_k^{\Omega} \rangle = 0 \quad \text{for} \quad j = 1, \ldots, N - 1
  \]
  \[
  \sum_{k=1}^{N} c_k \phi_k^{\Omega}(r^{\Omega}) = 0
  \]

- Non-trivial solution exists only if determinant of the system is zero. This is very restrictive condition for the model system $\phi^{\Omega}H$.

- Possible problem solving – use of approximative values for the overlap integrals $\langle \phi_j^{\Omega} | \phi_k^{\Omega} \rangle$
Improved Nestmann approximation

- **Objective:** to construct such an approximation for $\langle \phi_\Omega^j | \phi_\Omega^k \rangle$ that the conditions $\varphi_d(r_\Omega) = 0$ and $PQ = 0$ will be linearly dependent.

- Schrödinger equation for the $P$-component of the wave function
  
  $$
  (PHP + PHQ(\epsilon - QHQ)^{-1}QHP) P|\psi_\epsilon\rangle = \epsilon P|\psi_\epsilon\rangle
  $$

- $\Omega$-confined form, $\epsilon = E_\Omega^k$
  
  $$
  \left( b^g H^\Omega + \frac{P^\Omega H^\Omega |\varphi_d\rangle \langle \varphi_d | H^\Omega P^\Omega}{E_\Omega^k - \epsilon_d} \right) P^\Omega |\phi_\Omega^k\rangle = E_\Omega^k P^\Omega |\phi_\Omega^k\rangle
  $$

- Introduce residual potential: $b^g H^\Omega = \circ H^\Omega + V_{rsd}$

- Multiply by $\langle \phi_\Omega^j |$ from left, expand the projector $P^\Omega$

  \[ \downarrow \]
Improved Nestmann approximation

- Final (exact) implicit formula

\[
\langle \phi_j^\Omega \mid \phi_k^\Omega \rangle = \frac{v_{kj} + B_k \langle \phi_j^\Omega \mid H^\Omega \mid \varphi_d \rangle}{E_k^\Omega - E_j^\Omega}
\]

- Interaction of the discrete state with background continuum

\[
B_k = \sum_{\circ E_l^\Omega \in \Sigma_{\text{res}}} \langle \phi_l^\Omega \mid \phi_k^\Omega \rangle \frac{\langle \varphi_d \mid H^\Omega \mid \phi_l^\Omega \rangle}{E_k^\Omega - \epsilon_d}
\]

- Contribution of the residual potential

\[
v_{kj} = \sum_{\circ E_l^\Omega \in \Sigma_{\text{res}}} \langle \phi_l^\Omega \mid \phi_k^\Omega \rangle \langle \phi_j^\Omega \mid V_{rsd} \mid \phi_l^\Omega \rangle
\]
Improved Nestmann approximation

- Final implicit formula

\[
\langle \phi_j^\Omega | \phi_k^\Omega \rangle = B_k \frac{\langle \phi_j^\Omega | H^\Omega | \varphi_d \rangle}{E_k^\Omega - \epsilon^\Omega}
\]

- Interaction of the discrete state with background continuum

\[
B_k = \sum_{\circ E_l^\Omega \in \Sigma_{res}} \langle \phi_l^\Omega | \phi_k^\Omega \rangle \frac{\langle \varphi_d | H^\Omega | \phi_l^\Omega \rangle}{E_k^\Omega - \epsilon_d}
\]

- Contribution of the residual potential

\[
v_{kj} = \sum_{\circ E_l^\Omega \in \Sigma_{res}} \langle \phi_l^\Omega | \phi_k^\Omega \rangle \langle \phi_j^\Omega | V_{rsd} | \phi_l^\Omega \rangle \approx 0
\]
**Improved Nestmann approximation**

