The tale of tails: Sensitivity of quasi-free reactions on details of the bound-state overlap functions

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It is often stated that one-nucleon knockout in reactions with heavy ion targets are mostly sensitive to the tails of the bound-state wavefunctions. In contrast, (p,2p) and (p,pn) reactions are known to access information on the full overlap functions within the nucleus. We analyze the oxygen isotopic chain and explore the differences between single-particle wave functions generated with potential models, used in the experimental analysis of knockout reactions, and \textit{ab initio} computations from self-consistent Green’s function theory. Contrary to the common belief, we find that not only the tail of the overlap functions, but also partial information on their internal part are assessed in both reaction mechanisms, which are crucial to yield accurately determined spectroscopic information. The recent revival of (p,2p) reactions, this time in inverse kinematic experiments, will help improve studies of unstable nuclei if combined with a better experimental analysis with inputs from many-body \textit{ab initio} theories. We suggest that input from state-of-the-art \textit{ab initio} computations will be fundamental to quantify model dependencies in the analysis of experiments.

Introduction. In the last three decades, high energy (\( \gtrsim 100\) MeV/nucleon) neutron and proton removal (knockout) reactions with heavy targets (typically \(^{9}\)Be and \(^{12}\)C targets) have been one of the most successful tools to investigate the single-particle structure of the many-body wavefunction of nuclei far from the stability. A large number of such experiments have been carried out and an enormous amount of knowledge was collected on magicity, shell-evolution, two- and three-body halo configurations, spectroscopy of deep lying states, etc. The magnitude of the knockout cross sections, as well as the width of the momentum distribution of the fragments, have been the main source of information since the very beginning of this experimental campaign \([1,3]\). For these two quantities, theories have been developed which allow for a credible description of the experimental data \([4,5]\).

It is widely considered that knockout reactions are peripheral in nature and probe the tail of the nucleon removal wavefunction, due to absorption at low impact parameters (see, e.g., Refs. \([9,12]\)). The removal wavefunction is given by the overlap integral \(I(r) = \langle \Psi_i^{A-1}\mid \psi(r)\rangle \Psi_i^{A}\rangle\), where \(\Psi_i^{A}\rangle\) and \(\Psi_i^{A-1}\rangle\) respectively denote the (many-body) wavefunctions for the projectile and the residual fragment in its \(i\)-th excited state \([13,14]\). The operator \(\psi(r)\) removes a nucleon at position \(r\). The tail of this overlap function is proportional to the Whittaker function,

\[
I(r) = \langle \Psi_i^{A-1}\mid \psi(r)\rangle \Psi_i^{A}\rangle \rightarrow C \frac{1}{r} W_{-\eta, l+1/2}(2\kappa r),
\]

where \(\kappa = \sqrt{2\mu E_B}/\hbar\) is the wavenumber, \(\mu\) the reduced mass between the outgoing nucleon and the \((A-1)\) residual, \(E_B\) the removed nucleon separation energy, \(\eta = \mu Z_N Z_A e^2/\hbar\kappa\) is the Coulomb parameter, with \(Z_A\) and \(Z_N\) the target and projectile charges, and \(l\) the angular momentum of the removed nucleon.

Eikonal based theories for knockout reactions \([4,12,13]\) often imply that the total knockout cross section is proportional to the square of the integral \(I^2(r)\) and therefore, as long as the reaction is truly peripheral, to the squared asymptotic normalization coefficient (ANC): \(C^2\). In this case the ANC is the only messenger carrying information about the complex many-body wavefunctions \(\Psi_i^{A}\rangle\) and \(\Psi_i^{A-1}\rangle\) entering Eq. (1). In practice, most applications in the literature still assume that the tail of \(I(r)\) does not differ from a wavefunction computed via some independent–particle approximation (IPA), for example a Woods-Saxon plus spin-orbit tuned to the corresponding separation energy. When compared to the experimental data of nucleon knockout reactions, the square of \(C\) can be extracted and compared to predictions of many-body models (e.g., shell model calculations). This procedure is used to determine the spectroscopic factors \(S\) according to \([15,16]\):

\[
C^2_{\text{exp}} = S \cdot C^2_{\text{IPA}}.
\]
where $C_{\text{IPA}}$ is computed assuming that its IPA wavefunction is properly normalised to unity. Nuclear correlations have the effect of quenching the spectroscopic factor, $S \equiv \int f^2(r) \, dr$, and so the experimental value of $C_{\text{exp}}$ is smaller than its IPA. The many-body ANC, $C_{\text{MB}}$, computed from ab initio theory through Eq. (1) should be compared directly to $C_{\text{exp}}$. The primary goal of nucleon knockout experiments with heavy ion targets is to extract information on the spectroscopic factors and the $C_{\text{MB}}$.

