The Surface Operator for Transfers

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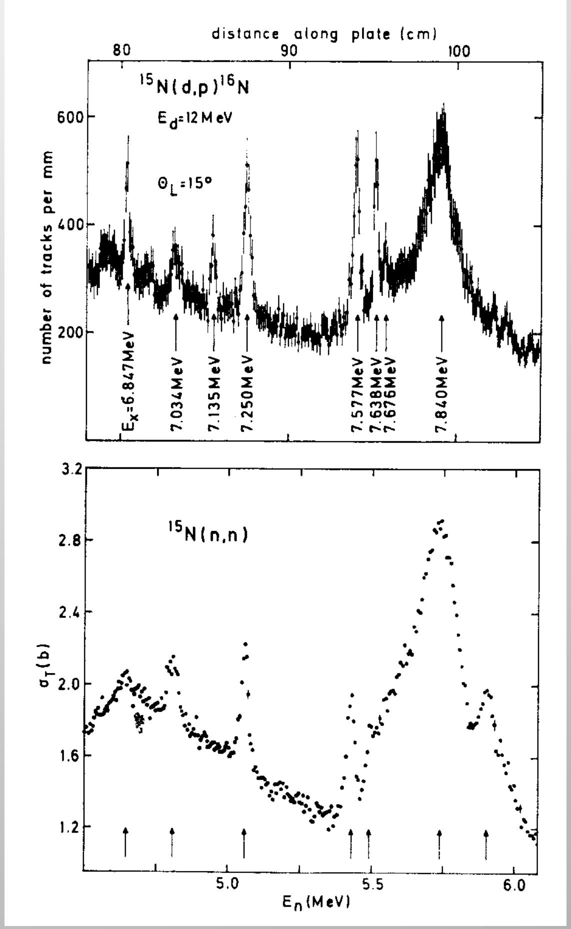
Outline

- Aim
- Splitting the Transfer Matrix Element
- Definition of Surface Operator
- Calculation in a partial-wave basis
- Implementation
- R-matrix fits (surface, interior, exterior)
- Role in transfer calculations

Role in transfer calculations

- Aim is to fit resonances in (d,p) cross sections in a region of the continuum.
- We see many wide and narrow resonances, often overlapping.
- Want to find neutron pole energies and partial widths, in entrance channel for (n,γ)



Splitting the Transfer Matrix Element

- Define $T_{post}(a,b)$ & $T_{prior}(a,b)$ with a < r' < b limits

Mukhamedzhanov (PRC **84**, 044616, 2011) showed for any ρ:

$T = T_{post}(0,\rho) + T_{surf}(\rho) + T_{prior}(\rho,\infty)$

where $T_{surf}(\rho) = \langle f_p^{(-)}\,\phi_n \,|[\overleftarrow{T} - \overrightarrow{T}]|\, \phi_d\, f_d^{(+)}\rangle_{(in)}$

- Evaluate:

$$\int_{r\leqslant R} \mathrm{d}\mathbf{r}\, f(\mathbf{r})[\overleftarrow{T} - \overrightarrow{T}]g(\mathbf{r})$$

$$= -\frac{1}{2\mu}\oint_{r=R} \mathrm{d}\mathbf{S}[g(\mathbf{r})\nabla_{\mathbf{r}} f(\mathbf{r}) - f(\mathbf{r})\nabla_{\mathbf{r}} g(\mathbf{r})]$$

$$= -\frac{1}{2\mu}R^2\int \mathrm{d}\Omega_{\mathbf{r}}\left[g(\mathbf{r})\frac{\partial f(\mathbf{r})}{\partial r} - f(\mathbf{r})\frac{\partial g(\mathbf{r})}{\partial r}\right]_{r=R}$$

