Expansion and perturbation methods for the Gamow Shell Model.

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Physical motivation.

In subatomic physics the expansion of many-body wavefunctions on single particle bases has been common practice.

In the traditional shell model the harmonic oscillator has served as a paradigmatic tool for describing bound nuclei.

The recent exploration of nuclear driplines has pushed traditional single particle methods to their limits of applicability.

In the description of weakly bound nuclei, coupling to unbound nuclear states such as resonances and virtual states has to be accounted for.

This may be accomplished by analytic continuation of the Newton completeness relation to the second energy sheet.
Why momentum space?

- Realistic NN - interactions derived from field theory given explicity in momentum space
- Boundary conditions automatically built into the integral equations
- Gamow states are non-oscillating decreasing functions in momentum
- Numerical procedures often easy to implement and check
- Convergence obtained by increasing number of integration points
In natural units $\hbar = c = 1$, the two-body momentum space Schrödinger equation in a partial wave decomposition reads

$$\frac{k^2}{2\mu} \psi_{nl}(k) + \frac{2}{\pi} \int_0^\infty dq q^2 V_l(k, q) \psi_{nl}(q) = E_{nl} \psi_{nl}(k).$$

$V_l(k, k')$ is given by a double Fourier-Bessel transform of the potential in $r$-space:

$$V_l(k, k') = \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 j_l(kr) j_l(k'r') V_l(r, r'). \quad (1)$$

- Hermitian Hamiltonian $\rightarrow$ real eigenvalues.
- Complete set of states forming a Hilbert space ($L^2$ - space)

$$1 = \sum_n |\psi_{nl}\rangle \langle \psi_{nl}| + \frac{1}{2} \int_{-\infty}^{\infty} dk k^2 |\psi_l(k)\rangle \langle \psi_l(k)|.$$
Momentum space Schrödinger equation.

- Resonant and virtual states can never be obtained from a Hermitian Hamiltonian.
- The Hermitian version of the Schrödinger equation is defined on the physical energy sheet.
- The momentum is a multivalued function of energy; \( k(E) = \sqrt{2\mu E} \). Multivalued functions may be represented by Riemann surface or branch cuts.
- Riemann surface with two sheets:
  1. The physical energy sheet is a mapping of the upper half \( k \)-plane.
  2. The non-physical sheet is a mapping of the lower half \( k \)-plane.
Analytic continuation.

To reach into the non-physical energy sheet where anti-bound and resonant states are located, one has to analytic continue the scattering equations through the cut along the real energy axis and into the lower half complex energy plane.

Analytic continuation of the scattering equations into the non-physical energy sheet may be done by the contour deformation method.
The most general Berggren completeness relation on an arbitrary inversion symmetric contour $C = C^+ + C^-$ can be written as

$$1 = \sum_{n \in \mathcal{C}} |\psi_{nl}\rangle \langle \psi_{nl}^*| + \int_{C^+} dk k^2 |\psi_l(k)\rangle \langle \psi_l^*(k)|,$$

Inversion symmetric contours gives

$$\int_{C^-} dk k^2 |\psi_l(k)\rangle \langle \psi_l^*(k)| = \int_{C^+} dk k^2 |\psi_l(k)\rangle \langle \psi_l^*(k)|$$
Contour deformation method

From the general Berggren completeness relation one may deduce the corresponding eigenvalue equation.

\[ \frac{k^2}{2\mu} \psi_{nl}(k) + \frac{2}{\pi} \int_{C^+} dk' k'^2 V_l(k, k') \psi_{nl}(k') = E_{nl} \psi_{nl}(k). \]

General rule: Continuing an integral in the complex plane, the moving singularities of the integrand must not intersect the integration contour. The only moving singularities are given by the interaction potential \( V_l(k, k') \). Choice of \( C^+ \) determined by analytic properties of \( V_l(k, k') \)

- Non-hermitian Hamiltonian \( \rightarrow \) complex eigenvalues
- Bound states invariant under this transformation
- Eigen states form a biorthogonal set.
- Normalization given by the generalized \( c \)-product, \( \langle \psi^*_{nl} | \psi_{n'l} \rangle = \delta_{n,l} \).
The line segment $L_1$ is given by a rotation $z_1 = k_1 \exp(-i\theta)$ and $L_2$ is given by a translation $z_2 = k_2 - ib\sin(\theta)$. May give virtual states in the spectrum.
The Malfliet-Tjon interaction.

