QMC Calculations of Light Nuclei – *More Than Just Energies* –

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WORK WITH

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WORK NOT POSSIBLE WITHOUT EXTENSIVE COMPUTER RESOURCES Argonne Laboratory Computing Resource Center (Fusion) Argonne Math. & Comp. Science Division (SiCortex) Argonne Leadership Computing Facility (BlueGene/P)

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GOALS

Understand nuclei at the level of elementary interactions between individual nucleons, including

- Binding energies, excitation spectra, relative stability, widths
- Densities, electroweak transitions, cluster-cluster overlaps & spectroscopic factors
- Low-energy $NA \& AA'$ scattering, astrophysical reactions, asymptotic normalizations

REQUIREMENTS

- Two-nucleon potentials that accurately describe elastic NN scattering data
- Consistent three-nucleon potentials and electroweak current operators
- Precise methods for solving the many-nucleon Schrödinger equation

RESULTS

- Quantum Monte Carlo methods can evaluate realistic Hamiltonians accurate to \sim 1–2%
- About 100 states calculated for $A \leq 12$ nuclei in good agreement with experiment
- 5 He = $n\alpha$ scattering and low-energy electroweak astrophysical reactions
- Applications to elastic & ineleastic e, π scattering, $(e, e'p)$, (d, p) reactions, etc.

$$
H = \sum_{i} K_i + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk}
$$

 K_i : Non-relativistic kinetic energy, m_n-m_p effects included

Argonne v₁₈: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_{p}(r_{ij})O_{ij}^{p}$

- 18 spin, tensor, spin-orbit, isospin, etc., operators
- full EM and strong CD and CSB terms included
- predominantly local operator structure
- fits Nijmegen PWA93 data with χ^2 /d.o.f.=1.1

Urbana & Illinois: $V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{3\pi} + V_{ijk}^{R}$

- Urbana has standard $2\pi P$ -wave + short-range repulsion for matter saturation
- Illinois adds $2\pi S$ -wave + 3π rings to provide extra $T=3/2$ interaction
- Illinois-7 has four parameters fit to 23 levels in $A \le 10$ nuclei

Pieper, Pandharipande, Wiringa, & Carlson, PRC **64**, 014001 (2001) Pieper, AIP CP **1011**, 143 (2008)

QUANTUM MONTE CARLO

Variational Monte Carlo (VMC): construct Ψ_V that

- Are fully antisymmetric and translationally invariant
- Have cluster structure and correct asymptotic form
- Contain non-commuting 2- & 3-body operator correlations from v_{ij} & V_{ijk}
- Are orthogonal for multiple J^{π} states
- Minimize $E_V = \langle \Psi_V | H | \Psi_V \rangle \ge E$

These are $\sim 2^A \binom{A}{Z}$ component spin-isospin vectors in 3A dimensions

Green's function Monte Carlo (GFMC): project out the exact eigenfunction

- $\Psi(\tau) = \exp[-(H E_0)\tau]\Psi_V = \sum_n \exp[-(E_n E_0)\tau]a_n\Psi_n \Rightarrow \Psi_0$ at large τ
- Propagation done stochastically in small time slices $\Delta \tau$
- Exact $\langle H \rangle$ for local potentials; mixed estimates $\langle \Psi_V | O | \Psi(\tau) \rangle$ for other operators
- Constrained-path propagation controls fermion sign problem for $A \geq 5$
- Multiple excited states for same J^{π} stay orthogonal

Many tests demonstrate 1–2% accuracy for realistic $\langle H \rangle$

Pudliner, Pandharipande, Carlson, Pieper, & Wiringa, PRC **56**, 1720 (1997) Wiringa, Pieper, Carlson, & Pandharipande, PRC **62**, 014001 (2000) Pieper, Varga, & Wiringa, PRC **66**, 044310 (2002) Pieper, Wiringa, & Carlson, PRC **70**, 054325 (2004)

APPLICATIONS TO LIGHT-ION REACTIONS

The availability of radioactive-ion beams has renewed interest in reactions like (d,p) in inverse kinematics

We have helped analyze ^a number of RIB experiments such as $d({}^{8}\text{Li},p){}^{9}\text{Li}$ (ATLAS) & $d({}^{9}\text{Li},t){}^{8}\text{Li}$ (TRIUMF)

- PTOLEMY DWBA calculations for transfer
- (d,p) vertex from AV18
- \bullet (d,t), $({}^{8}\text{Li}, {}^{9}\text{Li})$, etc. vertices computed as A-body overlaps using VMC $\langle \Psi_V(A-1)|a|\Psi_V(A)\rangle$
- Norm is spectroscopic factor
- Absolute prediction for $d\sigma/d\Omega$
- Good predictions of n -knockout from 10 Be and 10 C (NSCL)