Choice of boundary ρ: see in Jutta's talk

Definition of Surface Operator

- Normal post-form source term:

$$S_\beta^{\mathrm{CDCC:post}}(R') = \langle \phi_\beta(r') Y_\beta(\hat{R}', \hat{r}') | \mathcal{V}_{\mathrm{post}} | \psi^{JM}_{\mathrm{CDCC}}(\mathbf{R}, \mathbf{r}) \rangle$$

- To use in transfer exit-channel eqn:

$$[H_\beta(R') - E_\beta] u_\beta(R') + S^{\mathrm{surf}}_{\beta\alpha}(R') = 0 \ .$$

- Surface form of source term:

$$= -\frac{\hbar^2 \rho^2}{2\mu_n} \left[\frac{\partial \phi_\beta(r')}{\partial r'} - \phi_\beta(r') \frac{\partial}{\partial r'} \right] \left\langle Y_\beta(\hat{R}', \hat{r}') \middle| \psi_{\mathrm{CDCC}}(\mathbf{R}, \mathbf{r}) \right\rangle_{r'=\rho}$$

  - depends on bound state and its derivative only at r' = ρ

Calculation in a partial-wave basis

- In a partial wave basis with channel α, the derivative terms (wrt r') are:

$$\hat{\mathcal{S}}^{D}_{\beta\alpha} = -\frac{\hbar^2\rho^2}{2\mu_n}\phi_\beta(\rho) \left\langle Y_\beta(\hat{R}',\hat{r}')\delta(r'-\rho)\right| \frac{\partial}{\partial r'} \langle \hat{R},\hat{r}\,|\alpha\rangle \frac{1}{rR}\varphi_\alpha(r)u_\alpha(R)\Big\rangle$$

- Need derivatives of spherical harmonics $Y_\ell(\hat{\mathbf{r}})$ when $\mathbf{r} = p\mathbf{r}' + q\mathbf{R}'$

$$\frac{\partial}{\partial r'}Y^m_\ell(\hat{\mathbf{r}}) = -\frac{p\ell}{r}\,\hat{\mathbf{r}}\cdot\hat{\mathbf{r}'}\,Y^m_\ell(\hat{\mathbf{r}}) + p\sqrt{\frac{4\pi\ell(2\ell+1)}{3}}\,\frac{1}{r}\sum_{\lambda=-1}^{1} Y^{m-\lambda}_{\ell-1}(\hat{\mathbf{r}})Y^\lambda_1(\hat{\mathbf{r}'})\langle \ell{-}1\; m{-}\lambda, 1\lambda|\ell m\rangle$$

- So $\frac{\partial}{\partial r'}Y^m_\ell(\hat{\mathbf{r}})\frac{\varphi_\alpha(r)}{r}$ is

$$= \frac{p}{r}\left\{\sqrt{\frac{4\pi\ell(2\ell+1)}{3}}\frac{\varphi_\alpha(r)}{r}\sum_{\lambda=-1}^{1}\langle \ell{-}1\; m{-}\lambda, 1\lambda|\ell m\rangle Y^{m-\lambda}_{\ell-1}(\hat{\mathbf{r}})Y^\lambda_1(\hat{\mathbf{r}'}) + Y^m_\ell(\hat{\mathbf{r}})\hat{\mathbf{r}}\cdot\hat{\mathbf{r}'}\left[\varphi'_\alpha(r) - \frac{\ell+1}{r}\varphi_\alpha(r)\right]\right\}$$

Derivatives of products of 2 wfns

$$\frac{\partial}{\partial r'}\langle \hat{R}, \hat{r}\,|\alpha\rangle \frac{1}{rR}\,\varphi_\alpha(r)u_\alpha(R) = \frac{1}{rR}\sum_{M_L m_\ell} C_\alpha^{M_L m_\ell : M}$$

$$\Bigg(Y_L^{M_L}(\hat{\mathbf{R}})u_\alpha(R)\frac{p}{r}\Bigg\{\sqrt{\frac{4\pi\ell(2\ell{+}1)}{3}}\sum_{\lambda=-1}^{1}\langle \ell{-}1\ m{-}\lambda, 1\lambda|\ell m\rangle Y_{\ell-1}^{m-\lambda}(\hat{\mathbf{r}})Y_1^{\lambda}(\hat{\mathbf{r}'})\frac{\varphi_\alpha(r)}{r}$$

