Why Green’s functions?

Ab initio and

as a framework to analyze experimental data (and extrapolate and predict properties of exotic nuclei)

→ dispersive optical model (DOM)

Focus on recent DOM → DSM developments

Some surprises!

Conclusions
What do nucleons do in the nucleus?

- Shell model from 1949 with residual interaction? Not enough!
- Why do nuclei have the central density they have? Unanswered
- Do they sit in independent-particle model orbits all the time?
- Even electrons do other things some of the time!

Hydrogen 1s wave function “seen” experimentally in (e,2e) reaction

\[
\phi_{1s}(p) = \frac{2^{3/2}}{\pi} \frac{1}{(1 + p^2)^2}
\]

But in other atoms slight deviations!

- Properly executed --> Green’s function answers a question from Sir Denys Wilkinson: “What does a nucleon do in the nucleus?”
Remarks

• Given a Hamiltonian, a perturbation expansion can be generated for the single-particle propagator

• Dyson equation determines propagator in terms of nucleon self-energy

• Self-energy is causal and obeys dispersion relations relating its real and imaginary part

• Data constrained self-energy acts as ideal interface between ab initio theory and experiment
Propagator / Green's function

- Lehmann representation
  \[ G_{\ell j}(k, k'; E) = \sum_m \frac{\langle \Psi_0^A | a_{k\ell j} | \Psi_{m+1}^A \rangle \langle \Psi_{m+1}^A | a_{k'\ell j}^\dagger | \Psi_0^A \rangle}{E - (E_{m+1}^A - E_0^A) + i\eta} \]
  \[ + \sum_n \frac{\langle \Psi_0^A | a_{k'\ell j}^\dagger | \Psi_{n-1}^A \rangle \langle \Psi_{n-1}^A | a_{k\ell j} | \Psi_0^A \rangle}{E - (E_0^A - E_{n-1}^A) - i\eta} \]

- Any other single-particle basis can be used

- Overlap functions \( \rightarrow \) numerator

- Corresponding eigenvalues \( \rightarrow \) denominator

- Spectral function
  \[ S_{\ell j}(k; E) = \frac{1}{\pi} \text{Im} \ G_{\ell j}(k, k; E) \]
  \[ = \sum_n \left| \langle \Psi_{n-1}^A | a_{k\ell j} | \Psi_0^A \rangle \right|^2 \delta(E - (E_0^A - E_{n-1}^A)) \]

- Spectral strength in the continuum
  \[ S_{\ell j}(E) = \int_0^\infty dk \ k^2 \ S_{\ell j}(k; E) \]

- Discrete transitions
  \[ \sqrt{S_{\ell j}^n} \ \phi_{\ell j}^n(k) = \langle \Psi_{n-1}^A | a_{k\ell j} | \Psi_0^A \rangle \]

- Positive energy \( \rightarrow \) see later

reactions and structure
Propagator from Dyson Equation and “experiment”

Equivalent to ...

\[ E_n^- = E_0^A - E_{n}^{A-1} \]

**Self-energy**: non-local, energy-dependent potential

With energy dependence: spectroscopic factors \(< 1\)

\( \Rightarrow \) as extracted from (e,e'p) reaction

\[ \frac{k^2}{2m} \phi_{\ell_j}^n(k) + \int dq \, q^2 \, \Sigma^*_\ell_j(k, q; E_n^-) \, \phi_{\ell_j}^n(q) = E_n^- \, \phi_{\ell_j}^n(k) \]

**Spectroscopic factor**

\[ S_{\ell_j}^n = \int dk \, k^2 \, \left| \langle \Psi_n^{A-1} | a_{k\ell_j} | \Psi_0^A \rangle \right|^2 < 1 \]

Dyson equation also yields

\[ [\chi_{\ell_j}^{elE}(r)]^* = \langle \Psi_{elE}^{A+1} | a_{r\ell_j}^\dagger | \Psi_0^A \rangle \quad \text{for positive energies} \]

**Elastic scattering wave function for protons or neutrons**

Dyson equation therefore provides:

Link between scattering and structure data from **dispersion relations**

reactions and structure
Propagator in principle generates

- Elastic scattering cross sections for p and n
- Including all polarization observables
- Total cross sections for n
- Reaction cross sections for p and n
- Overlap functions for adding p or n to bound states in Z+1 or N+1
- Plus normalization --> spectroscopic factor
- Overlap function for removing p or n with normalization
- Hole spectral function including high-momentum description
- One-body density matrix; occupation numbers; natural orbits
- Charge density
- Neutron distribution
- p and n distorted waves
- Contribution to the energy of the ground state from $V_{NN}$
Dispersive Optical Model