Macfarlane & Pieper, PTOLEMY, ANL-76-11, Rev. 1 (1978) Wuosmaa *et al.*, PRL **94**, 082502 (2005) ⁺ ... Kanungo *et al.*, PLB **660**, 26 (2008) Grinyer *et al.*, PRL **106**, 162502 (2011)

ONE-NUCLEON OVERLAPS IN VMC/GFMC

For antisymmetric and translationally invariant parent $\Psi_A(\alpha)$ and daughter $\Psi_{A-1}(\gamma)$ wave functions, with $\alpha \equiv [J_A^{\pi}, T_A, T_{z_A}], \gamma \equiv [J_{A-1}^{\pi}, T_{A-1}, T_{z_{A-1}}]$, and single-nucleon quantum numbers $\nu \equiv [l, s, j, t, t_z]$, the translationally invariant overlap function is:

$$
R(\alpha, \gamma, \nu; r) = \sqrt{A} \left\{ \left[\Psi_{A-1}(\gamma) \otimes \mathcal{Y}(\nu)(\hat{r}') \right]_{J_A, T_A} \left| \frac{\delta(r - r')}{r^2} \right| \Psi_A(\alpha) \right\}
$$

where $\mathcal{Y}(\nu)(\hat{r}') = [Y_l(\hat{r}') \otimes \chi_s]_i \chi_t$ and $|\Psi_{A-1}(\gamma)|^2 = 1$, $|\Psi_A(\alpha)|^2 = 1$.

The corresponding spectroscopic factor is the norm of the overlap:

$$
S(\alpha, \gamma, \nu) = \int |R(\alpha, \gamma, \nu; r)|^2 r^2 dr
$$

Overlap functions R satisfy a one-body Schrödinger equation with appropriate source terms. Asymptotically, at $r \to \infty$, these source terms contain core-valence Coulomb interaction at most, and hence for paren^t states below core-valence separation thresholds:

$$
R(\alpha,\gamma,\nu;r)\xrightarrow{r\to\infty}C(\alpha,\gamma,\nu)\frac{W_{-\eta,l+1/2}(2kr)}{r},
$$

where $W_{-\eta, l+1/2}(2kr)$ is a Whitakker function with $k = \sqrt{2\mu B}/\hbar$, B is the separation energy, and $C(\alpha, \gamma, \nu)$ is the asymptotic normalization coefficient or ANC.

GFMC evaluation of R is by extrapolation requiring two mixed estimates minus the VMC result:

 $R(\alpha, \gamma, \nu; r; \tau) \approx \langle R(\alpha, \gamma, \nu; r; \tau) \rangle_{M_A} + \langle R(\alpha, \gamma, \nu; r; \tau) \rangle_{M_{A-1}} - \langle R(\alpha, \gamma, \nu; r) \rangle_{V},$

where M_A denotes a mixed estimate where parent $\Psi_A(\alpha; \tau)$ has been propagated in GFMC and M_{A-1} is a mixed estimate where daughter $\Psi_{A-1}(\gamma;\tau)$ has been propagated.

Imaginary time evolution of overlaps in the $p_{3/2}$ channel of the overlap $\langle ^6He + p| ^7Li \rangle$

A convenient parametrization for input to PTOLEMY or other direct reaction code is provided by fitting a single-particle potential to reproduce the overlap $R\mathrm{:}$

$$
V(r) = V_{WS} \left[\frac{1}{1 + \exp((r - R_{WS})/a_{WS})} - \beta \exp(-(r/\rho)^2) \right] +
$$

$$
\left(4\vec{l} \cdot \vec{s} \right) \frac{V_{so}}{r} \frac{d}{dr} \left[\frac{1}{1 + \exp((r - R_{so})/a_{so})} \right] + V_{Coul}
$$

The potential parameters are adjusted to minimize χ^2 under the constraint that the overlap tail falls off with the correct core-valence separation energy B . This helps in extraction of the ANCs.

Brida, Pieper, & Wiringa, in preparation

Example: (³H,⁴He), s_{1/2} overlap

Example: (⁶He, ⁷Li), p_{3/2} overlap

GFMC separation energies

- total energies are within 1% around exp. values
- Sep. energies are within 3% around exp. values
- · use exp. sep. energies for ANCs accounting for uncertainties

s-shell: spectroscopic factors

GFMC systematic uncertainties are 2-3% or less exp. values: Pandharipande et al, RMP 69 (1997) 981

s-shell: ANCs

GFMC systematic uncertainties are 5% or less exp. values: Timofeyuk (2010), Girard (1979), Locher (1978, Purcell (2010), Blimov (1985, Blokhintsev (1977)

s-shell: comparing with HH

p-shell: spectroscopic factors

SFs for overlaps with $\sqrt[7]{\text{Be(g.s)}}$ are close to $\sqrt[7]{\text{Li(g.s)}}$ Shell-model SFs quenched by as much as 40%. GFMC systematic uncertainties are 2-3% or less exp. values: Wuosmaa (2008), Lapikas (1999), Ju (2010), Li (1969), Towner (1969), Schiffer (1967)

p-shell: ANCs

ANCs for overlaps with ${}^{7}Be(g.s)$ are close to ${}^{7}Li(g.s)$ GFMC systematic uncertainties are 5% or less exp. values: Gulamov (1995), Bekbaev (1991)

