Consistently treating bound and scattering states in many-body methods

Mack C. Atkinson



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 - No-core shell model with continuum (NCSMC) ab initio
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- I will present different reaction calculations that benefit from their simultaneous bound/scattering states
- Results of these calculations warrant futher investigation of the nuclear force

³He (α, γ) ⁷Be important for solar-model predictions



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Adelberger et al., Rev Mod Phys 83 195 (2011)

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$$\sigma(E) = \frac{S_{34}(E)}{E} \exp\left\{-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2E/m}}\right\}$$

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³He(α, γ)⁷Be important for solar-model predictions

- Reaction rates too low at solar energies in the lab
- Current evaluations depend on both theory and experiment
- Ideally, theory will accurately predict $S_{34}(E)$





$$\left\langle \Psi_{bs}\left(^{7}\mathrm{Be}\right)\left|\hat{\mathcal{M}}_{\mathrm{EM}}\right|\Psi_{sc}\left(^{3}\mathrm{He}+\alpha\right)
ight
angle$$

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$$\hat{H}=\hat{T}+\hat{V}_{NN}+\hat{V}_{NNN}$$
 $\hat{H}\ket{\Psi^A}=E\ket{\Psi^A}$

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 $\left\langle \Psi_{bs}\left(^{7}\mathrm{Be}\right) \middle| \hat{\mathcal{M}}_{\mathrm{EM}} \middle| \Psi_{sc}\left(^{3}\mathrm{He} + \alpha\right) \right\rangle$



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \stackrel{(A)}{\Longrightarrow} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \, \gamma_{\nu}(\vec{r}) \, \hat{A}_{\nu} \left| \stackrel{\bullet}{\underbrace{\bullet}}_{\substack{(A-a)}} , \nu \right\rangle$$

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$$\uparrow |^{7} \text{Be} \rangle$$

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$$\uparrow \qquad \uparrow \qquad \uparrow$$

$$|^{7} \text{Be} \rangle \qquad |\alpha\rangle \otimes |^{3} \text{He} \rangle$$

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NCSMC Calculation of ³He+⁴He well-converged, levels need shifting



V. Soma *et al*, PRC **101**, 014318 (2020) U. van Kolck, PRC **49**, 2932 (1994) D.R. Entem and R. Machleidt, PRC **68**, 041001(R) (2003)

Mack C. Atkinson LLNL M.C. Atkinson et al., arXiv:2409.09515 (In Press PLB)



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• Compare to SONIK elastic scattering results to further probe ψ_{sc}



Paneru et al., arXiv:2211.14641 (2022)

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- Experiment done at TRIUMF in 2022 \rightarrow lowest *E* measured to date



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• What is the source of discrepancy at large angles?

Paneru et al., arXiv:2211.14641 (2022)

6

• More repulsion is needed in the $1/2^+$ channel



- More repulsion is needed in the $1/2^+$ channel
- Explicitly add repulsion

$${\cal H}^{1/2^+}_{
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 10^{2}

 $d\sigma/d\Omega_{c.m.}$

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-10

 $1/2^+$
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• With NN + 3N interaction treated consistently, two possibilities:

• Calculation could be missing channels

 Including p+⁶Li channel could have strong effect on phase shift

Ohiral interaction

- Phase shift shows some dependence on interaction
- Need to compare more interactions



Comparison with other theories





• Excitation spectrum provides evidence of many-body correlations beyond mean-field



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M.C. Atkinson et al., PRC 98, 044627 (2018)

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$$rac{\hat{oldsymbol{p}}^2}{2\mu}\psi(oldsymbol{r})+\int doldsymbol{r}'\Sigma^*(oldsymbol{r},oldsymbol{r}';E)\psi(oldsymbol{r}')=E\psi(oldsymbol{r})$$



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$$\Sigma^*(\mathbf{r},\mathbf{r'};E) = \Sigma^*\left(rac{r+r'}{2};E
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Can this also describe negative energy observables?

$$\Sigma^{*}(\mathbf{r},\mathbf{r}';E) = \Sigma^{*}\left(\frac{r+r'}{2};E\right)e^{\frac{-(r-r')^{2}}{\beta^{2}}}\pi^{-\frac{3}{2}}\beta^{-3}$$