- **Claude Mahaux 1980s**
  - connect traditional optical potential to bound-state potential
  - crucial idea: use the dispersion relation for the nucleon self-energy
  - smart implementation: use it in its subtracted form
  - applied successfully to $^{40}$Ca and $^{208}$Pb in a limited energy window
  - employed traditional volume and surface absorption potentials and a local energy-dependent Hartree-Fock-like potential

- **Radiochemistry group at Washington University in St. Louis:**
  Charity and Sobotka propose to use it for a sequence of Ca isotopes $\rightarrow$ data-driven extrapolations to the drip line
  - First results 2006 PRL
  - Subsequently $\rightarrow$ attention to data below the Fermi energy related to ground-state properties $\rightarrow$ Dispersive Self-energy Method (DSM)
Optical potential \(\longleftrightarrow\) nucleon self-energy

- e.g. Bell and Squires \(\rightarrow\) elastic T-matrix = reducible self-energy
  - relate dynamic (energy-dependent) real part to imaginary part
  - employ subtracted dispersion relation

### General dispersion relation for self-energy:

\[
\text{Re } \Sigma(E) = \Sigma^{HF} - \frac{1}{\pi} \mathcal{P} \int_{E^+_T}^\infty dE' \frac{\text{Im } \Sigma(E')}{E - E'} + \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{E^+_T} dE' \frac{\text{Im } \Sigma(E')}{E - E'}
\]

Calculated at the Fermi energy \(\varepsilon_F = \frac{1}{2} \left\{ (E_{0}^{A+1} - E_0^A) + (E_0^A - E_{0}^{A-1}) \right\}\)

\[
\text{Re } \Sigma(\varepsilon_F) = \Sigma^{HF} - \frac{1}{\pi} \mathcal{P} \int_{E^+_T}^\infty dE' \frac{\text{Im } \Sigma(E')}{\varepsilon_F - E'} + \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{E^+_T} dE' \frac{\text{Im } \Sigma(E')}{\varepsilon_F - E'}
\]

Subtract

\[
\text{Re } \Sigma(E) = \text{Re } \Sigma^{HF}(\varepsilon_F) - \frac{1}{\pi} (\varepsilon_F - E) \mathcal{P} \int_{E^+_T}^\infty dE' \frac{\text{Im } \Sigma(E')}{(E - E')(\varepsilon_F - E')} + \frac{1}{\pi} (\varepsilon_F - E) \mathcal{P} \int_{-\infty}^{E^+_T} dE' \frac{\text{Im } \Sigma(E')}{(E - E')(\varepsilon_F - E')}
\]
Recent local DOM analysis
--> towards global

J. Mueller et al.
PRC83,064605 (2011), 1-32

reactions and structure
Elastic scattering data for protons and neutrons

- Abundant for stable targets
Local DOM ingredients and transfer reactions

- Overlap function
- p and n optical potential
- ADWA (developed by Ron Johnson)
- MSU-WashU:

\[ {^{40,48}}Ca, {^{132}}Sn, {^{208}}Pb(d,p) \]

N. B. Nguyen, S. J. Waldecker, F. M. Nuñes, R. J. Charity, and W. H. Dickhoff

\[
\begin{align*}
E & \quad \text{CH+ws} & \quad \text{DOM} \\
2 & \quad 0.94 & \quad 0.72 \\
13 & \quad 0.82 & \quad 0.67 \\
19.3 & \quad 0.77 & \quad 0.68 \\
56 & \quad 1.1 & \quad 0.70
\end{align*}
\]
$^{132}\text{Sn}(d,p)$

- Does it work when the potentials are extrapolated?

- $E_d = 9.46$ MeV $^{132}\text{Sn}(d,p)^{133}\text{Sn}$
- CH89+ws $\rightarrow S_{1f7/2} = 1.1$
- DOM $\rightarrow S_{1f7/2} = 0.72$
Nonlocal DOM implementation PRL112,162503(2014)

• Particle number --> nonlocal imaginary part
• Microscopic FRPA & SRC --> different nonlocal properties above and below the Fermi energy
• Include charge density in fit
• Describe high-momentum nucleons <-->(e,e'p) data from JLab

