The Optical Potential in direct and compound nucleus reactions

Gregory Potel Aguilar

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LLNL-PRES-XXXXXX
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Part 1

Introduction: nuclear reactions and the Optical Potential



Nuclear reactions: why do we care? Nuclear reactions around us





nuclear medicine





Why do we care? Nuclear reactions as an experimental tool





Nuclear reactions of astrophysical interest (light elements)



Big Bang nucleosynthesis

reaction networks



Nuclear reactions of astrophysical interest (heavy elements)



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Features of nuclear spectra probed by nuclear reactions







Which reaction theories, and where?





The Optical Potential is a projection of the many-body Hamiltonian on the elastic channel



- The "optical reduction" transforms a many-body operator into a one-body operator
- It is a well-defined, in principle exact, mathematical operation

The OP accounts for the composite nature of the target nucleus





The OP accounts for the composite nature of the target nucleus





The OP accounts for the composite nature of the target nucleus



- The computed OP is energy dependent, non-local, complex, and dispersive
- The OP verifies the Kramers-Kronig dispersion relations between the real and the imaginary part



Nuclear reaction theorist's roadmap



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Nuclear reaction theorist's roadmap





There are different strategies for calculating the nucleon-nucleus optical potential (OP)





RPA calculation with

coupled-cluster ab initio with non-zero η parameter



- Phenomenological fits are widely used, but are disconnected from the structure and extrapolation away from stability is risky
- Microscopic theories often struggle to get absorption right
- Ab-initio approaches are only feasible for light nuclei



OP	EN	ACO	CESS

IOP Publishing

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Optical potentials for the rare-isotope beam era

C Hebborn^{1,2}, F M Nunes^{1,3}, G Potel², W H Dickhoff⁴, J W Holt⁵, M C Atkinson^{2,6}, R B Baker⁷, C Barbieri^{8,9}, G Blanchon^{10,11}, M Burrows¹², R Capote¹³, P Danielewicz^{1,3}, M Dupuis^{10,11}, Ch Elster⁷, J E Escher², L Hlophe², A Idini¹⁴, H Jayatissa¹⁵, B P Kay¹⁵, K Kravvaris², J J Manfredi¹⁶, A Mercenne¹⁷, B Morillon^{10,11}, G Perdikakis¹⁸, C D Pruitt², G H Sargsyan², I J Thompson², M Vorabbi^{19,20} and T R Whitehead¹





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6 authors are attending this conference





• experiment	— MBR	JLMB
— KD	MST-B	NSM
— DOM (STL)	MST-V	KDUQ
MR (2007)	SCGF	WLH

KD	Koning–Delaroche
KDUQ	Koning-Delaroche with Uncertainty Quantification
DOM (STL)	Dispersive Optical Model (Saint Louis)
MR	Morillon–Romain
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SCGF	Self-Consistent Green's Function
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	Mass	Energy	D.	Mic.	UQ
KD	$24 \leqslant A \leqslant 209$	$1 \text{ keV} \leq E \leq 200 \text{ MeV}$	×	×	×
KDUQ	$24 \leqslant A \leqslant 209$	$1 \text{ keV} \leq E \leq 200 \text{ MeV}$	×	×	\checkmark
DOM	C, O, Ca, Ni,	$-\infty < E < 200 \text{ MeV}$		×	\checkmark
(STL)	Sn, Pb isotopes				
MR	12 < Z < 83	E < 200 MeV	\checkmark	×	×
MBR	12 < Z < 83	E < 200 MeV	\checkmark	×	×
NSM	⁴⁰ Ca, ⁴⁸ Ca, ²⁰⁸ Pb	E < 40 MeV	$\overline{\checkmark}$	\checkmark	×
SCGF	O, Ca, Ni isotopes	E < 100 MeV	$\overline{\checkmark}$	\checkmark	×
MST-B	$A \leqslant 20$	$E \gtrsim 70 \text{ MeV}$	×	\checkmark	×
MST-V	$4 \leqslant A \leqslant 16$	$E\gtrsim 60 { m MeV}$	×	\checkmark	×
WLH	$12 \leqslant A \leqslant 242$	$0 \leqslant E \leqslant 150 \text{ MeV}$	×	\checkmark	1
JLMB	A > 30	1 keV < E < 340 MeV	×	\checkmark	×