The Malfliet-Tjon interaction in a partial wave decomposition reads:

\[
V_l(k, k') = V_R \frac{1}{2kk'}Q_l(x_R) + V_A \frac{1}{2kk'}Q_l(x_A)
\]  \hspace{1cm} (2)

Here \(Q_l(x)\) is a Legendre function of the second kind. The arguments of the Legendre functions are \(x_{R,A} = (k^2 + k'^2 + \mu_{R,A}^2)/2kk'\). Analytic continue Schrödinger equation to the non-physical energy sheet. The Legendre functions are singular for \(x = \pm 1\), and this condition determine the analyticity region of the interaction in the complex \(k\)-plane.

\[
(k \pm k')^2 + \mu_{R,A}^2 = 0,
\]  \hspace{1cm} (3)

which gives:

\[
\text{Re}[k] = \pm\text{Re}[k'] \quad \text{and} \quad \text{Im}[k] = -\mu_{R,A} \pm \text{Im}[k'].
\]
Continuation in the 3’rd quadrant.

Continuation in the third quadrant:
If the translation into the complex $k$-plane exceeds $\mu/2$ it is not possible to construct overlapping domains of analyticity which contain the distorted contour.

\[
\frac{k^2}{2\mu} \psi_{nl}(k) + \frac{2}{\pi} \int_{C^+} dk' k'^2 V_l(k, k') \psi_{nl}(k') = E_{nl} \psi_{nl}(k).
\]
Continuation in the third quadrant:
If the translation into the complex $k$-plane is less than $\mu/2$ it is possible to construct overlapping domains of analyticity which contain the distorted contour.

\[ \frac{k^2}{2\mu} \psi_{nl}(k) + \frac{2}{\pi} \int_{C^+} dk' k'^2 V_l(k, k') \psi_{nl}(k') = E_{nl} \psi_{nl}(k). \]
Virtual states in the M-T interaction.

<table>
<thead>
<tr>
<th>$\nu_A$</th>
<th>Column A Energy</th>
<th>Column B Energy</th>
<th>Column C Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2.6047</td>
<td>-0.066674</td>
<td>-0.066653</td>
<td>-0.066653</td>
</tr>
<tr>
<td>-2.5</td>
<td>-0.310114</td>
<td>-0.310115</td>
<td>-0.310115</td>
</tr>
<tr>
<td>-2.3</td>
<td>-1.229845</td>
<td>-1.229845</td>
<td>-1.229845</td>
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<tr>
<td>-2.1</td>
<td>-2.679069</td>
<td>-2.678979</td>
<td>-2.678979</td>
</tr>
</tbody>
</table>

Calculation of the neutron-proton virtual state as function of increasing attractive strength $\nu_A$ for the $s$-wave Malfliet-Tjon interaction. Column A used $N_1 = 30$, $N_2 = 50$ integration points, column B used $N_1 = 100$, $N_2 = 100$ integration points and column C used $N_1 = 150$, $N_2 = 250$ integration points.
Gamow shell model

Construct antisymmetric many-particle basis based on the single particle Berggren basis.

The unperturbed many-particle energy is the tensorial product of all single particle energies. May be problematic to locate physical resonances.

Choose a suitable contour which separates the many-particle resonances from the dense distribution of complex continuum states. $C_{R+T}$ is a good choice.

$C_{R+T}$ allows for continuation in the third quadrant, i.e. anti-bound states treated on equal footing with bound- and resonant states.
A model example: $^5\text{He}$.

- Unbound nucleus, with two known resonant states moving in $p_{3/2}$ and $p_{1/2}$ orbitals.

- The single particle motion may be described phenomenologically with the SBB - potential, consisting of Gaussian terms.

The SBB potential in momentum space takes the analytic form,

$$V_l(k,k') = V_0 \frac{\pi}{4\alpha^2} \frac{1}{\sqrt{kk'}} \exp\left(-\left(\frac{k^2 + k'^2}{4\alpha^2}\right)\right) I_{l+1/2}\left(\frac{kk'}{2\alpha^2}\right). \quad (4)$$

$I_{l+1/2}(z)$ is a Bessel function of the first kind.

- The SBB-potential diverges exponentially for $|\text{Im}[k]| > |\text{Re}[k]|$. $C_{R}^+$

  $\Rightarrow \theta < \pi/4$.