Implications

• Changes the description of hadronic reactions because interior nucleon wave functions depend on non-locality
• Consistency test of the interpretation of (e,e'p) possible
• Independent “experimental” statement on size of three-body contribution to the energy of the ground state--> two-body only:

$$E/A = \frac{1}{2A} \sum_{\ell j} (2j + 1) \int_0^\infty dk k^2 \frac{k^2}{2m} n_{\ell j}(k) + \frac{1}{2A} \sum_{\ell j} (2j + 1) \int_0^\infty dk k^2 \int_{-\infty}^{\varepsilon_F} dE \ E S_{\ell j}(k; E)$$
Differential cross sections and analyzing powers

\[ d\sigma/d\Omega [\text{mb/sr}] \]

\[ \theta_{\text{cm}} [\text{deg}] \]

\[ E_{\text{lab}} > 100 \]
\[ 40 < E_{\text{lab}} < 100 \]
\[ 20 < E_{\text{lab}} < 40 \]
\[ 10 < E_{\text{lab}} < 20 \]
\[ 0 < E_{\text{lab}} < 10 \]
Reaction (p&n) and total (n) cross sections

\[ \text{Lab } E \]

\[ \sigma [\text{mb}] \]

\[ \sigma_0 \]

\[ \sigma_1 \]

\[ \sigma_2 \]

\[ \sigma_3 \]

\[ \sigma_\text{tot} \]

\( \text{Ca}^{40} \)

\( \text{p}^{+} \)

\( \text{n}^{+} \)

\( \sigma_\text{react} \)

\( \sigma_\text{tot} \)

\( E_{\text{Lab}} [\text{MeV}] \)
Nonlocal imaginary self-energy:
proton number $\rightarrow 19.88$
neutron number $\rightarrow 19.79$

$S_{0d3/2} = 0.76$
$S_{1s1/2} = 0.78$
0.15 larger than NIKHEF analysis!

$\ell \leq 5$

Below $\varepsilon_F$

$^{40}\text{Ca}$ spectral function

Old $(p,2p)$ data from Liverpool
or $(e,e'p)$ from Saclay

reactions and structure
Linking nuclear reactions and nuclear structure $\rightarrow$ DOM

**Correlations from nuclear reactions**

In $(e,e'p)$ proton still has to get out of the nucleus $\rightarrow$ optical potential

*Nucl. Phys. A553, 297c (1993)*

Consistency study in progress

Different optical potentials $\rightarrow$ different reduction factors $\rightarrow$ for transfer reactions

Spectroscopic factors $> 1$??

**PRL 93, 042501 (2004) HI**

**PRL 104, 112701 (2010) Transfer**

Recent summary $\rightarrow$ Jenny Lee

Different reactions different results??

**PRL 93, 042501 (2004) HI**

**PRL 104, 112701 (2010) Transfer**
Linking nuclear reactions and nuclear structure

- Extracting information on correlations beyond the independent particle model requires optical potentials in \((e,e'p), (d,p),(p,d),(p,pN)\), etc.
- Quality of \textit{ab initio} to describe elastic scattering or optical potentials should be improved substantially and urgently

\[40\text{Ca}\]

\frac{d\sigma}{d\Omega}(E_{\text{c.m.}} = 9.6 \text{ MeV})

\begin{align*}
\text{Coupled cluster calculation using overlap functions} \\
\text{PRC86,021602(R)(2012)} \\
\text{Probably limited to low energy}
\end{align*}

\begin{align*}
\text{Green's function result } \rightarrow \text{ optical potential with emphasis on SRC only} \\
\text{PRC84,044319(2011)}
\end{align*}
High-momentum components

Rohe, Sick et al. JLab data for Al and Fe (e,e'p) per proton
Jefferson Lab data per proton

- Pion/isobar contributions cannot be described
- Rescattering contributes some cross section (Barbieri, Lapikas)
Critical experimental data

Local version
radius correct...
PRC82,054306(2010)

Charge density $^{40}\text{Ca}$
Non-locality essential
PRL112,162503(2014)

High-momentum nucleons $\rightarrow$ JLab can also be described $\rightarrow$ E/A
Historical perspective...

- The following authors identify the single-particle propagator (or self-energy) as central quantities in many-body systems:

  - Abrikosov, Gorkov, Dzyaloshinski
    (Methods of Quantum Field Theory in Statistical Physics, 1963 Dover Revised edition 1975),

  - Pines
    (The Many-body Problem, 1961 Addison Wesley reissued 1997),

  - Nozieres
    (Theory of Interacting Fermi Systems, 1964 Addison-Wesley reissued 1997),

  - Thouless

  - Anderson
    (Concepts in Solids, Benjamin 1963; World Scientific reissued 1998),

  - Schrieffer
    (Theory of Superconductivity, 1964 Benjamin revised 1983),

  - Migdal
    (Theory of Finite Fermi Systems and Applications to Atomic Nuclei (Interscience, 1967),