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11 potentials were surveyed in this work

• 5 dispersive potentials

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- 6 microscopic (based on nuclear structure)



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NSM	⁴⁰ Ca, ⁴⁸ Ca, ²⁰⁸ Pb	E < 40 MeV	\checkmark	\checkmark	×
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Recommendations

• Theory-experiment collaboration to address isospin dependence away from stability



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- Include UQ
- Efforts in both ab-initio and beyond mean field structure calculations for improved collectivity and level density



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- Integrate dispersivity and non-locality



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- Theory-experiment collaboration to address isospin dependence away from stability
- Include UQ
- Efforts in both ab-initio and beyond mean field structure calculations for improved collectivity and level density
- Integrate dispersivity and non-locality
- Extension to nucleus-nucleus OP



Part 2

How we* do it

* G. Sargsyan (MSU, FRIB Theory Fellow), J. Escher, K. Kravvaris, GP (LLNL)





We calculate the OP by coupling the system to all excited states



- Excited states, static potential, and couplings, come from structure theory input
- But how do we get the Green's function?

The solution strategy is based on an iterative procedure

$$\bigvee = - \bigcirc + \bigvee i$$

$$V(\mathbf{r}, \mathbf{r}'; E) = U_0(r) + \sum_i U_{0i}(\mathbf{r})G(E - E_i, \mathbf{r}, \mathbf{r}')U_{i0}(\mathbf{r}')$$

$$G(\mathbf{r}, \mathbf{r}', E) = \lim_{\eta \to 0} (E - T - V(\mathbf{r}, \mathbf{r}'; E) + i\eta)^{-1}$$





The solution strategy is based on an iterative procedure

$$V(\mathbf{r}, \mathbf{r}'; E) = U_0(r) + \sum_i U_{0i}(\mathbf{r})G(E - E_i, \mathbf{r}, \mathbf{r}')U_{i0}(\mathbf{r}')$$

$$G(\mathbf{r}, \mathbf{r}', E) = \lim_{\eta \to 0} (E - T - V(\mathbf{r}, \mathbf{r}'; E) + i\eta)^{-1}$$
Dyson equation verified
$$G = G_0 + G_0 VG$$



Both elastic and absorption cross sections can be calculated from the OP



$(E-T-V(\mathbf{r},\mathbf{r}';E))\,\phi=0$ \Longrightarrow elastic scattering from phase shifts

$$\sigma_{abs} \sim \langle \phi | Im(\Sigma_{i}) | \phi \rangle \Longrightarrow$$

absorption from imaginary part of polarization potential



⁴⁰Ca OP calculated in a weak coupling, collective model approximation

$$V(\mathbf{r}, \mathbf{r}'; E) = U_0(r) + \sum_i U_{0i}(\mathbf{r}) G(E - E_i, \mathbf{r}, \mathbf{r}') U_{i0}(\mathbf{r}')$$



- the static potential is a simple Woods-Saxon
- a small imaginary part *W* is included to account for the lack of absorption of the model
- this is a consequence of the oversimplification of the spectrum
- The small imaginary part spoils dispersivity

From Rao, Reeves, and Satchler, NPA 207 (1973) 182



⁴⁰Ca OP calculated in a weak coupling, collective model approximation

$$V(\mathbf{r}, \mathbf{r}'; E) = U_0(r) + \sum_i U_{0i}(\mathbf{r})G(E - E_i, \mathbf{r}, \mathbf{r}')U_{i0}(\mathbf{r}')$$



 the spectrum of ⁴⁰Ca is approximated by 6 collective vibrational states

• the deformation parameters β_{λ} are constrained by the experimental inelastic scattering cross section

$$\left| \Phi(^{41}\text{Ca}) \right\rangle_i \approx \left| \Phi(^{40}\text{Ca}) \right\rangle_i \otimes \left| \chi(n) \right\rangle_i$$

$\hat{\lambda}_n^{\pi}$	• 1-	2+	2+	3-	4+	5-
E_n (MeV) $\beta_i(n)$	18.0 0.087	3.9 0.143	8.0 0.309	3.73 0.354	8.0 0.254	4.48 0.192
$\sigma_{\mathbf{A}}$ (mb)	17	43	176	164	78	37