- A contour of type $C_{R+T}^+$ allows for continuation in the third quadrant.
A model example: $^5$He.

```
<table>
<thead>
<tr>
<th>$n_R$</th>
<th>$n_T$</th>
<th>Re[E]</th>
<th>Im[E]</th>
<th>Re[E]</th>
<th>Im[E]</th>
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<td>-0.329830</td>
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<tr>
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<td>20</td>
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<td>2.154139</td>
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<tr>
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<td>30</td>
<td>0.752476</td>
<td>-0.328033</td>
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<tr>
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<td>40</td>
<td>0.752476</td>
<td>-0.328033</td>
<td>2.154147</td>
<td>-2.912162</td>
</tr>
</tbody>
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```
Two particle resonances in $^6$He.

Expand the two-particle shell model equation in the unperturbed single particle basis:

\[(h_0 + V_{12}) \Psi_{\alpha}^{JM}(1, 2) = E_{\alpha}^{JM} \Psi_{\alpha}^{JM}(1, 2)\]  \hspace{1cm} (5)

\[\Psi_{\alpha}^{JM}(1, 2) = \sum_{a \leq b} C_{a,b}^{J,\alpha} \tilde{\Phi}_{a,b}^{JM}(1, 2)\]  \hspace{1cm} (6)

Here $\tilde{\Phi}_{a,b}^{J}(1, 2)$ is an antisymmetric two-particle basis-state in j-j coupling.

\[\tilde{\Phi}_{a,b}^{J}(1, 2) = \frac{1}{\sqrt{2(1 + \delta a, b)}} \left( \Phi_{a,b}^{J,M}(1, 2) - (-1)^{j_a + j_b - J} \Phi_{b,a}^{J,M}(1, 2) \right)\]  \hspace{1cm} (7)

The two-particle Berggren completeness reads

\[1 = \sum_{a \leq b} |\tilde{\Phi}_{a,b}^{J}(1, 2)\rangle \langle \tilde{\Phi}_{a,b}^{J}(1, 2)|^*\]  \hspace{1cm} (8)
The residual n-n interaction, $V_{12}$, is for simplicity chosen to be of Gaussian type, and separable in $r_1, r_2$.

$$V_{12}(r_1, r_2) = V_0 \exp(-\alpha^2 (r_1^2 + r_2^2)) \sum_\lambda (Y_\lambda(1) \cdot Y_\lambda(2))$$

We fit the interaction strength to reproduce the $0^+$ binding energy ($\approx -0.98\text{MeV}$) in $^6\text{He}$ in both cases.

Observe that position of $2^+$ resonance energy is dependent on the range $\alpha$ of the Gaussian.

The many-particle resonant spectrum is dependent on the radial shape of the interaction, which stresses the need for a realistic derived n-n interaction.
0\(^+\) in \(^6\)He, \(\rho_{3/2}\) s.p. motion.

<table>
<thead>
<tr>
<th>(N_R)</th>
<th>(N_T)</th>
<th>(N_{2p})</th>
<th>(\text{Re}[E])</th>
<th>(\text{Im}[E])</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>12</td>
<td>300</td>
<td>-0.980067</td>
<td>-0.000759</td>
</tr>
<tr>
<td>20</td>
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<td>820</td>
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<td>0.000000</td>
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<td>25</td>
<td>25</td>
<td>1275</td>
<td>-0.979509</td>
<td>0.000000</td>
</tr>
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Convergence of 0\(^+\) bound state energy in \(^6\)He as the number of integration points along the rotated \(C_R\) and the translated part \(C_T\) of the contour increases. \(N_{2p}\) gives the dimension of the two-particle anti symmetrized basis.


\textbf{2$^+$ resonance in $^6\text{He}$, $\rho_{3/2}$ s.p. motion.}

<table>
<thead>
<tr>
<th>$N_R$</th>
<th>$N_T$</th>
<th>$N_{2p}$</th>
<th>Re[E]</th>
<th>Im[E]</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>12</td>
<td>300</td>
<td>1.215956</td>
<td>-0.267521</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>820</td>
<td>1.216495</td>
<td>-0.267745</td>
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<td>25</td>
<td>25</td>
<td>1275</td>
<td>1.216496</td>
<td>-0.267745</td>
</tr>
</tbody>
</table>