  - Fetter and Walecka

- but apart from qualitative features, they don’t answer what it looks like for a real system like a nucleus!
Energy of the ground state

- **Energy sum rule** (Migdal, Galitski & Koltun)

\[
\frac{E}{A} = \frac{1}{2A} \sum_{\ell j} (2j + 1) \int_0^{\infty} dk k^2 \frac{k^2}{2m} n_{\ell j}(k) + \frac{1}{2A} \sum_{\ell j} (2j + 1) \int_0^{\infty} dk k^2 \int_{-\infty}^{E_F} dE\ E S_{\ell j}(k; E)
\]

- **Not** part of fit because it can only make a statement about the two-body contribution

- **Result:**
  - DOM ---> 7.91 MeV/A  
  - T/A ---> 22.64 MeV/A
  - 10% of the particles (those with momenta above 1.4 fm-1) provide \( \sim \frac{2}{3} \) of the binding energy!
  - Exp. 8.55 MeV/A
  - Three-body ---> 0.64 MeV/A attraction
  - *Argonne GFMC* \( \sim \) 1.5 MeV/A attraction for three-body \( \leftrightarrow \) *Av18*
Do elastic scattering data tell us about correlations?

- **Scattering T-matrix**
  \[ \Sigma_{\ell,j}(k, k'; E) = \Sigma_{\ell,j}^*(k, k'; E) + \int dq q^2 \Sigma_{\ell,j}^*(k, q; E)G^{(0)}(q; E)\Sigma_{\ell,j}(q, k'; E) \]

- **Free propagator**
  \[ G^{(0)}(q; E) = \frac{1}{E - \hbar^2 q^2 / 2m + i\eta} \]

- **Propagator**
  \[ G_{\ell,j}(k, k'; E) = \frac{\delta(k - k')}{k^2} G^{(0)}(k; E) + G^{(0)}(k; E)\Sigma_{\ell,j}(k, k'; E)G^{(0)}(k; E) \]

- **Spectral representation**
  \[ G_{\ell,j}^p(k, k'; E) = \sum_n \frac{\phi_{\ell,j}^{n+}(k) \left[ \phi_{\ell,j}^{n+}(k') \right]^*}{E - E_n^{A+1} + i\eta} + \sum_c \int_{T_c}^\infty dE' \frac{\chi_{cE'}_{\ell,j}(k) \left[ \chi_{cE'}_{\ell,j}(k') \right]^*}{E - E' + i\eta} \]

- **Spectral density**
  \[ S_{\ell,j}^p(k, k'; E) = \frac{i}{2\pi} \left[ G_{\ell,j}^p(k, k'; E^+) - G_{\ell,j}^p(k, k'; E^-) \right] = \sum_c \chi_{cE}_{\ell,j}(k) \left[ \chi_{cE}_{\ell,j}(k') \right]^* \]

- **Coordinate space**
  \[ S_{\ell,j}^p(r, r'; E) = \sum_c \chi_{cE}_{\ell,j}(r) \left[ \chi_{cE}_{\ell,j}(r') \right]^* \]

- **Elastic scattering explicit**
  \[ \chi_{\ell,j}^{eE}(r) = \left[ \frac{2mk_0}{\pi\hbar^2} \right]^{1/2} \left\{ j_\ell(k_0 r) + \int dk k^2 j_\ell(kr)G^{(0)}(k; E)\Sigma_{\ell,j}(k, k_0; E) \right\} \]

reactions and structure
Adding an $s_{1/2}$ neutron to $^{40}\text{Ca}$

- Inelastically!
- Zero when there is no absorption!

Multiplied by $r^2$
• **One node now**

\[ d_{3/2} \]

\[ l = 2 \]
No nodes

- Asymptotically determined by inelasticity

\[ l = 4 \ (g92) \]

\[ S - |\chi|^2 \] [MeV$^{-1}$ fm$^{-1}$]

\[ E \] [MeV]

\[ r \] [fm]
Determine location of bound-state strength

• Fold spectral function with bound state wave function
  \[ S_{\ell j}^{m+}(E) = \int dr \ r^2 \int dr' \ r'^2 \phi_{\ell j}^{n-}(r) S_{\ell j}^{p}(r, r'; E) \phi_{\ell j}^{n-}(r') \]

• \( \rightarrow \) Addition probability of bound orbit

• Also removal probability
  \[ S_{\ell j}^{n-}(E) = \int dr \ r^2 \int dr' r'^2 \phi_{\ell j}^{n-}(r) S_{\ell j}^{h}(r, r'; E) \phi_{\ell j}^{n-}(r') \]