$$+\,Y_\ell^m(\hat{\mathbf{r}})\ \hat{\mathbf{r}}\cdot\hat{\mathbf{r}'}\left[\varphi'_\alpha(r) - \frac{\ell{+}1}{r}\varphi_\alpha(r)\right]\Bigg\}$$

$$+\,Y_\ell^{m_\ell}(\hat{\mathbf{r}})\varphi_\alpha(r)\frac{P}{R}\Bigg\{\sqrt{\frac{4\pi L(2L{+}1)}{3}}\sum_{\Lambda=-1}^{1}\langle L{-}1\ M_L{-}\Lambda, 1\Lambda|LM_L\rangle Y_{L-1}^{M_L-\Lambda}(\hat{\mathbf{R}})Y_1^{\Lambda}(\hat{\mathbf{r}'})\frac{u_\alpha(R)}{R}$$

$$+\,Y_L^{M_L}(\hat{\mathbf{R}})\ \hat{\mathbf{R}}\cdot\hat{\mathbf{r}'}\left[u'_\alpha(R) - \frac{L{+}1}{R}u_\alpha(R)\right]\Bigg\}\quad\Bigg)$$

$$\mathbf{r} = p\mathbf{r}' + q\mathbf{R}'$$

$$\mathbf{R} = P\mathbf{r}' + Q\mathbf{R}'$$

Source term complete for r,R wfns

$$S^{\rm surf}_{\beta\alpha}(R') = -\frac{\hbar^2\rho^2}{2\mu_n} \sum_{M'_L m'_\ell M_L m_\ell} F_\beta^{M'_L m'_\ell:M*} C_\alpha^{M_L m_\ell:M} \langle Y_{L'}^{M'_L}(\hat{\mathbf{R}}')\ Y_{\ell'}^{m'_\ell}(\hat{\mathbf{r}}')|_{r'=\rho}\frac{1}{rR}$$

$$\Bigg[\phi'_\beta(\rho)\ \ Y_\ell^{m_\ell}(\hat{\mathbf{r}})\ Y_L^{M_L}(\hat{\mathbf{R}})\quad \varphi_\alpha(r)\ u_\alpha(R)$$

$$-\ \phi_\beta(\rho)\Bigg(Y_L^{M_L}(\hat{\mathbf{R}})u_\alpha(R)\frac{p}{r}\Bigg\{\sqrt{\frac{4\pi\ell(2\ell{+}1)}{3}}\sum_{\lambda=-1}^{1}\langle\ell{-}1\ m{-}\lambda, 1\lambda|\ell m\rangle Y_{\ell-1}^{m-\lambda}(\hat{\mathbf{r}})Y_1^\lambda(\hat{\mathbf{r}'})\frac{\varphi_\alpha(r)}{r}$$

$$+\ Y_\ell^m(\hat{\mathbf{r}})\ \hat{\mathbf{r}}\cdot\hat{\mathbf{r}'}\left[\varphi'_\alpha(r) - \frac{\ell{+}1}{r}\varphi_\alpha(r)\right]\Bigg\}$$

$$+\ Y_\ell^{m_\ell}(\hat{\mathbf{r}})\varphi_\alpha(r)\frac{P}{R}\Bigg\{\sqrt{\frac{4\pi L(2L{+}1)}{3}}\sum_{\Lambda=-1}^{1}\langle L{-}1\ M_L{-}\Lambda, 1\Lambda|LM_L\rangle Y_{L-1}^{M_L-\Lambda}(\hat{\mathbf{R}})Y_1^\Lambda(\hat{\mathbf{r}'})\frac{u_\alpha(R)}{R}$$

$$+\ Y_L^{M_L}(\hat{\mathbf{R}})\ \hat{\mathbf{R}}\cdot\hat{\mathbf{r}'}\left[u'_\alpha(R) - \frac{L{+}1}{R}u_\alpha(R)\right]\Bigg\}\quad\Bigg)\Bigg].$$

The $F_\beta^{M'_L m'_\ell:M*} C_\alpha^{M_L m_\ell:M}$ are the channel-defining Clebsch-Gordon coefs.