From Rao, Reeves, and Satchler, NPA **207** (1973) 182



⁴⁰Ca OP calculated in a weak coupling, collective model approximation

8.0

78

0.254

4.48

37

0.192

3.73

164

0.354

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3.9

43

0.143

8.0

176

0.309

18.0

17

0.087

V (MeV)

 $\hat{\lambda}_n^{\pi}$

 $\beta_{\lambda}(n)$

 E_n (MeV)

 $\sigma_{\rm A}$ (mb)



We benchmark our results against Rao et al., and look at the effect of iterations

p+⁴⁰Ca elastic scattering at 30.3 MeV 10² 10^{3} converged result 1 iteration 10² 10^{1} da/dΩ (mb/sr) dơ/dơ_{Ruth} 10^{1} 10'converged resu 10^{0} with no added WV 10^{-1} 10^{-1} 1 iteration 10^{-2} 10^{-2} 180 $\begin{array}{c} 80 & 100\\ \theta \mbox{ (degrees)} \end{array}$ 160 $\theta = 0$ 100 θ (degrees) 0 20 60 120 140 180 20 40 60 120 140 40 0

- 1 iteration calculation agrees with Rao et al. (not shown)
- Converged result different at large angles ۲

Good result for neutrons just by removing Coulomb

160

180

Added non-dispersive imaginary part W not needed for the converged result

۲

²⁴Mg+n with valence shell model




²⁴Mg+n with valence shell model





²⁴Mg+n with valence shell model



step 3: Iterative procedure

10

8

$$V(\mathbf{r}, \mathbf{r}'; E) = U_0(r) + \sum_i U_{0i}(\mathbf{r})G(E - E_i, \mathbf{r}, \mathbf{r}')U_{i0}(\mathbf{r}')$$
$$G(\mathbf{r}, \mathbf{r}', E) = (E - T - V(\mathbf{r}, \mathbf{r}'; E))^{-1}$$

- Iterate until convergence is achieved
- Consistency between potential and Green's function is achieved, as expressed by Dyson's equation:

 $G(\mathbf{r}, \mathbf{r}'; E) = G_0(\mathbf{r}, \mathbf{r}'; E) + G_0(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}, \mathbf{r}'; E)G(\mathbf{r}, \mathbf{r}'; E)$ $G_0(\mathbf{r}, \mathbf{r}'; E) = (E - T - U_0(r))^{-1}$

As a bonus, we obtain the Green's function



The dynamical polarization potential is complex, energydependent, dispersive, and non-local















-2 -4 -6 -8



The OP, the level density, and the γ strength function are connected through the same underlying physics



We can explicitly check the limits of the statistical model (Hauser-Feshbach approach)



Part 3

Extending the scope: Green's Function Transfer (GFT)







































same as for x-A scattering!









 $\langle \chi_b(\mathbf{r}_b;\mathbf{k}_b) | \Psi_0(\mathbf{r}_{xA},\mathbf{r}_b) = \langle \chi_b(\mathbf{r}_b;\mathbf{k}_b) | \left(F(\mathbf{r}_a)\phi_a(\mathbf{r}_{xb}) + G(E-E_b)\mathcal{P}(\mathbf{r}_b) \left[\mathcal{V}(E-E_b) + U_b(\mathbf{r}_b) \right] F(\mathbf{r}_a)\phi_a(\mathbf{r}_{xb}) \right)$

project over **b** state to get **x**-A wavefunction









 $\sigma_{i0}^{DWBA} \sim |\langle \psi_i | V | \psi_0 \rangle|^2 \qquad \sigma_R^{GFT}(E) \sim \langle G(E) \left(\mathcal{V}(E) + U_b \right) \psi^{HM} | \text{Im} \mathcal{V}(E) | G(E) \left(\mathcal{V}(E) + U_b \right) \psi^{HM} \rangle$















 $\sigma_{i0}^{DWBA} \sim |\langle \psi_i | V | \psi_0 \rangle|^2 \qquad \sigma_R^{GFT}(E) \sim \langle G(E) \left(\mathcal{V}(E) + U_b \right) \psi^{HM} | \text{Im} \mathcal{V}(E) | G(E) \left(\mathcal{V}(E) + U_b \right) \psi^{HM} \rangle$