A whole new set of experiments have been carried out or are planned using $(p,pN)$, with $N = p, n$, reactions in inverse kinematics [17–20] and new reaction theories have also been developed which differ in essence from those appropriate for knockout reactions with heavy targets [21,22]. Knockout and $(p,pN)$ reactions differ in the property that protons probes are more sensitive to the inner parts of the nuclear wavefunction, specially for light nuclear projectiles [23]. Since both knockout as well as $(p,pN)$ reactions are notable spectroscopic tools of unstable nuclei, it is imperative to understand to what extent experimental conclusions can be affected by assumptions in modeling $I(r)$. For this goal we will compare the outcome of $(p,pN)$ and heavy ion knockout calculations using both ab initio many-body overlap functions and those obtained from phenomenological optical potentials.

**Overlaps with ab initio methods.** The ab initio overlaps have been calculated from the Hamiltonian

$$H(A) = T - T^{[A-1]}_{\text{c.m.}} + V + W,$$

where $T^{[A-1]}_{\text{c.m.}}$ is the intrinsic kinetic energy for the recoiling system of mass $A-1$ nucleons, while $V$ and $W$ are the two- and three-body interactions. This formulation is conveniently suited for the calculation of overlap functions and the corresponding nucleon separation energies, $E_h$ [23]. The three-body term $W$ is reduced to an effective two-body operator as outlined in [24].

We used self-consistent Green’s function (SCGF) theory within the third order algebraic diagrammatic construction (ADC(3)) truncation scheme that accounts for all $2p1h, 2h1p$ intermediate state configurations [25,26]. The SCGF self-energy was obtained in an harmonic oscillator basis including 14 major shells ($N_{\text{max}} = 13$) and frequency $\hbar \Omega = 20$ MeV. The correct asymptotic tail of our ab initio overlap $I_{\text{GF}}^l(r)$ is ensured by a final Dyson diagonalization in the full (non truncated) momentum space [27],

$$E_h - \frac{k^2}{2\mu} I_{\text{GF}}^l(k) = \int dq \, q^2 \Sigma^*_{lj}(k; q; E_h) I_{\text{GF}}^l(q),$$

where $\Sigma^*$ is the ADC(3) self-energy, $\mu$ is the reduced mass of the $(A-1)$-body system plus the ejected nucleon, and $I(k)$ represents the Fourier-Hankel transform of Eq. (1).

We perform computations using the NNLOsat interaction because of its good saturation properties [28]. Both radii and binding energies are known to be well reproduced for the oxygen chain nuclei used in this analysis [29], allowing for a meaningful comparison with reactions from Woods-Saxon–based calculations.

Next we show the results for $(p,pN)$ quasi-free reaction cross sections using overlap functions obtained with: (a) SCGF formalism with the chiral NNLOsat interaction, denoted by $I_{\text{GF}}(r)$; (b) Single particle wavefunctions, $u_{WS}(r)$ generated in a potential model (Woods-Saxon + Coulomb), herewith denoted by $WS$. The WS radii and diffuseness parameters were taken as $R = 1.2A^{1/3}$ fm and $a = 0.65$ fm, respectively. A homogeneously charged sphere with radius $R$ was used to generate the Coulomb potential. For case (a) the spectroscopic factors are given by $S_{\text{GF}} = \int dr I_{\text{GF}}^l(r)$ and are computed directly from the associated SCGF propagators. For case (b) the calculations for the quasi-free cross sections are usually obtained by multiplying the cross section by a spectroscopic factor $S_{WS}$ chosen to reproduce the experimental data. Thus, our task reduces in checking if the procedure used in (a) yields compatible results as the procedure in (b).