Convergence of 2$^+$ resonant state energy in $^6\text{He}$ as the number of integration points along the rotated $C_R$ and the translated part $C_T$ of the contour increases. $N_{2p}$ gives the dimension of the two-particle anti-symmetrized basis.
The choice of contour ($C_{R+T}$) makes transparent all physical two-particle states. One may also do a search for which state that has largest overlap with the unperturbed state where both particles move in single particle resonant states.
0\(^+\) in \(^6\text{He}, \, p_{3/2}, \, p_{1/2}\) s.p. motion.

<table>
<thead>
<tr>
<th>(N_R)</th>
<th>(N_T)</th>
<th>(N_{2p})</th>
<th>(\text{Re}[E])</th>
<th>(\text{Im}[E])</th>
<th>(\text{Re}[E])</th>
<th>(\text{Im}[E])</th>
</tr>
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<tr>
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<td>600</td>
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<td>25</td>
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<td>-0.979148</td>
<td>0.000000</td>
<td>4.286181</td>
<td>-3.882876</td>
</tr>
</tbody>
</table>

Convergence of \(0_{1}^{+}\) bound and the \(0_{2}^{+}\) resonant state energy in \(^6\text{He}\) as the number of integration points along the rotated \(C_R\) and the translated part \(C_T\) of the contour increases. \(N_{2p}\) gives the dimension of the two-particle anti symmetrized basis.
\[ 2_{1,2}^+ \text{ in } ^6\text{He, } p_{3/2}, p_{1/2} \text{ s.p. motion.} \]

<table>
<thead>
<tr>
<th>( N_R )</th>
<th>( N_T )</th>
<th>( N_{2p} )</th>
<th>( \text{Re}[E] )</th>
<th>( \text{Im}[E] )</th>
<th>( \text{Re}[E] )</th>
<th>( \text{Im}[E] )</th>
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<tbody>
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<td>3775</td>
<td>1.150527</td>
<td>-0.203060</td>
<td>2.372817</td>
<td>-2.123254</td>
</tr>
</tbody>
</table>

Convergence of the \( 2_{1}^+ \) and \( 2_{2}^+ \) resonance energy in \(^6\text{He}\) as the number of integration points along the rotated \( C_R \) and the translated part \( C_T \) of the contour increases. \( N_{2p} \) gives the dimension of the two-particle anti symmetrized basis.
$0^+ \text{ strength distribution in } ^6\text{He.}$

Expansion coefficients of the $0^+_{1,2}$ bound and resonant state in $^6\text{He}$. Here $p_{3/2}$ and $p_{1/2}$ single particle states are included.

|        | $|p_{3/2}^2\rangle$ | $|p_{1/2}^2\rangle$ |
|--------|----------------------|----------------------|
|        | Re[$C^2$] | Im[$C^2$] | Re[$C^2$] | Im[$C^2$] |
| RR     | 1.10488 | -0.83161 | 0.22620 | -0.16120 |
| RC     | -0.06036 | 0.88137 | -0.19842 | 0.22423 |
| CC     | -0.09716 | -0.04974 | 0.02486 | -0.06305 |

|        | $|p_{3/2}^2\rangle$ | $|p_{1/2}^2\rangle$ |
|--------|----------------------|----------------------|
|        | Re[$C^2$] | Im[$C^2$] | Re[$C^2$] | Im[$C^2$] |
| RR     | -0.01136 | -0.08003 | 0.90189 | 0.33029 |
| RC     | 0.04282 | -0.03939 | 0.05966 | -0.24478 |
| CC     | 0.00617 | 0.00494 | 0.00082 | 0.02896 |
2\(^+\) strength distribution in \(^6\) He.

Expansion coefficients of the \(2^+_{1,2}\) resonances in \(^6\)He. Here \(p_{3/2}\) and \(p_{1/2}\) single particle states are included.

|       | \(|p^2_{3/2}\rangle\) | \(|p_{3/2}p_{1/2}\rangle\) |
|-------|-------------------------|-----------------------------|
|       | Re[\(C^2\)] | Im[\(C^2\)] | Re[\(C^2\)] | Im[\(C^2\)] |
| RR    | 0.96962     | 0.05539     | 0.11394    | -0.00494    |
| RC    | -0.05247    | -0.02727    | -0.03250   | -0.01265    |
| CC    | -0.00089    | -0.00282    | 0.00229    | -0.00772    |

|       | \(|p^2_{3/2}\rangle\) | \(|p_{3/2}p_{1/2}\rangle\) |
|-------|-------------------------|-----------------------------|
|       | Re[\(C^2\)] | Im[\(C^2\)] | Re[\(C^2\)] | Im[\(C^2\)] |
| RR    | 0.08911      | -0.03742      | 0.88847     | -0.03742    |