Racah-algebra or m-state evaluation?

Two methods:

1. Convert all $\hat{\mathbf{R}} \cdot \hat{\mathbf{r}'}$ dot-products and all spherical-harmonic products, to sums of single harmonics.

2. Evaluate *m*-sums directly in suitable coordinate frame. Follow Tamura & Udagawa (1979):

Choose z-axis parallel to R,

and x-axis in plane with R and R'.

Then: r and r' also in this plane.

Remaining numerical variable is $\cos\theta \doteq \hat{\mathbf{R}} \cdot \hat{\mathbf{R}}'$

Evaluation in Tamura frame

- Integral operators, for given $\mathbf{R}'$, $\mathbf{r}'$:

$$\int d\hat{\mathbf{R}}' \int d\hat{\mathbf{r}}' \; \delta(r' - \rho) = \left. \frac{8\pi^2 \rho}{2abRR'} \right|_{u=(\rho^2 - a'^2 R^2 + b'^2 R'^2)/(2abRR')}$$

- No u integral needed.
All spherical harmonics in the x-z plane ($\phi = 0$).

$$Y_L^{M_L}(\hat{\mathbf{R}}) = \delta_{M_L,0} \sqrt{\frac{4\pi}{2L+1}}$$

$$r = \sqrt{(a^2 R^2 + b^2 R'^2 + 2abRR'u)}$$

$$\cos(\theta_{R'}) = u$$

$$\cos(\theta_{r'}) = (a'R + b'R'u)/r' \quad \text{from} \quad \mathbf{r}' = a'\mathbf{R} + b'\mathbf{R}'$$

$$\cos(\theta_r) = (aR + bR'u)/r$$

$$\hat{\mathbf{R}} \cdot \hat{\mathbf{r}}' = \hat{\mathbf{r}}'_z = \cos(\theta_{r'}).$$

Implementation

- As $\mathbf{R}' \neq \mathbf{R}'$, transfer couplings are still non-local
- With A, B, C as non-local operators, the transfer-channel exit equation is

$$[H_\beta - E_\beta]u_\beta + \phi'_\beta(\rho)\ \mathsf{A}_{\beta\alpha} u_\alpha + \phi_\beta(\rho)\ \mathsf{B}_{\beta\alpha} u_\alpha + \phi_\beta(\rho)\ \mathsf{C}_{\beta\alpha} \left[u'_\alpha - \frac{L_\alpha + 1}{R} u_\alpha\right] = 0$$

- More complicated than standard transfers, because of derivative $u'_\alpha(R)$

R-matrix continuum parameterisation

- Definition $\mathsf{R}(e_\beta) = \frac{1}{\rho}\frac{\phi(\rho;e_\beta)}{\phi'(\rho;e_\beta)}$
- Parameterization: $\mathsf{R}(e_\beta) = \sum_{p=1}^{N} \frac{\gamma_p^2}{\varepsilon_p - e_\beta}$ (N-pole case)
- From $\mathsf{R}(e_\beta)$, get S-matrix $\mathsf{S}(e_\beta)$ and wf $\phi_\beta(\rho;e_\beta)$ by usual theory, for every energy $e_\beta = E_{\rm tot} - E_\beta$
- Then exit channel eqn, for continuous E_β is

$$[H_\beta - E_\beta]u_\beta + \phi_\beta(\rho;e_\beta)\left\{\frac{1}{\rho\mathsf{R}_\beta(e_\beta)}\mathsf{A}_{\beta\alpha}u_\alpha + \mathsf{B}_{\beta\alpha}u_\alpha + \mathsf{C}_{\beta\alpha}\left[u'_\alpha - \frac{L_\alpha+1}{R}u_\alpha\right]\right\} = 0$$

Note that A, B, C and u_α are independent of exit energy E_β.