Our comparison of the cross section calculations will follow the reaction theory developed in Ref. [13] keeping all other input parameters the same, such as separation energies, nuclear densities, etc.
In Table I we list separation energies, $E_B$, root mean square radii of the overlap wavefunction, $\langle r^2 \rangle^{1/2}$, asymptotic normalization coefficients (ANC), $(p,pN)$ quasi-free cross sections, $\sigma_{qf}$ and nucleon knockout cross sections, $\sigma_{ko}$, with $^9\text{Be}$ targets, for 350 MeV/nucleon oxygen projectiles. WS denotes wavefunctions calculated with a potential model (Woods-Saxon) and GF denotes many-body \textit{ab initio} overlap functions from self-consistent Green’s function method.

In Table I we list separation energies, $E_B$, root mean square radii, $\langle r^2 \rangle^{1/2}$, asymptotic normalization coefficients, $C_{WS}$, quasi-free proton/neutron knockout ($p,pN$) cross sections, $\sigma_{qf}$, for 350 MeV protons in inverse kinematics, and proton(neutron) knockout reactions, $\sigma_{ko}$, for oxygen isotopes incident on $^9\text{Be}$ targets at 350 MeV/nucleon. A selected set of neutron and proton states in oxygen isotopes were chosen. Note that overlaps from SCGF calculations are not single particles but represent correlated states with the corresponding angular momentum and parity. The same quantum numbers have more than one fragment and it is only the sum of those fragments that normalizes the overlap function to 1. The last column in this table lists the spectroscopic factors, as computed from \textit{ab initio} SCGF. To simplify the comparison and focus on the ANC contribution, in this study we keep all GF overlap and WS functions normalized to one, i.e., the cross sections have not been multiplied by the GF overlap functions stemming from the No-Core-Shell-Model (NCSM). Similar issues are now fully resolved both for both NCSM and for SCGF theories. In our case, the projection of Eq. (4) into momentum space, as discussed in Refs. [23, 25] always yields the correct