| RC    | -0.00175     | -0.02524      | 0.01170     | 0.02338     |
| CC    | 0.00115      | -0.00220      | 0.01131     | -0.00447    |

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Model example: $^7\text{He}$ ($J = 3/2$) resonance.

Three-particle shell model equations in j-j coupling:

$$
\left( h_0 + \sum_{i<j}^3 V_{i,j} \right) \Psi^{JM}_\alpha (1, 2, 3) = E^{JM}_\alpha \Psi^{JM}_\alpha (1, 2, 3)
$$

(9)

The wave function is expanded in a three-particle antisymmetric Berggren basis

$$\Psi^J_\alpha (1, 2, 3) = \sum_{a \leq b \leq c} C^J_{(a,b)c} \tilde{\Phi}^c_{(a,b)c} (1, 2, 3)$$

where the completeness reads:

$$1 = \sum_{a \leq b \leq c} |\langle \tilde{\Phi}^c_{(a,b)c} (1, 2, 3) | \tilde{\Phi}^c_{(a,b)c} (1, 2, 3) \rangle|^2$$

and

$$1 = \sum_{a \leq b \leq c} (C^J_{(a,b)c})^2$$
Model example: $^7\text{He}$ ($J = 3/2$) spectrum.

The $J = 3/2$ energy spectrum of $^7\text{He}$ obtained in a full diagonalization, using only $p_{3/2}$ single particle motion. The shell-model dimension is in this case $N = 9224$. $J = 3/2$ resonance energy: $E = -0.1207 - 0.1222i$ MeV.
Model example: $^7\text{He}$ ($J = 3/2$) resonance.

| $|p_{3/2}^3\rangle$ | Re$[C^2]$  | Im$[C^2]$  |
|---------------------|------------|------------|
| RRR                 | 1.295549   | -0.986836  |
| RRC                 | -0.184544  | 1.099729   |
| RCC                 | -0.115738  | -0.110375  |
| CCC                 | 0.004733   | -0.002518  |

Expansion coefficients of the $3/2^-$ ground state in $^7\text{He}$. Here only $p_{3/2}$ single particle states are included.

Full diagonalization: $E = -0.1207 - 0.1222i$ MeV.

Diag. within $|RRR\rangle, |RRC\rangle, |RCC\rangle$: $E = -0.0677 - 0.0878i$ MeV.
Lee-Suzuki similarity transformation.

For $n \geq 3$ one has to handle the extreme growth of the shell model dimension.

In j-j coupling one has typically,

\[ n_{1p} = 20 - 30 \Rightarrow n_{2p} = 1000 - 3000 \Rightarrow n_{3p} = 10000 - 50000. \]

As continuum-resonance and continuum-continuum couplings play an important role, the configuration mixings in the full-space has to be accounted for in some way.

Construction of a two-particle effective in a reduced space.

The Lee-suzuki similarity transformation for complex interactions.

The multireference perturbation method.
Lee-Suzuki similarity transformation.

Two-body Schrödinger equation:

\[(h_0 + V_{12})|\psi_n\rangle = E_n |\psi_n\rangle\]

We introduce projection operators \(P_{1p}, Q_{1p} \Rightarrow P_{2p}, Q_{2p}\)

\[P = \sum_{\alpha_P} |\alpha_P\rangle \langle \tilde{\alpha}_P|, \quad Q = \sum_{\alpha_Q} |\alpha_Q\rangle \langle \tilde{\alpha}_Q|\]

The two-particle states follows the Berggren metric,

\[\langle \tilde{\alpha}' | \alpha \rangle = \langle \alpha' | \alpha \rangle = \delta_{\alpha', \alpha}\]

And the projection operators fulfill the relations,

\[P^2 = P, \quad Q^2 = Q, \quad P^T = P\]
\[Q^T = Q, \quad P + Q = 1, \quad PQ = 0.\]
Lee-Suzuki similarity transformation.

Construct an effective two-body interaction within the model space, reproducing exactly the $n_P$ eigenvalues of the full Hamiltonian. This can be accomplished by a similarity transformation,

$$
\tilde{H} = e^{-\omega} H e^{\omega}
$$

$\omega$ is defined by $\omega = Q\omega P$, and it follows that $\omega^2 = \omega^3 = \ldots = 0$ and $e^{\omega} = P + Q + \omega$. The two-body Schrödinger equation can then be written in a 2x2 block structure,

$$
\begin{pmatrix}
P\tilde{H}P & P\tilde{H}Q \\
Q\tilde{H}P & Q\tilde{H}Q
\end{pmatrix}
\begin{pmatrix}
P\psi_n \\
Q\psi_n
\end{pmatrix}
= E_n
\begin{pmatrix}
P\psi_n \\
Q\psi_n
\end{pmatrix}
$$

If $P\tilde{H}P$ is to be the two-particle effective interaction the decoupling condition $P\tilde{H}Q = Q\tilde{H}P = 0$ must be fulfilled.
Lee-Suzuki similarity transformation.