• Overlap function
  \[ \sqrt{S_{\ell j}^{n}} \phi_{\ell j}^{n-}(r) = \langle \Psi_{n}^{A-1} | a_{r, \ell j} | \Psi_{0}^{A} \rangle \]

• Sum rule
  \[ 1 = n_{n\ell j} + d_{n\ell j} = \int_{-\infty}^{\varepsilon_{F}} dE \ S_{\ell j}^{n-}(E) + \int_{\varepsilon_{F}}^{\infty} dE \ S_{\ell j}^{n-}(E) \]
Spectral function for bound states

• $[0,200]$ MeV $\rightarrow$ constrained by elastic scattering data

---

proton number $\rightarrow$ 19.88
neutron number $\rightarrow$ 19.79
$S_{0d3/2} = 0.76$
$S_{1s1/2} = 0.78$
0.15 larger than NIKHEF analysis!
Quantitatively

- Orbit closer to the continuum → more strength in the continuum
- Note “particle” orbits
- Drip-line nuclei have valence orbits very near the continuum

Table 1: Occupation and depletion numbers for bound orbits in $^{40}$Ca. $d_{nlj}[0, 200]$ depletion numbers have been integrated from 0 to 200 MeV. The fraction of the sum rule that is exhausted, is illustrated by $n_{nlj} + d_{nlj}[\varepsilon_F, 200]$. Last column $d_{nlj}[0, 200]$ depletion numbers for the CDBonn calculation.

<table>
<thead>
<tr>
<th>orbit</th>
<th>$n_{nlj}$</th>
<th>$d_{nlj}[0, 200]$</th>
<th>$n_{nlj} + d_{nlj}[\varepsilon_F, 200]$</th>
<th>$d_{nlj}[0, 200]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0s$_{1/2}$</td>
<td>0.926</td>
<td>0.032</td>
<td>0.958</td>
<td>0.035</td>
</tr>
<tr>
<td>0p$_{3/2}$</td>
<td>0.914</td>
<td>0.047</td>
<td>0.961</td>
<td>0.036</td>
</tr>
<tr>
<td>1p$_{1/2}$</td>
<td>0.906</td>
<td>0.051</td>
<td>0.957</td>
<td>0.038</td>
</tr>
<tr>
<td>0d$_{5/2}$</td>
<td>0.883</td>
<td>0.081</td>
<td>0.964</td>
<td>0.040</td>
</tr>
<tr>
<td>1s$_{1/2}$</td>
<td>0.871</td>
<td>0.091</td>
<td>0.962</td>
<td>0.038</td>
</tr>
<tr>
<td>0d$_{3/2}$</td>
<td>0.859</td>
<td>0.097</td>
<td>0.966</td>
<td>0.041</td>
</tr>
<tr>
<td>0f$_{7/2}$</td>
<td>0.046</td>
<td>0.202</td>
<td>0.970</td>
<td>0.034</td>
</tr>
<tr>
<td>0f$_{5/2}$</td>
<td>0.036</td>
<td>0.320</td>
<td>0.947</td>
<td>0.036</td>
</tr>
</tbody>
</table>

$^{48}$Ca in progress → more later this week
In progress

- $^{48}\text{Ca} \rightarrow$ charge density has been measured
- Recent neutron elastic scattering data $\rightarrow$ PRC83,064605(2011)
- Local DOM OLD Nonlocal DOM NEW

![Graphs showing $d\sigma/d\Omega$ vs. $\theta_{cm}$ for different energy bins for $n^{40}\text{Ca}$, $n^{48}\text{Ca}$, and $p^{48}\text{Ca}$ reactions.]
Preliminary results $^{48}\text{Ca}$

- Density distributions
- DOM $\rightarrow$ neutron distribution $\rightarrow R_n - R_p$

$^{48}\text{Ca}$ nuclear charge distribution

![Graph showing the $^{48}\text{Ca}$ nuclear charge distribution with different distributions and their labels: Neutron matter distribution, DOM, Experiment.](image-url)
Conclusions

• It is possible to link nuclear reactions and nuclear structure

• Vehicle: nonlocal version of Dispersive Optical Model (Green’s function method) pioneered by Mahaux → DSM

• Can be used as input for analyzing nuclear reactions

• Can predict properties of exotic nuclei

• “Benchmark” for ab initio calculations: e.g. $V_{NNN}$ → binding

• Can describe ground-state properties
  - charge density & momentum distribution
  - spectral properties including high-momentum Jefferson Lab data

• Elastic scattering determines depletion of bound orbitals

• Outlook: reanalyze many reactions with nonlocal potentials...

• For $N \gg Z$ exhibits sensitivity to properties of neutrons → weak charge in progress