| Nucleus (state) | $E_B$ [MeV] | $\langle r^2 \rangle^{1/2}_{WS}$ [fm$^2$] | $\langle r^2 \rangle^{1/2}_{GF}$ [fm$^2$] | $C_{WS}$ | $C_{GF}$ | $\sigma_{qf}^{WS}$ [mb] | $\sigma_{qf}^{GF}$ [mb] | $\sigma_{ko}^{WS}$ [mb] | $\sigma_{ko}^{GF}$ [mb] | $S_{ij}$ |
|----------------|-------------|---------------------------------|---------------------------------|---------|---------|----------------|----------------|----------------|----------------|--------|
| $^{14}\text{O}$ ($\pi 1p_{3/2}$) | 8.877 | 2.386 | 2.961 | 6.665 | 7.060 | 20.72 | 21.28 | 26.28 | 28.15 | 0.548 |
| $^{14}\text{O}$ ($\pi 1p_{1/2}$) | 6.181 | 2.991 | 3.160 | 4.872 | 5.401 | 21.08 | 16.89 | 28.61 | 31.33 | 0.760 |
| $^{16}\text{O}$ ($\nu 1p_{3/2}$) | 21.33 | 2.513 | 2.722 | 11.39 | 14.64 | 30.55 | 32.80 | 21.13 | 23.92 | 0.773 |
| $^{16}\text{O}$ ($\pi 1s_{1/2}$) | 15.89 | 2.295 | 2.233 | 13.06 | 13.81 | 7.870 | 7.696 | 16.97 | 15.81 | 0.074 |
| $^{16}\text{O}$ ($\pi 1p_{3/2}$) | 17.43 | 2.612 | 2.832 | 15.29 | 18.27 | 17.41 | 18.58 | 19.83 | 22.70 | 0.805 |
| $^{16}\text{O}$ ($\pi 1p_{1/2}$) | 10.65 | 2.816 | 3.077 | 8.624 | 10.70 | 9.094 | 9.913 | 22.54 | 26.29 | 0.794 |
| $^{16}\text{O}$ ($\nu 1p_{3/2}$) | 20.71 | 2.580 | 2.807 | 11.96 | 13.88 | 27.88 | 30.26 | 18.81 | 21.66 | 0.801 |
| $^{22}\text{O}$ ($\pi 1p_{1/2}$) | 13.83 | 2.767 | 3.032 | 6.684 | 7.578 | 14.64 | 16.47 | 21.20 | 24.89 | 0.790 |
| $^{22}\text{O}$ ($\pi 1p_{3/2}$) | 29.26 | 2.554 | 2.884 | 43.74 | 63.52 | 14.37 | 17.08 | 13.07 | 14.50 | 0.274 |
| $^{22}\text{O}$ ($\pi 1s_{1/2}$) | 25.67 | 2.606 | 2.820 | 35.00 | 54.07 | 13.30 | 14.20 | 12.93 | 15.10 | 0.443 |
| $^{22}\text{O}$ ($\nu 1d_{3/2}$) | 23.58 | 2.634 | 2.916 | 30.49 | 51.49 | 6.607 | 7.253 | 13.27 | 16.21 | 0.731 |
| $^{24}\text{O}$ ($\pi 1p_{3/2}$) | 6.670 | 3.328 | 3.533 | 4.519 | 4.685 | 45.30 | 46.63 | 21.36 | 24.28 | 0.806 |
| $^{24}\text{O}$ ($\nu 2s_{1/2}$) | 28.57 | 2.609 | 2.886 | 45.76 | 66.45 | 12.13 | 13.29 | 11.37 | 14.01 | 0.675 |
| $^{24}\text{O}$ ($\nu 1p_{1/2}$) | 31.88 | 2.566 | 2.847 | 55.88 | 95.22 | 11.94 | 13.11 | 10.98 | 13.70 | 0.042 |
| $^{24}\text{O}$ ($\nu 1d_{5/2}$) | 25.28 | 2.657 | 2.985 | 37.04 | 57.21 | 6.054 | 6.881 | 11.81 | 15.11 | 0.740 |
| $^{24}\text{O}$ ($\nu 1d_{3/2}$) | 4.120 | 4.190 | 4.479 | 3.971 | 4.130 | 13.94 | 19.95 | 31.81 | 36.45 | 0.844 |
| $^{24}\text{O}$ ($\nu 1d_{5/2}$) | 6.961 | 3.436 | 3.557 | 2.056 | 2.106 | 40.53 | 41.95 | 19.51 | 21.11 | 0.832 |
analyses of \((p,pN)\) reactions require a closer collaboration of experiment and theory than typically done in the analysis of knockout reactions with heavy ions. Just the ANC, or spectroscopic factor, is not enough. The full knowledge of the single particle wavefunction is necessary.

To clarify the latest point, and show that knockout reactions with heavy ions are also partially sensitive to details of the inner part of the wavefunctions, consider the probability for one-nucleon stripping in a collision with the core (surviving spectator) having an impact parameter \(b\) with the target, while the removed nucleon has an impact parameter \(b_n\). The stripping probability is given by \(7\).

\[
P_{ko}(b) = S_n(b) \left( 1 - |S_n(b_n)|^2 \right) = S_n(b) \int d^3r |\phi_{nlj}(r)|^2 \left( 1 - |S_n(b_n)|^2 \right) \tag{5}\]

where \(\phi_{nlj}(r)\) denotes the wave function with quantum numbers \(nlj\) expressed in terms of the relative core-neutron distance \(r\). \(S_n(S_n)\) is the scattering matrix for the core(nucleon)-target and \(|\phi_{nlj}|^2\) is the probability to find the nucleon at \(r\). The impact parameter \(b_n \equiv (b_n, \phi_n)\) and the w.f. intrinsic coordinate \(r \equiv (r, \theta, \phi)\) are related by \(7\)

\[
b = \sqrt{r^2 \sin^2 \theta + b_n^2 - 2rb_n \sin \theta \cos(\phi - \phi_n)}. \tag{6}\]

We apply this equation to obtain the heavy ion proton knockout from \(^{24}\)O, \(1p3/2\), with \(E_B = 31.88\) MeV. In Fig. [3]we compare the GF and WS wavefunctions, noticing that while the tails are similar to a Whittaker function (only seen in a logarithmic scale), there are visible differences in their overall shapes. The calculated proton stripping probabilities, calculated with help of Eq. [5], are shown in Fig. [4]. One sees that the probabilities are larger for the GF wavefunctions, yielding larger cross sections, as expected by inspecting Table [1].