ALTERNATE ROUTE TO ANCS

The VMC wave functions account fairly well for short-range correlations but may have poor asymptotic behavior, particularly in p-shell.

Fitting $C = rR(r)/W(2kr)$ is generally difficult because long-range shapes can be wrong, and Monte Carlo sampling of the tails is difficult.

In the s-shell, however, it works ok:

INTEGRAL REALTION FOR THE ANC

There is ^a better way than explicit overlaps, ideally suited to QMC methods

Consider the A-body wave function Ψ_A and its overlap with Ψ_{A-1} plus a final proton with separation energy B .

Write the Schrödinger equation as

$$
(H-E)\,\Psi_A=0
$$

and expand H and E into parts internal to Ψ_{A-1} and parts involving the last particle

$$
\left(H_{\mathrm{int}}+T_{\mathrm{rel}}+U_{\mathrm{rel}}+V_C-V_C-E_{\mathrm{int}}+B\right)\Psi_A=0
$$

Then

$$
\Psi_A = -[T_{\text{rel}} + V_C + B]^{-1} (U_{\text{rel}} - V_C) \Psi_A -[T_{\text{rel}} + V_C + B]^{-1} (H_{\text{int}} - E_{\text{int}}) \Psi_A
$$

The second line is zero since $(H_{int} - E_{int})\Psi_{A-1} = 0$

Rewriting the Green's function $[T_{rel} + V_C + B]^{-1}$ in terms of special functions turns

$$
\Psi_A = -[T_{\text{rel}} + V_C + B]^{-1} (U_{\text{rel}} - V_C) \Psi_A
$$

into

$$
\Psi_{A-1}^{\dagger} \chi^{\dagger} Y_{lm}^{\dagger} \Psi_A = \frac{2\mu}{k\hbar^2 w} \mathcal{A} \int \frac{M_{-\eta, l+\frac{1}{2}}(2kr_<)W_{-\eta, l+\frac{1}{2}}(2kr_>)}{r_< r_>} \times \Psi_{A-1}^{\dagger} \chi^{\dagger} Y_{lm}^{\dagger}(\hat{\mathbf{r}}_{cc}) \left(U_{\text{rel}} - V_C\right) \Psi_A d\mathbf{R}
$$

so at large radius

$$
C_{lj} = \frac{2\mu}{k\hbar^2 w} \mathcal{A} \int \frac{M_{-\eta,l+\frac{1}{2}}(2kr_{cc})}{r_{cc}} \Psi_{A-1}^{\dagger} \chi^{\dagger} Y_{lm}^{\dagger}(\hat{\mathbf{r}}_{cc}) \left(U_{\text{rel}} - V_C\right) \Psi_A d\mathbf{R}
$$

 $M_{-\eta, l+\frac{1}{2}}(2kr)$ is the "other" Whittaker function, irregular at $r \to \infty$. Here U_{rel} is

$$
U_{\text{rel}} = \sum_{i < A} v_{iA} + \sum_{i < j < A} V_{ijA}
$$

and at large separation of the last nucleon, $U_{rel} \rightarrow V_C$, so $(U_{rel} - V_C) \rightarrow 0$. This makes the integrand terminate at \sim 7 fm for AV18+UIX.

This is grea^t for QMC methods, which are good at integration over the wave function interior, but bad in the tails.

ANC: ${}^{3}\text{He} \rightarrow dp$

Points are Monte-Carlo sampled integrand; solid curves are cumulative integrals

For ³He → dp, we get $C_s^{dp} = 2.131(8)$ fm^{-1/2}, $C_d^{dp} = -0.0927(10)$ fm^{-1/2} Corresponding HH values are 2.16 & [−]0.⁰⁸⁶⁵ Corresponding GFMC values are 2.10 & [−]0.0794

 C_d^{dp} converges just where sampling gets sparse in the explicit overlap

ANC: ${}^{8}\text{Li} \rightarrow {}^{7}\text{Li} + n$

Here is ^a case where fitting to VMC samples is impossible, but the integral method using the laboratory separation energy works beautifully:

RESULTS FOR ONE-NUCLEON REMOVAL $3 < A < 9$

- Small error bars are VMC statistics
- Large ones are "experimental"
- Sensitivity to wave function construction seems weak but hard to quantify
- $A \leq 4$ clearly dominated by systematics, also old
- With ^a few exceptions, these are the first *ab initio* ANCs in $A > 4$

Nollett and Wiringa, PRC **83**, 041001(R) (2011)

QMC FOR CONTINUUM STATES

We generally treat nuclei as particle-stable systems – probably good for energies of narrow resonances, but no prediction for widths. For wide states we need full scattering solution.