The decoupling condition:

\[ QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0 \]

\( \omega \) acts as a transformation P-space to Q-space:

\[
\langle \tilde{\alpha}_Q | \psi_n \rangle = \sum_{\alpha_P} \langle \tilde{\alpha}_Q | \omega | \alpha_P \rangle \langle \tilde{\alpha}_P | \psi_n \rangle.
\]

No unique solution to \( \omega \). \( \omega \) may be obtained as long as the matrix \( \langle \tilde{\alpha}_P | \psi_n \rangle \) is invertible and non-singular. Based on this we choose those \( n_p \) exact solutions with the largest overlap with the two particle model space. With the solution \( \omega \) the non-symmetric effective interaction \( R \) is given by,

\[
R = P\tilde{H}P - Ph_0P = PV_{12}P + PV_{12}Q\omega. \quad (11)
\]
Lee-Suzuki similarity transformation.

It would be preferable to obtain a complex symmetric effective interaction, to take advantage of the anti-symmetrization of the two-particle basis. This may be accomplished by a complex orthogonal transformation:

\[ V_{eff} = U^{-1}(h_0 + V_{12})U - h_0 \]

here \( U \) is complex orthogonal, i.e.

\[ U = \exp(-S), \quad S = \text{arctanh}(\omega - \omega^T) \]
\[ U^T U = UU^T = 1, \quad U^T = U^{-1} \]

*Complex orthogonal transformations* preserves the Berggren metric \( x^T x \) of any vector \( x \) in \( C^n \). This gives the complex symmetric interaction:

\[ V_{eff} = (P + \omega^T \omega)^{1/2}(PHP + PHQ\omega)(P + \omega^T \omega)^{-1/2} - h_0 \]
To obtain the complex symmetric effective interaction, $V_{eff}$, one has to find the matrix square root of $A \equiv (P + \omega^T \omega)$. In the case of $A$ being real and positive semi-definite,

\[ A = X^2, \quad A = ZDZ^T, \quad D = (D)^{1/2}(D)^{1/2}, \quad Z^T Z = ZZ^T = 1 \]
\[ \Rightarrow A = ZD^{1/2}Z^T ZD^{1/2}Z^T, \quad A^{1/2} = ZD^{1/2}Z^T \]

It can be shown that the matrix square root is related to the matrix sign function (N.J.Higham). In the case of $A$ being complex and having all eigenvalues in the open right half complex plane, iterations based on the matrix sign are generally more more stable:

\[
\text{sign} \begin{pmatrix}
0 & A \\
I & 0
\end{pmatrix} = \begin{pmatrix}
0 & A^{1/2} \\
A^{-1/2} & 0
\end{pmatrix}
\]
Lee-Suzuki similarity transformation.

One stable iteration scheme for the matrix sign was derived by Denman and Beavers, as a special case of a method for solving the algebraic Riccati equation:

\[
Y_0 = A, \quad Z_0 = I, \quad (12)
\]

\[
Y_{k+1} = \frac{1}{2}(Y_k + Z_k^{-1}) \quad (13)
\]

\[
Z_{k+1} = \frac{1}{2}(Z_k + Y_k^{-1}), \quad k = 0, 1, 2, \ldots, \quad (14)
\]

provided \( A \) has no non-positive eigenvalues this iteration has quadratic rate of convergence. Typically in our calculations convergence is obtained after 2-3 iterates.
Model example: $^7\text{He}$ resonance.

\[
| (p_{3/2})^3; \ 3/2 \rangle = \frac{1}{6} | (p_{3/2})^2 p_{3/2}; \ 3/2 \rangle - \sqrt{\frac{5}{6}} | (p_{3/2})^2 p_{3/2}; \ 3/2 \rangle
\]

Convergence of the $J = 3/2$ resonance in $^7\text{He}$, using the Lee-Suzuki similarity transformation (solid line), compared with the bare interaction (dashed line). $N_{tot} = 9224$
Multireference perturbation method.

Extensively used in quantum chemistry (Ex.: C. Buth et.al (2003) and Chen et al (2002)). Define a suitable $n$-particle reference (model) space $P$ which describes most of the many-body correlations, and gives a weak coupling between the reference and the complement space.

\[
\begin{pmatrix}
H^{PP} & H^{PQ} \\
H^{QP} & H^{QQ}
\end{pmatrix}
\begin{pmatrix}
P\psi_n \\
Q\psi_n
\end{pmatrix}
= E_n
\begin{pmatrix}
P\psi_n \\
Q\psi_n
\end{pmatrix}
\]

Then we write:

\[
\begin{pmatrix}
H^{PP} & H^{PQ} \\
H^{QP} & H^{QQ}
\end{pmatrix}
= \begin{pmatrix}
H^{PP} & 0 \\
0 & D^{QQ}