• The DOM makes use of complex analysis to formulate a consistent self-energy

Calculation could be missing channels

$$\operatorname{Re}\Sigma_{\ell j}(r, r'; E) = \operatorname{Re}\Sigma_{\ell j}(r, r'; \epsilon_F) - \frac{1}{\pi}(\epsilon_F - E)\mathcal{P}\int_{\epsilon_T^+}^{\infty} dE' \operatorname{Im}\Sigma_{\ell j}(r, r'; E') \left[\frac{1}{E - E'} - \frac{1}{\epsilon_F - E'}\right] + \frac{1}{\pi}(\epsilon_F - E)\mathcal{P}\int_{-\infty}^{\epsilon_T^-} dE' \operatorname{Im}\Sigma_{\ell j}(r, r'; E') \left[\frac{1}{E - E'} - \frac{1}{\epsilon_F - E'}\right]$$

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- (subtracted) Dispersion relation constrains self-energy at all energies
- This constraint ensures bound and scattering quantities are simultaneously described

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 \bullet Parameters of self-energy varied to minimize χ^2

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M.C. Atkinson et al., PRC 98, 044627 (2018)

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M.C. Atkinson et al., PRC 98, 044627 (2018)

• Parameters of self-energy varied to minimize χ^2



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- Parameters of self-energy varied to minimize χ^2
- Reproducing the data means self-energy is found



0.09

0.08

0.07

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Experiment DOM

DOM calculation of ${}^{40}Ca(e, e'p){}^{39}K$

• DWIA for exclusive reaction (C. Giusti's DWEEPY code)

$$J^{\mu}(\mathbf{q}) = \int \chi^{(-)*}_{E\alpha}(\mathbf{r}) j^{\mu}(\mathbf{r}) \phi_{E\alpha}(\mathbf{r}) [S_{F\alpha}(E)]^{1/2} e^{i\mathbf{q}\cdot\mathbf{r}} d^3r$$



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p,

 (\mathbf{q},ω)

A-1

e

Want to study knockout in exotic nuclei too



Experimental sketch for exotic nuclei (RIB)





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$$T \approx \int d\mathbf{R} t_{NN} \chi_1^{(-)*}(\mathbf{R}) \chi_2^{(-)*}(\mathbf{R}) \chi_0^{(+)}(\mathbf{R}) e^{-i\alpha_R \mathbf{K}_0 \cdot \mathbf{R}} \phi_{ljm}^n(\mathbf{R}).$$

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"S _F "	(p, 2p)	(e, e'p)
DOM	0.560	0.71 ± 0.04



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- Remember that S_F comes directly from Σ^*_{DOM}
- Main difference is the probe \implies problem is likely V_{pp}

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• Try varying V_{NN} to see effect on S_F



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S _F	V_{NN}	(<i>p</i> , 2 <i>p</i>)
DOM	FL	0.560 ± 0.05
DOM	Mel	0.489 ± 0.05
DOM	Mel (free)	0.515 ± 0.05

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- Dependence of S_F on choice of V_{NN} is another sign the problem lies in V_{NN}



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• $G_{pp} \approx \int G_{\rm DOM} \times G_{\rm DOM}$



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- Similar to *G*-matrix, except this is calculated in finite nuclei



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- $G_{pp} \approx \int G_{\rm DOM} \times G_{\rm DOM}$
- Similar to *G*-matrix, except this is calculated in finite nuclei
- Good approximation for typical (p, 2p) energies



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- Ab initio calculation of ${}^{3}\text{He}(\alpha,\gamma){}^{7}\text{Be capture reaction using the NCSMC}$
 - Simultaneous analysis of elastic and capture data reveals mild tension
 - Lack of repulsion in $1/2^+$ channel could be due to V_{NN} or the lack of $p+^6$ Li channel
- So The DOM accurately predicts ${}^{40}Ca(e, e'p){}^{39}K$ but not the very similar ${}^{40}Ca(p, 2p){}^{39}K$ reaction
 - Likely cause of discrepancy in these knockouts is the pp interaction used in the DWIA
- In both examples of the NCSMC and the DOM, the ability to simultaneously describe bound and scattering states helped isolate areas of improvement
- Resolution of these issues will lead to improved nucleus-induced reaction calculations

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- Willem Dickhoff
- Hossein Mahzoon



- Cole Pruitt
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- Louk Lapikás
- Henk Blok







• Kazuki Yoshida

Japan Atomic Energy Agency