METHOD

- Pick a logarithmic derivative, χ , at some large boundary radius ($R_B \approx 9$ fm)
- GFMC propagation, using method of images to preserve χ at R, finds $E(R_B, \chi)$
- Phase shift, $\delta(E)$, is function of R_B , χ , E
- Repeat for a number of χ until $\delta(E)$ is mapped out
- need E accurate to $\sim 1/3\%$

⁵He AS $n+4$ He SCATTERING

Black curves: Hale phase shifts from R-matrix analysis up to $J = \frac{9}{2}$ of data AV18 with no V_{ijk} underbinds ⁵He(3/2⁻) & overbinds ⁵He(1/2⁻) AV18+UIX improves 5 He(1/2⁻) but still too small spin-orbit splitting AV18+IL2 reproduces locations and widths of both P-wave resonances

Nollett, Pieper, Wiringa, Carlson, & Hale, PRL **99**, 022502 (2007)

WIDTHS AS ANCS

Mapping $E(\gamma) \to \delta(E)$ is laborious, requires many solutions, and sensitive to calculational precision Reliable widths of narrow states will be difficult by this method

But widths are closely related to ANCs, so maybe there's ^a cheap way to estimate them

An unbound wave function at large radius looks like

 $\psi(r \to \infty) \propto F_l(kr) \cos \delta + G_l(kr) \sin \delta$

so that at resonance ($\delta = 90^{\circ}$; as our pseudobound states should have)

$$
\psi(r \to \infty) = C_{lj} \phi_1 \phi_2 G_l(kr)
$$

The flux per unit time through the surface is $|C_{lj}|^2 v = \frac{\hbar k}{\mu} |C_{lj}|^2$

From $\Gamma \simeq \hbar / \tau$, we get $\Gamma \simeq \frac{\hbar^2 k}{\mu} |C_{lj}|^2$

One could also consider Gamow's decaying complex-energy states and getthe same answer

WIDTHS AS ANCS

The relation

$$
\psi(r \to \infty) = C_{lj} \phi_1 \phi_2 G_l(\eta, kr)
$$

for resonant states is mathematically almost the same as

$$
\psi(r \to \infty) = C_{lj} \phi_1 \phi_2 W_{-\eta, l + \frac{1}{2}}(2kr)
$$

for bound states

You can get from one to the other by considering the bound k and η as $\pm i$ times their scattering-state counterparts

The integral method also applies to resonant states, except that now F_l appears in the integral instead of

$$
M_{-\eta,l+\frac{1}{2}}
$$

This is used as a mathematical tool to get the asymptotics right in α and p decays (e.g. Esbensen & Davids (2000) deformed proton emitters)

TESTING THE INTEGRAL RELATION FOR Γ

The integral estimate should apply to states that are in some sense narrow Here are low-lying states in $A \leq 9$ with width mainly/all in nucleon emission

Nollett & Wiringa, in preparation

Lots of widths come out close to experiment

Widths not close to experiment generally have some unaccounted-for width (e.g. α or 3-body channel) or isospin mixing, or are broad

Pseudobound ⁵He states yield wildly unreasonable widths, probably because they're very broad

Width integral appears to be better than just using the Wigner limit and S_{lj}

FUTURE WORK

GFMC one-nucleon overlaps for $A \geq 8$ nuclei

Two-nucleon overlaps like $\langle \alpha nn|^6$ He \rangle and $\langle \alpha d|^6$ Li \rangle under development – first VMC calculations made

Generalize integral method for ANCs and widths to α and other cluster breakups

Utilize integral method with GFMC wave functions and IL7 potential

Integral method may provide way of extracting surface amplitudes from GFMC for coupled-channel scattering problems

Still need to do full scattering calculations for wide states like ${}^{8}Be(2^{+}, 4^{+})$ but integral method will probably give best estimate of width of ${}^{8}Be(0^{+})$

Example: 2N overlaps for ⁶He

2N overlaps in the past:

three-body calculations

- 3-body w.f.s are the 2N overlaps
- inert core, simple interactions, ...
- microscopic calculations
	- I.Brida and F.M.Nunes, NPA 847(2010) 1 phenomenological N-N forces
	- spec. factors greater by 30%-70% than in 3-body

 10°

Present:

VMC:

- fully ab-initio
- preliminary VMC results:

Future: GFMC