Exterior-Prior Contributions in R fits

- Jutta shows that these are often needed.
- Even in CDCC, because of energy dependence of the neutron optical potential.
- If ρ is outside the neutron binding potential, then the continuum wfn is just asymptotic form for given S-matrices $\mathsf{S}(e_\beta)$:

$$\phi_\beta(r'; e_\beta) = \frac{i}{2}[H^-(k_\beta r') - \mathsf{S}(e_\beta) H'^-(k_\beta r')]$$

- So, fortunately, these do depend just on the R pole and reduced width parameters via $\mathsf{S}(e_\beta)$

Interior-Post Contributions in R fit

- Jutta shows that these are often needed
- This contribution may be small sometimes, but does depend on the interior neutron wfns.
- Hence depends on the Spectroscopic Factor (the interior square norm of the wfn).
- Can imagine a method where ANC is main observable, and the SF is subsidiary result with larger uncertainties.

Calculating the Interior-Post in R fits

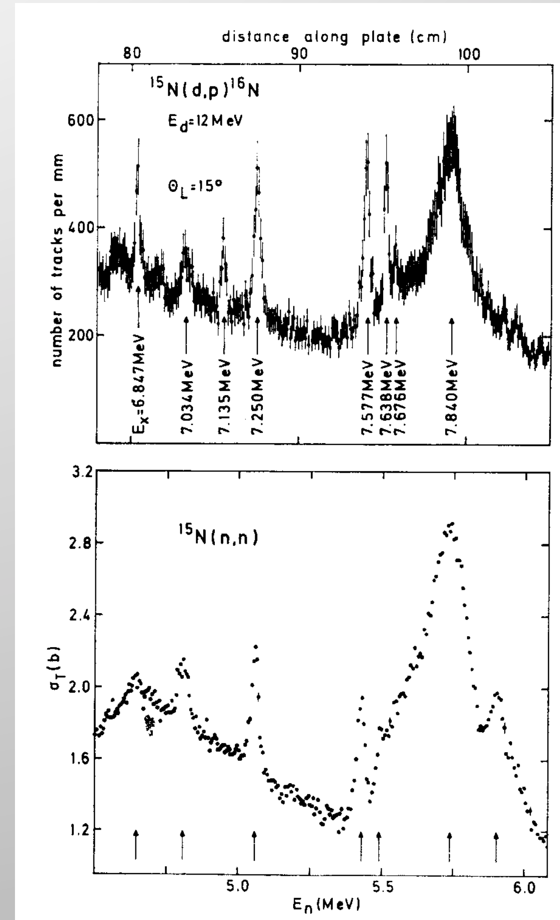
- This depend on wfs $w_p(r')$ that are eigenfunctions of interior Hamiltonian at the R-matrix pole energies ε_p, and normalized to unity over radial interval $[0, \rho]$.
- Given these, the scattering wf at any energy e_β is

$$\phi_\beta(r') = \sum_{p=1}^{N} \frac{\hbar^2}{2\mu\rho} \frac{w_p(\rho)}{\varepsilon_p - e_\beta} \phi'_\beta(\rho) w_p(r')$$

- Note that $\gamma_p = \sqrt{\frac{\hbar^2}{2\mu\rho}}\, w_p(\rho)$, so only shape of $w_p(r')$ is needed, as long as normalized correctly, & at ε_p

Role in transfer calculations

- Aim is to fit neutron pole energies and partial widths to (d,p) cross sections across a resonance.
- We see many wide and narrow resonances, often overlapping.
- Can be generalized to multichannel exit wfs $\phi_\beta(\rho; e_\beta)$



Data from Hewka et al, NP **88**, 561 (1966)

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