- Coefficients $B_k$ are determined from the condition $\varphi_d(r) = 0$ for $r \geq r_\Omega$, which is equivalent to

  $$\left( P\phi_k^\Omega \right)(r) = \phi_k^\Omega(r) \quad \text{for} \quad r \geq r_\Omega,$$

  as

  $$B_k = \left( \sum_{\circ E_i^\Omega \in \Sigma_{res}} \frac{\langle \circ \phi_i^\Omega | H^\Omega | \varphi_d \rangle^{\circ} \phi_i^\Omega(r_\Omega)}{E_k^\Omega - \circ E_i^\Omega} \right)^{-1} \phi_k^\Omega(r_\Omega)$$

- Iterative process, starting from

  $$\varphi_d^{(1)}(r) = \phi_i^\Omega(r)$$

  $$\langle \circ \phi_j^\Omega | H^\Omega | \varphi_d \rangle^{(1)} = E_i^\Omega \langle \circ \phi_j^\Omega | \phi_k^\Omega \rangle^{(0)}$$
Recapitulation of Improved Nestmann approximation

- **Discrete state expansion** is determined in a self-consistent iterative process via solving system of equations

\[
\sum_{E_k^\Omega \in \Sigma_{res}} c_k \langle \circ \phi_j^\Omega | \phi_k^\Omega \rangle = 0 \quad \text{for} \quad \circ E_j^\Omega \in \Sigma_{res}
\]

- In order to ensure \( \varphi_d(r^\Omega) = 0 \) the overlap integrals \( \langle \circ \phi_j^\Omega | \phi_k^\Omega \rangle \) are approximated as

\[
\langle \circ \phi_j^\Omega | \phi_k^\Omega \rangle = B_k \frac{\langle \circ \phi_j^\Omega | H^\Omega | \varphi_d \rangle}{E_k^\Omega - \circ E_j^\Omega}
\]

\[
B_k = \left( \sum_{\circ E_i^\Omega \in \Sigma_{res}} \frac{\langle \circ \phi_i^\Omega | H^\Omega | \varphi_d \rangle \circ \phi_i^\Omega (r^\Omega)}{E_k^\Omega - \circ E_i^\Omega} \right)^{-1} \phi_k^\Omega (r^\Omega)
\]
Advantages of Improved Nestmann approximation

- Influence of the model potential is reduced.

- Difficult and time consuming explicit numerical evaluation of multi-dimensional integrals $\langle \phi_j^\Omega | \phi_k^\Omega \rangle$ is avoided.

- The algorithm requires only the knowledge of the poles $E_k^\Omega$ and $E_j^\Omega$, and amplitudes $\phi_k^\Omega(r_\Omega)$ and $\phi_j^\Omega(r_\Omega)$.

- Possible simplification: $\langle \phi_j^\Omega | H^\Omega | \varphi_d \rangle$ is assumed to be $j$-independent constant. Iterative process is avoided, but the algorithm becomes less stable and strongly dependent on unphysical parameters $r_\Omega$ and $\Sigma_{res}$. 

Feshbach-Fano-R-matrix (FFR) method – p.14/26
Having defined the discrete state \( \varphi_d(r) \), we can construct projector onto the background subspace \( P \)

\[
P^\Omega = 1^\Omega - |\varphi_d\rangle\langle\varphi_d|
\]

- Background R-matrix spectrum

\[
P^\Omega H^\Omega(r) P^\Omega_{bg} \phi^\Omega_l(r) = bg H^\Omega bg \phi^\Omega_l(r) = bg E^\Omega_{l} bg \phi^\Omega_l(r)
\]

- Expansion into original R-matrix basis

\[
bg \phi^\Omega_l(r) = \sum_k b_{lk} \phi^\Omega_k(r)
\]

- Discrete state-continuum coupling (depending on discrete index \( l \))

\[
V^\Omega_{dl} = \langle bg \phi^\Omega_l | H^\Omega | \varphi_d \rangle = \sum_{E_i^\Omega \in \Sigma_{res}} b_{li} E^\Omega_{i} c_i
\]
Discrete state-continuum coupling

- Background scattering states

\[ \psi_{\epsilon}^{(+)}(r) = \frac{1}{2} \sum_k \phi_k(r) \frac{\phi_k^\Omega(r)}{E_k^\Omega - \epsilon} \left( \frac{d}{dr} \psi_{\epsilon}^{(+)}(r) \right) \bigg|_{r=r^\Omega} \]