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$$G(E) = (E - T - \mathcal{V}(E))^{-1}$$

- Consistency between structure and reactions
- Same ingredients as **x**-A scattering
- Need for tools for inverting Hamiltonians with non-local potentials





- Absorption of the neutron as a function of excitation energy and spin computed with GFT formalism
- We used the phenomenological Koning-Delaroche OP







- γ rays observed in coincidence with protons
- transitions from both ⁹⁵Mo and ⁹⁶Mo are identified

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PHYSICAL REVIEW LETTERS 122, 052502 (2019)

Towards Neutron Capture on Exotic Nuclei: Demonstrating $(d,p\gamma)$ as a Surrogate Reaction for (n,γ)

A. Ratkiewicz,^{1,2,*} J. A. Cizewski,² J. E. Escher,¹ G. Potel,^{3,4} J. T. Burke,¹ R. J. Casperson,¹
M. McCleskey,⁵ R. A. E. Austin,⁶ S. Burcher,² R. O. Hughes,^{1,7} B. Manning,² S. D. Pain,⁸
W. A. Peters,⁹ S. Rice,² T. J. Ross,⁷ N. D. Scielzo,¹ C. Shand,^{2,10} and K. Smith¹¹



- The obtained Hauser-Feshbach parameters are used to calculate (n,γ)
- We found an excellent agreement with the direct measurement.









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Cavallaro et al., PRL 118, 012701 (2017)

Barranco, GP, Vigezzi, Broglia PRC 101, 031305(R) (2020)




Applications: population of low-lying dipole states in ¹²⁰Sn(1⁻) with (d,p) reactions

PHYSICAL REVIEW LETTERS 127, 242501 (2021)









connection between direct and indirect R-matrix parameters example:

- direct: α scattering $(T_{i0}(E))$
- indirect: $(^{6}\text{Li},d)$. $(T'_{i0}(E))$



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- direct: α scattering $(T_{i0}(E))$
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indirect
T-matrix
$$T_{i0}^{I}(E) = \int T_{i0}(E_k) g(\mathbf{k}; E) d\mathbf{k}.$$

direct
T-matrix



connection between direct and indirect R-matrix parameters example:

- direct: α scattering $(T_{i0}(E))$
- indirect: $(^{6}\text{Li},d)$. $(T'_{i0}(E))$

indirect
T-matrix
$$E_{k} = \frac{\hbar^{2}k^{2}}{2\mu}$$

$$T_{i0}^{I}(E) = \int T_{i0}(E_{k}) g(\mathbf{k}; E) d\mathbf{k}.$$
direct
T-matrix

















- If the broadening distribution is narrow, the T-matrix can be evaluated at the peak
- This is essentially the approximation made by Barker in Aust. J. Phys. 20 (341) 1967 for isolated resonances

$$T_{i0}^{I} = \int \sqrt{P_{i}(E_{k})P_{0}(E_{k})} \sum_{pq} \frac{\gamma_{ip}\gamma_{0q}}{(E_{p} - E_{k})\delta_{pq} - \sum_{c}\gamma_{ic}\gamma_{jc}(S_{c}(E_{k}) + iP_{c}(E_{k})))} g(\mathbf{k}) d\mathbf{k}.$$

$$T_{i0}^{I} \approx \sqrt{P_{i}(E_{k}^{max})P_{0}(E_{k}^{max})} \sum_{pq} \frac{\gamma_{ip}\gamma_{0q}}{(E_{p} - E_{k}^{max})\delta_{pq} - \sum_{c}\gamma_{ic}\gamma_{jc}(S_{c}(E_{k}^{max}) + iP_{c}(E_{k}^{max})))} \int g(\mathbf{k}) d\mathbf{k}.$$

T

Conclusions and some perspectives

- The calculation of the OP provides a flexible and versatile connection between structure and reactions, including 3-body reactions (with GFT)
- It can be used across different regimes (compound vs direct; bound vs unbound...)

what's next?