\end{pmatrix} + \begin{pmatrix}
0 & H^{PQ} \\
H^{QP} & \tilde{H}^{QQ}
\end{pmatrix}
= H^0 + H^1
\]

Here $D^{QQ}$ is the diagonal part of $H^{QQ}$ and $\tilde{H}^{QQ}$ the off-diagonal part.
Multireference perturbation method.

Diagonalize $H^0$ and obtain the zero-order correction to the exact energy and wavefunction. $\Psi^0 = [\phi^T, 0]^T$ and $E^0 = \phi^T H^{PP} \phi$. We define $M = \phi^T H^{PQ}$ which gives the orthogonal transformation of the coupling block. The energy corrections up to third order may then be shown to be:

\[ E^0_i = \phi^T_i H^{PP} \phi_i, \quad E^1_i = 0 \]

\[ E^2_i = \sum_{j=n_p+1}^N \frac{M^2_{i,j}}{E^0_i - H^0_{j,j}} \]  

(15)

\[ E^3_i = \sum_{j,k=n_p+1}^N \frac{M_{i,j} H^{QQ}_{j,k} M^T_{k,i}}{(E^0_i - H^0_{j,j})(E^0_i - H^0_{k,k})}, \quad j \neq k \]

(16)

(17)
Multireference perturbation method.

3-particle model space used in the multireference perturbation calculations:

\[ P_{3p} \equiv \{|RRR\rangle, |RRC\rangle, |RCC\rangle\}, \tag{18} \]
\[ \text{Re}(e_a + e_b + e_c) < \text{Re}[E]_{\text{cut}}, \tag{19} \]
\[ \text{Im}(e_a + e_b + e_c) > \text{Im}[E]_{\text{cut}}. \tag{20} \]
Convergence of real (left) and imaginary (right) part of \(3/2^-\) resonance in \(^7\)He. The dashed line uses the effective interaction generated by the Lee-Suzuki similarity transformation method, and the solid line uses the multireference perturbation method (mrpm).
Effective interaction scheme for GSM.

Choose an optimal set of $n_{sp}$ single particle states, defining modelspace: $P_{1p}, P_{2p}, ...$.

Construct a two-particle effective interaction (Lee-Suzuki similarity transform) within $P_{2p}$.

Within $P_{3p}$ we define a new three-particle model (and complement) space:

$$P'_{3p} \equiv \{ |RRR\rangle, |RRC\rangle, |RCC\rangle \}, \quad Q'_{3p} \equiv \{ |CCC\rangle \}$$

Use multireference perturbation theory to obtain energy corrections to a specific order.

Start from top with a larger set $P_{1p}$ until convergence is reached.
Convergence of real and imaginary part of $3/2^-$ resonance in $^7$He. The solid line uses the effective interaction generated by the Lee-Suzuki similarity transformation method and subsequently the mcppm, and the dashed line uses the multireference within the full space. 9224 $\rightarrow$ 350.
Conclusions.

- The choice of contour considered, allows for a clear distinction between physical resonant states and the remaining complex-continuum states, even for $n > 3$.

- The shell-model dimension increases dramatically when several valence particles and partial waves are included.

- The clear distinction of unperturbed resonances from the rest, allows for a perturbation treatment of the unperturbed resonant state, when configuration mixing is taken into account.

- Have seen that MCPM combined with the similarity transformation method reduces the dimension of the full problem to about $3 - 4\%$. 
Ongoing work and perspectives.

Why include anti-bound states in many-particle problems? Treating the many-particle problem in some pertubative scheme, we need to define a reference (model) space which describes most of the many-body correlations.

The scheme outlined here, allows for calculation of anti-bound states, and a pertubative treatment many-body states in which anti-bound states are included (Ex. $^{11}\text{Li}$).

Self consistent Hartree-Fock single particle energies and realistic effective interactions (the G-matrix), using the Berggren ensemble may give an understanding of many-body resonances from a microscopic viewpoint.

Solve the problem of vector-transformation brackets for complex momenta.
The charge dependent Bonn potential (CD-Bonn):

- A realistic nonlocal nucleon - nucleon interaction.
- One boson-exchange interaction → Yukawa - terms.
