Effective interactions for reaction calculations

Nuclear Theory & Modeling, LLNL

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**Goal:** Replace phenomenological input for reaction calculations by theoretically predicted quantities in order to enable reaction calculations for areas with little/no available systematics.

**Deliverable:**
Nucleon-nucleus optical model
For use in direct-reaction calculations and in modeling of statistical reactions (compound-nucleus formation).

**Our Strategy:**
- Employ state-of-the-art nuclear theory input (e.g. nuclear structure input from DFT, information on interactions)
- Employ large-scale computational resources to minimize/eliminate those inputs that lump together physics that cannot be described properly with traditional tools (e.g. “channels”)

**Applications**
Reaction predictions

**Structure Model**
Methods: HF, DFT, RPA, CI, CC, ...

**Folding Code**

**Coupled Channels**
Code: FRESCO

**Transitions Code**

**Optical Potential**

**Applications**
Reaction predictions
Large-scale coupled-channels calculations

Practical approach:

- Implement a large-scale coupled-channels framework that is able to exploit the available (predicted) nuclear structure input.
- Develop/determine and test the ingredients that cannot be supplied by DFT.

Coupled-channels equations:

\[ \left\{ E - E_c^{ex} + \frac{\hbar^2}{2\mu_c} \frac{d^2}{dr^2} - \frac{l_c(l_c+1)}{2\mu_c r^2} - V_{cc'}^J(r) \right\} u_c(r) = \sum_{c' \neq c} V_{cc'}^J(r) u_{c'}(r) \]

The coupling potentials \( V_{cc'}^J(r) \) contain information on the structure of the target nucleus and on the effective NN interaction between the projectile (nucleon) and target nucleons, via terms of the type:

\[ \frac{2}{\pi} \int_0^\infty dq \, q^2 \, j_L(qr) \, \nu^{\text{ST}}(q) \, \rho_{L\Sigma J}^T(q) \, f_i(q) \]

Number and type of channels to be coupled determined in large-scale reaction calculations.
(See Nobre talk)

Transition densities for target states, obtained from a nuclear-structure calculation based on DFT results.
(See, e.g., Terasaki talk).

Effective NN interaction between a particle in the continuum and a nucleon in the target - to be determined!
Effective interactions for reaction calculations

Effective interactions:
- Provide crucial link to interactions considered by UNEDF collaboration.
- Have important impact on the outcome of the reaction calculations.
  E.g. their energy and density dependence determine strength of coupling to various channels and energy dependence of reaction cross section.

To be addressed:
- **Need for folding codes**: Formalism and code to convolute relevant interactions with densities to provide coupling potentials for coupled-channels calculations.
- **Which effective interaction?** The same that was employed for the structure calculation? How should it be modified?
- **What is the level of uncertainty** in scattering predictions due to incomplete information about the effective interaction?
- **Can we connect features of effective interactions to specific reaction observables?** If so, can we identify constraints for selecting a good effective interaction?

**Coupling potentials require folding of effective interaction with transition densities (in r or q space):**

\[
\frac{2}{\pi} \int_0^\infty dq \, q^2 \, j_L(qr) \, V_{ST}(q) \, \rho_{LSJ}^{Tq} \, \hat{n}(q)
\]
Progress in Year 3

Progress and findings:

• Developed formalism and code to extend folding procedure to Gogny and density-dependent M3Y interactions, including exchange.
  – Skyrme-type interactions are next.
  – Recently-developed extensions to Skyrme will need to be considered.

• **Studied energy and density dependence of the resulting folding potentials.**
  – Effective interactions considered so far show some differences in energy and density dependence.
  – Scattering is sensitive to behavior at low densities, reaction cross section will test energy dependence.

• Found exchange contributions, as expected, to be very important. Decided that more detailed work is needed:
  – Comparison of exact and approximate treatments (e.g. of the non-local density matrices used) for different interactions guides level of sophistication implemented in CC calculations
  – Are non-local transition potentials needed? How do non-localities due to exchange and dynamic polarization potentials interfere with each other?

• Obtained HFB/QRPA code (Terasaki/Engel) which will allow for wider range of nuclei to be included in our work.
Energy & Density Dependence

From Jeukenne et al., PRC 16 (1977) 80.

Volume integral provides measure for strength of interaction in the nuclear surface; strength impacts reaction predictions.

Gogny interaction - isoscalar, central term

Density-dependent M3Y

\[ F(\rho) = C[1 - \alpha \exp(-\beta \rho)] \]

\[ F(\rho) = C[1 - \gamma \rho] \]
Importance of Exchange

Features:

- Non-local, large and important
- Their size relative to the direct term depends on the type of interaction considered
- Treatment in the context of large coupled-channels calculations requires consideration of:
  - Various possible approximations for non-local density
  - Interference of non-local exchange with non-locality of dynamical polarization potential

Gogny interaction - isoscalar, central term

Gogny interaction - isovector, central term
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Plan for Year 3 and Year 4

Year 3:

- Finalize folding codes; including Skyrme.
- Use transition potentials in large-scale CC calculations & determine sensitivity of cross sections to choice of effective interaction.
- Draw conclusions about proper treatment of exchange terms.

Year 4:

- Extend calculations to additional nuclei, using HFB/QRPA transition densities from Terasaki-Engel code
- Study nucleon scattering for even-even \( ^{40-48}\text{Ca} \) isotopes
- Investigate whether features of effective interactions can be connected to specific reaction observables
- Study in detail interference of non-localities due to exchange terms in effective interactions and to dynamic polarization potential.
- Recommend interactions for reaction calculations.
- Consider extension to deformed systems (to connect to UNEDF effort to develop deformed QRPA code)
Some details...

Nucleon scattering for even-even $^{40-48}$Ca isotopes:

- Scattering data available for all even-even isotopes, for large number of energies.
- Wide range of proton data available.
- Neutron data enhanced by recent measurements at LANL ($^{48}$C).
- Comparison to existing optical model calculations possible.
- Relevant to goal of going to exotic, neutron-rich systems.

From Charity et al., PRL 97 (2006) 162503.
Density dependence of the effective interaction

Constructing diagonal coupling potentials from effective interactions with/without density dependence:

- Effective nucleon-nucleon interaction:
  \[ V(E, \rho, r) = F(\rho) \, v(r) \]

  Where \( v \) is a M3Y interaction
  \[ v(r) = \sum_{i=1,3} G_i \exp(-\mu_i r)/(\mu_i r) + J_{00} \]
  \[ F(\rho) = C(1 + \alpha \exp(-\beta \rho)) \]
  \[ J_{00} = -G_8(1-0.0005E/A) \]

- Density from a Skyrme (SkM*) HF calculation

Coupling potentials compared

\( ^{90}\text{Zr} \)