- Implement the recommendations of the community.
- Disentangle direct, pre-equilibrium, and compound reactions.
- Explore the limits of validity of the statistical model.
- Systematic implementation for deformed nuclei



Thank you!





is ⁹He parity-inverted?

the parity of the unbound ⁹He ground state is still controversial





is ⁹He parity-inverted?

the parity of the unbound ⁹He ground state is still controversial K. Fossez, J. Rotureau, W. Nazarewicz. Phys. Rev. C **98** (2018) 061302(R)



we use a structure approach with explicit inclusion of the continuum (K. Fossez)



3

2

-2

-3

 $E-E(^{4}\mathrm{He})(\mathrm{MeV})$

 $1/2^{-}$

3/2

He chain

5



is ⁹He parity-inverted?

the parity of the unbound ⁹He ground state is still controversial we use a structure approach with explicit inclusion of the continuum (K. Fossez)

A

K. Fossez, J. Rotureau, W. Nazarewicz. Phys. Rev. C **98** (2018) 061302(R)

 $5/2^{-}$

G-DMRG 🛋

 $= 5/2^+$

 $\frac{1/2^{-}}{1/2^{+}}$ _ 0⁺

9

10

🛰 Exp



with the GFT formalism we can "translate" neutron elastic scattering into (d,p) cross sections





we are partnering with experimentalists Y. Ayyad and A. Macchiavelli to prepare a proposal for the ⁸He(d,p)⁹He measurement at FRIB



Thank you for your attention!



Thanks to my collaborators:

Jutta Escher, Kostas Kravvaris



K. Fossez (FSU)A. O. Macchiavelli (ORNL)Y. Ayyad (U of Santiago de Compostela)

Grigor Sargsyan



Theory Alliance facility for rare isotope beams ⁹⁵Mo: A. Ratkiewicz, J. Escher, J. Burke, R. Casperson, R. Hughes, N. Scielzo (LLNL), J. Cizewski, S. Burcher, B. Manning, S. Rice, C. Shand (Rutgers), M. McCleskey (TAMU), R. Austin (St Mary's), S. Pain (ORNL), W. Peters (U of Tennessee), T. Ross (U of Richmond) and K. Smith (LANL).

¹²⁰Sn: M. Weinert, M. Müscher, J. Wilhelmy, A. Zilges (U of Cologne), M. Spieker (FSU), N. Tsoneva (ELI-NP).









- The absorption probability of the neutron is calculated with the OP
- Within the Hauser-Feshbach formalism, it is encoded in the transmission coefficients









- Neutron emission competes with γ emission
- γ emission probability is calculated from the γ strength function
- if γ wins, the neutron is captured in a bound state





- Neutron scattering cannot be performed on radioactive nuclei
- Surrogate inverse kinematics (d,pγ) reactions can be performed instead
- The process is described within Green's Function Transfer (GFT) formalism





- As a first step, the OP breaks the deuteron
- We assume that the proton doesn't play any subsequent role (spectator approximation)





 The Green's function is used to describe the neutron-nucleus propagation





 The Green's function is used to describe the neutron-nucleus propagation





 The Green's function is used to describe the neutron-nucleus propagation









- The rest is history!
- The photon is detected in coincidence with the proton



Capture processes: direct capture





Capture processes: direct capture



$$T_{if}^d = \langle \phi_i^s | A | \phi_f \rangle$$

- process favored if strong resonances are not present
- electromagnetic T-matrix accounts for the quantum amplitude from the scattering state to the final bound state



nucleon in vacuum with external field U $\left(E-T-U\right)\chi_0=0$



nucleon in vacuum with external field U $(E - T - U) \chi_0 = 0$ nucleon in a medium with 2 intrinsic states ϕ_0 and ϕ_1 $\Psi = \phi_0 \chi_0 + \phi_1 \chi_1$



nucleon in vacuum with external field U $(E - T - U) \chi_0 = 0$ nucleon in a medium with 2 intrinsic states ϕ_0 and ϕ_1 $\Psi = \phi_0 \chi_0 + \phi_1 \chi_1$ the nucleon couples to the medium $(E - T - U) \chi_0 = U_{01} \chi_1$ $(E - \epsilon_1 - T - U) \chi_1 = U_{01}^* \chi_0$



the nucleon couples to the medium $(E - T - U) \chi_0 = U_{01}\chi_1$ $(E - \epsilon_1 - T - U) \chi_1 = U_{01}^* \chi_0$ we manipulate the second equation