- Given explicitly in momentum space → CDM appropriate.

\[ V(k, q) \propto \sum_{\alpha = \pi^0, \pi^\pm, \rho, \omega, \sigma_1, \sigma_2} \bar{V}_\alpha(k, q) F^2_\alpha(k, q; \Delta_\alpha). \]

Both \( \bar{V}_\alpha(k, q) \) and \( F^2_\alpha(k, q; \Delta_\alpha) \) contain Yukawa terms

\[ \frac{1}{(k - q)^2 + m^2_\alpha}, \]

The poles of the interaction are determined by the various meson masses \( m_\alpha \) and cut-off masses \( \Delta_\alpha \).
Virtual/bound states in CDBonn; $^1S_0, ^3S_1$

Calculation of $^3S_1 - ^3D_1$ bound and $^1S_0$ virtual states using a rotated + translated contour.

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<th>Energy</th>
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Expansion and perturbation methods for the Gamow Shell Model. – p.47/53
Green’s function.

The resolvent (Green’s operator) $g^{II}(\omega)$ and the corresponding free Green’s operator $g_0^{II}(\omega)$ are defined:

$$g_0^{II}(\omega) = \frac{1}{\omega - H_0}, \quad (21)$$

$$g^{II}(\omega) = \frac{1}{\omega - H}. \quad (22)$$

They are related through the Dyson equation

$$g^{II}(\omega) = g_0^{II}(\omega) + g_0^{II}(\omega)V g^{II}(\omega) \quad (23)$$

The physical interpretation of the Green’s functions is that $g_0^{II}$ describes the propagation of two noninteracting particles, and $g^{II}$ describes the propagation of two interacting particles in free space.
By expanding the unit operator on a complete set of physical eigenstates of $H$, we can write the interacting Green’s operator in a spectral decomposition:

$$g^{II}(\omega) = \sum_b \frac{|\psi_b\rangle \langle \psi_b|}{\omega - E_b} + \int_0^\infty dE_c \frac{|\psi_c\rangle \langle \psi_c|}{\omega - E_c}. \quad (24)$$

The Green’s function is analytic on the entire physical energy sheet except at the spectrum of the Hamiltonian, and a branch cut along the positive energy axis:

The discontinuity of the Green’s function across the cut is

$$g^{II}(E + i\eta) - g^{II}(E - i\eta) = -2\pi i |\psi_c\rangle \langle \psi_c|. \quad (25)$$
Green’s function in Berggren basis.

Analytic continuation can be used to extend the values of an analytic function across a branch cut in the complex plane.

Expanding *unity* on a complete set of Berggren states, the Green’s function becomes analytic through the cut, and is extended into the non-physical energy sheet.

The branch cut along the real axis is then transformed onto the deformed contour $C^+$.

\[
g^{II}(\omega) = \sum_i \frac{|\psi_i\rangle\langle\psi_i|}{\omega - E_i} + \int_{C^+} dE_{cc} \frac{|\psi_{cc}\rangle\langle\psi_{cc}|}{\omega - E_{cc}}. \tag{26}
\]

$i \in [a,b,c,d]$, *cc* denotes complex continuum states.
T-matrix in Berggren basis.

The $t$-matrix is defined in terms of the interacting Green’s function:

$$t(\omega) = V + V g^{II}(\omega)V,$$  \hspace{1cm} (27)

Using the Berggren representation for $g^{II}$, and decomposing into partial waves, the $t$-matrix reads:

$$t_l(k, k', \omega) = V_l(k, k') + \frac{4}{\pi^2} \int_{C^+} \int_{C^+} dq' \, dq' \, q^2 q'^2 V_l(k, q) g^{II}(q, q'; \omega) V_l(q', k'),$$

In free space scattering, $\omega$ is defined on the energy shell, $\omega \propto k^2$, here $k, k'$ are real. By an appropriate choice of contour CDM gives an alternative to the standard principal value prescription in solving numerically for the $t$-matrix.
T-matrix for M-T interaction.

\[ t_l(k, k', \omega) = V_l(k, k') + \frac{4}{\pi^2} \int_{C^+} \int_{C^+} dq \ dq' \ q^2 q'^2 V_l(k, q) g^{II}(q, q'; \omega) V_l(q', k'), \]

For \( k, k' > k_{\text{max}} \) the contour \( C_1^+ \) will pass through the singularity of the interaction \( V_l(k, k') \).

\[ \theta < \arctan \left( \frac{\mu}{k_{\text{max}}} \right). \]
T-matrix for M-T interaction.

K_{\text{max}} = 529 \text{ [MeV]}