A simple question raises: do the heavy ion knockout cross sections scale with the square of the ANCs? The answer is negative. The respective ANCs scale as \((C_{GF}/C_{WS})^2 \sim 3\), whereas the cross sections scale as \(\sigma_{GF}/\sigma_{WS} \sim 1.25\). The reason for this intriguing difference is best understood if the stripping probability is plotted logarithmically for large values of \(b\). This is shown in Fig. [3]. While at very large distances, the probability seems as if it scales with a single factor (the ratio between the ANCs), at lower but still large impact parameters they visibly differ from simple scaling. This result is understood by considering the stripping probability in Eq. [3]. Even for large \(b\), when the core and the target pass by as much as 10 fm apart, the inner parts of the wavefunction are still probed because the integrand is too small to make substantial contributions to the probability if \(b_n \gg 1\), as the \(1 - |S_n|^2\) goes to rapidly to zero there. We have observed the same behavior for all the cases displayed in Table [1].
The imprints of the details of the many-body overlap functions are summarized in Figure 6 for the 17 reactions considered in Table I. The horizontal scale is a list of the reactions in Table I from top to bottom of the table. The vertical scale represents \((\sigma_{GF} - \sigma_{WS})/\sigma_{WS}\) in percent for (p,pN) reactions. Except for two cases, the quasi-free cross sections calculated with GF overlaps are larger than those with WS wavefunctions. The squares (diamonds) [circles] [stars] represent these quantities for 350 MeV/nucleon \(^{14}\)O \(^{16}\)O \(^{22}\)O \(^{24}\)O projectiles. It is evident that the results change appreciably with a different form of the internal part of the overlap functions. Fig. 6 also demonstrates that variations with respect to the overlap functions are smaller in the (p,pN) case (full symbols). We interpret this as due to the capability of this reaction mechanism of better probing the internal part of the nucleus.

### Conclusions

In summary, we have shown in this work that, in contrast to a commonly considered idea, both heavy ion knockout reactions and \((p,pN)\) reactions have substantial sensitivity to the internal details of the overlap wave function. Thus, both experimental probes put strong constraints on the coordinate dependence of the many-body wavefunctions.

An accurate experimental analysis ideally requires not only the input of an accurately determined overlap function from many-body computations but also a direct comparison among possible predictions of it, so that one can assess the extent of the model dependence for the

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**Figure 3.** Wood Saxon (WS, red dashed line) wavefunction and Green Function (GF, black dotted line) overlap function for \(^{24}\)O, 1p3/2, \(E_B = 31.88\) MeV.

**Figure 4.** Probability to remove a proton from \(^{24}\)O, 1p3/2, \(E_B = 31.88\) MeV for Wood Saxon (WS, red dashed line) and Green Function (GF, black dotted line) in the \(M = 0\) (thin lines) and \(M = \pm 1\) (thick lines) channels calculated with Eq. (5).

**Figure 5.** Same as in Fig. 4 but for very large impact parameters \(b\), where the integrand in Eq. (5) is dominated by the tail of the s.p. w.f.

**Figure 6.** Percent deviation of cross sections calculated with Wood Saxon wavefunctions and Green Function overlaps for the 17 reactions considered in Table I for quasi free (full symbols) and knockout reactions (empty symbols). The cross sections calculated with GF overlaps are larger than those with WS wavefunctions, except for two states.
inferred spectroscopic factors. The latter task requires particular attention since a good reproduction of nuclear binding energies and radii is a fundamental constraint but only a fraction of currently available ab initio Hamiltonians offer satisfactory saturation properties [34–36]. While this poses a more difficult task for the study of single-particle configurations with heavy-ion knockout and (p,pN) reactions, it also opens opportunities for a better and more profound understanding of the many-body configurations and their single-particle overlaps.

In view of the recent advances in experimental facilities and detection techniques, it is suggested that heavy-ion knockout and (p,pN) reactions are analyzed using a consistent many-body model, because they are a formidable tool to extend our knowledge in nuclear spectroscopy only when many-body correlations are considered in the analysis.

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