$$\chi_1 = \lim_{\eta \to 0} \left(E - \epsilon_1 - T - U + i\eta \right)^{-1} U_{01}^* \chi_0 = G(E - \epsilon_1) U_{01}^* \chi_0$$



the nucleon couples to the medium $(E - T - U) \chi_0 = U_{01} \chi_1$ $(E - \epsilon_1 - T - U) \chi_1 = U_{01}^* \chi_0$ we manipulate the second equation $\chi_1 = \lim_{\eta \to 0} \left(E - \epsilon_1 - T - U + i\eta \right)^{-1} U_{01}^* \chi_0 = G(E - \epsilon_1) U_{01}^* \chi_0$ where we have defined the Green's function $G(E) = \lim_{n \to 0} (E - T - U + i\eta)^{-1}$



the nucleon couples to the medium $(E - T - U) \chi_0 = U_{01}\chi_1$ $(E - \epsilon_1 - T - U) \chi_1 = U_{01}^*\chi_0$

substituting in the first equation

$$(E - T - U) \chi_0 = U_{01}G(E - \epsilon_1)U_{01}^*\chi_0$$



the nucleon couples to the medium $(E - T - U) \chi_0 = U_{01}\chi_1$ $(E - \epsilon_1 - T - U) \chi_1 = U_{01}^*\chi_0$

substituting in the first equation

$$(E - T - U) \chi_0 = U_{01}G(E - \epsilon_1)U_{01}^*\chi_0$$

we define the optical potential

$$\mathcal{V}(E) = U + U_{01}G(E - \epsilon_1)U_{01}^*$$

 $(E - T - \mathcal{V}(E))\chi_0 = 0$


Self energy in a nutshell

the nucleon couples to the medium

$$(E - T - U) \chi_0 = U_{01}\chi_1$$
$$(E - \epsilon_1 - T - U) \chi_1 = U_{01}^*\chi_0$$

substituting in the first equation

$$(E - T - U) \chi_0 = U_{01} G(E - \epsilon_1) U_{01}^* \chi_0$$

we define the optical potentia

$$\mathcal{V}(E) = U + U_{01}G(E - \epsilon_1)U_{01}^*$$

$$(E - T - \mathcal{V}(E))\chi_0 = 0$$





Self energy in a nutshell





Dispersion (Kramers-Kronig) relations

$$\mathcal{V}(E) = \lim_{\eta \to 0} \frac{U_{01}^*(r)U_{01}(r')}{E - T - U + i\eta} = \lim_{\eta \to 0} \frac{U_{01}^*(r)U_{01}(r')(E - T - U - i\eta)}{(E - T - U)^2 + \eta^2}$$

$$\operatorname{Re}\mathcal{V}(E) = \frac{U_{01}^*(r)U_{01}(r')}{(E - T - U)}; \quad \operatorname{Im}\mathcal{V}(E) = -\pi U_{01}^*(r)U_{01}(r')\delta(E - T - U)$$

$$\operatorname{Re}\mathcal{V}(E) = -\frac{1}{\pi} \int \frac{\operatorname{Im}\mathcal{V}(E')}{(E - T - U)} \, dE'$$



Eur. Phys. J. A (2017) 53: 178

THE EUROPEAN Toward a complete theory for predicting inclusive deuteron **PHYSICAL JOURNAL A**





is ⁶¹Ca bound?







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An extension to holes: The Green's function knockout (GFK) and the asymmetry plot







An extension to holes: The Green's function knockout (GFK) and the asymmetry plot

PHYSICAL REVIEW C 107, 014607 (2023)

Green's function knockout formalism

C. Hebborn $\mathbb{D}^{1,2,*}$ and G. Potel $\mathbb{D}^{2,\dagger}$

(talk by J. Gómez Camacho)



When we include the coupling to the electromagnetic field, we can compute the (n,γ) cross section





When we include the coupling to the electromagnetic field, we can compute the (n,γ) cross section



where
$$T_{i,\lambda}$$
 is the partial γ width, calculated with, e.g., the shell model



An equivalent expansion in powers of the couplings can shed light on direct, preequilibrium, and compound processes





An equivalent expansion in powers of the couplings can shed light on direct, preequilibrium, and compound processes





An equivalent expansion in powers of the couplings can shed light on direct, preequilibrium, and compound processes





Some strong single-particle states are also strong γ absorbers/emitters