- Extension of the coupling to continuous energy

\[ V_{d\epsilon} = \langle \varphi_d | H | \psi_{\epsilon}^{(+)} \rangle = \frac{1}{2} \sum_{ki} b_{ki} E_i^\Omega c_i \phi_k^\Omega(r^\Omega) \left( \frac{d}{dr} \psi_{\epsilon}^{(+)}(r) \right) \bigg|_{r=r^\Omega} \]

- Resonance term of the T-matrix is determined by the coupling via \( \epsilon_d, \Gamma(\epsilon) \) and \( \Delta(\epsilon) \).

- Background term of the T-matrix is determined by the background R-matrix

\[ bg R(\epsilon) = \frac{1}{2} \sum_l \left| \frac{\phi_l^\Omega(r^\Omega)}{E_l^\Omega - \epsilon} \right|^2 \]
Application to potential scattering

\[ V(r) = \frac{\lambda}{2} r^2 e^{-R} \]

\[ \hat{V}(r) = \frac{\lambda_0}{4} e^{-(r-3)/2} \]
Application to potential scattering

R-matrix level closest to the resonance, $r_\Omega = 16$

![Graph showing wave function amplitude vs. r](image-url)
Application to potential scattering

Discrete state wave function, $r_\Omega = 16$
Application to potential scattering

Background phase shift, $r_\Omega = 16$

![Graph showing the background phase shift $\delta$ vs energy with different curves for full phase shift, $\delta_{bg}$, NA, and $\delta_{bg}$, INA.](image)
Application to potential scattering

Energy-dependent resonance width, $r_\Omega = 16$

![Graph showing energy-dependent resonance width]
Application to potential scattering

Energy-dependent resonance width, $r_\Omega = 15$

Feshbach-Fano-R-matrix (FFR) method – p.22/26
Application to low-energy electron-Cl$_2$ scattering – SEP level

Fixed-nuclei cross section

\[
\sigma_{FN}(E) \quad \text{vs. Energy [eV]}
\]

- R=3.2 a.u.
- R=3.3 a.u.
- R=3.4 a.u.
- R=3.5 a.u.
- R=3.6 a.u.
Application to low-energy electron-Cl\textsubscript{2} scattering – SEP level

Fixed-nuclei cross section

Energy [eV]

\(\sigma_{bg}(E)\)

\begin{align*}
R=3.2 \text{ a.u.} & \quad \quad \text{solid line} \\
R=3.3 \text{ a.u.} & \quad \quad \text{dotted line} \\
R=3.4 \text{ a.u.} & \quad \quad \text{dashed line} \\
R=3.5 \text{ a.u.} & \quad \quad \text{dotted-dashed line} \\
R=3.6 \text{ a.u.} & \quad \quad \text{dashed line}
\end{align*}

Feshbach-Fano-R-matrix (FFR) method – p.23/26
Application to low-energy electron-Cl$_2$ scattering – SEP level

Background fixed-nuclei cross section

![Graph showing the background fixed-nuclei cross section for different R values.]
Application to low-energy electron-Cl\textsubscript{2} scattering – SEP level

Resonance width and level shift function

![Graph showing resonance width and level shift function with different values of R (a.u.)]
Application to low-energy electron-Cl$_2$ scattering – SEP level

Diabatization of the R-matrix spectrum

Energy [eV] vs. r [a.u.]

- SE target
- SEP discrete state
- R-matrix poles
Conclusions

• The FFR method provides the discrete state, its potential curve and the associated coupling terms to the background continuum.

• It requires \textit{a priori} definition of the energy domain $\Sigma_{res}$ and the model potential.

• It can be applied to systems which can be investigated via the R-matrix method.

• Once the R-matrix calculations are done FFR is computationally very cheap method to analyze the results – only the R-matrix poles $E_k^\Omega$ and $E_j^\Omega$ and amplitudes $\phi_k^\Omega(r_\Omega)$ and $\phi_j^\Omega(r_\Omega)$ are required to obtain the discrete state position and coupling.