

Separable Approximation to Optical Potentials

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Outline

- **Fourier transform of Wood-Saxon**
- **Momentum space: Comparison with FRESCO**
 - scattering phase shifts
 - bound states
- **Rank-1 separable potentials**
 - Unitary pole approximation (UPA)
 - Extension to positive energies (EST)

Wood-Saxon potential Fourier transform

- Coordinate space potential

$$U_{\text{nucl}}(r) = V(r) + i(W(r) + W_s(r)).$$

where

$$V(r) = \frac{-V_r}{1 + \exp\left(\frac{r-R_r}{a_r}\right)},$$

$$W(r) = \frac{-V_i}{1 + \exp\left(\frac{r-R_i}{a_i}\right)}$$

$$W_s(r) = \frac{-V_s \times 4 \times \exp\left(\frac{-(r-R_s)}{a_s}\right)}{\left(1 + \exp\left(\frac{-(r-R_s)}{a_s}\right)\right)^2},$$

- From contour Integration (thanks R. C. Johnson)

$$\bar{V}(\mathbf{q}) = \frac{V_r}{\pi^2} \left\{ \frac{\pi a e^{-\pi a q}}{q(1 - e^{-2\pi a q})^2} \left[R_0 (1 - e^{-2\pi a q}) \cos(qR_0) - \pi a (1 + e^{-2\pi a q}) \sin(qR_0) \right] - a^3 e^{-\frac{R_0}{a}} \left[\frac{1}{(1 + a^2 q^2)^2} - \frac{2e^{-\frac{R_0}{a}}}{(4 + a^2 q^2)^2} \right] \right\}, \quad (18)$$

$$\begin{aligned} \bar{W}_s(\mathbf{q}) = & -4a_s \frac{V_s}{\pi^2} \left\{ \frac{\pi a e^{-\pi a q}}{(1 - e^{-2\pi a q})^2} \right. \\ & \left[\left(\pi a (1 + e^{-2\pi a q}) - \frac{1}{q} (1 - e^{-2\pi a q}) \right) \cos(qR_s) + R_s (1 - e^{-2\pi a q}) \sin(qR_s) \right] \\ & \left. + a^2 e^{-R_s/a} \left[\frac{1}{(1 + a^2 q^2)^2} - \frac{4e^{-R_s/a}}{(4 + a^2 q^2)^2} \right] \right\}, \quad (19) \end{aligned}$$

Scattering properties

- Lippmann-Schwinger equation

$$t_l(k, k') = v_l(k, k') + \int_0^\infty dk'' k''^2 v_l(k, k'') \frac{1}{E - k'^2/2\mu + i\varepsilon} t_l(k'', k'),$$

- solved as linear system with `zgesv` from `lapack` (~50 pts)

- partial wave projection

$$v_l(k, k') = 2\pi \int_{-1}^1 d\cos\theta P_l(\cos\theta) U(\sqrt{k^2 + k'^2 - 2kk'\cos\theta})$$

- evaluated by Gauss-Legendre integration (~ 15 pts)

- transition amplitude and S-matrix

$$\tau_l(E) = -\pi\mu k_0 t_l(k_0, k_0),$$

$$s_l(E) = 1 + 2i \tau_l(E)$$

- phase shifts and inelasticity

$$\delta_l = \frac{1}{2} \arctan\left(\frac{\Re\tau_l}{\frac{1}{2} - \Im\tau_l}\right)$$

$$\eta_l = \sqrt{1 + 4[(\Re\tau_l)^2 + (\Im\tau_l)^2 - \Im\tau_l]}$$

Half-Shell n-⁴⁸Ca potential (CH89) --- s-wave

top: $E_{cm} = 5$ MeV , bottom: $E_{cm} = 45$ MeV ---- $p^2 = 2 \mu E_{cm}$

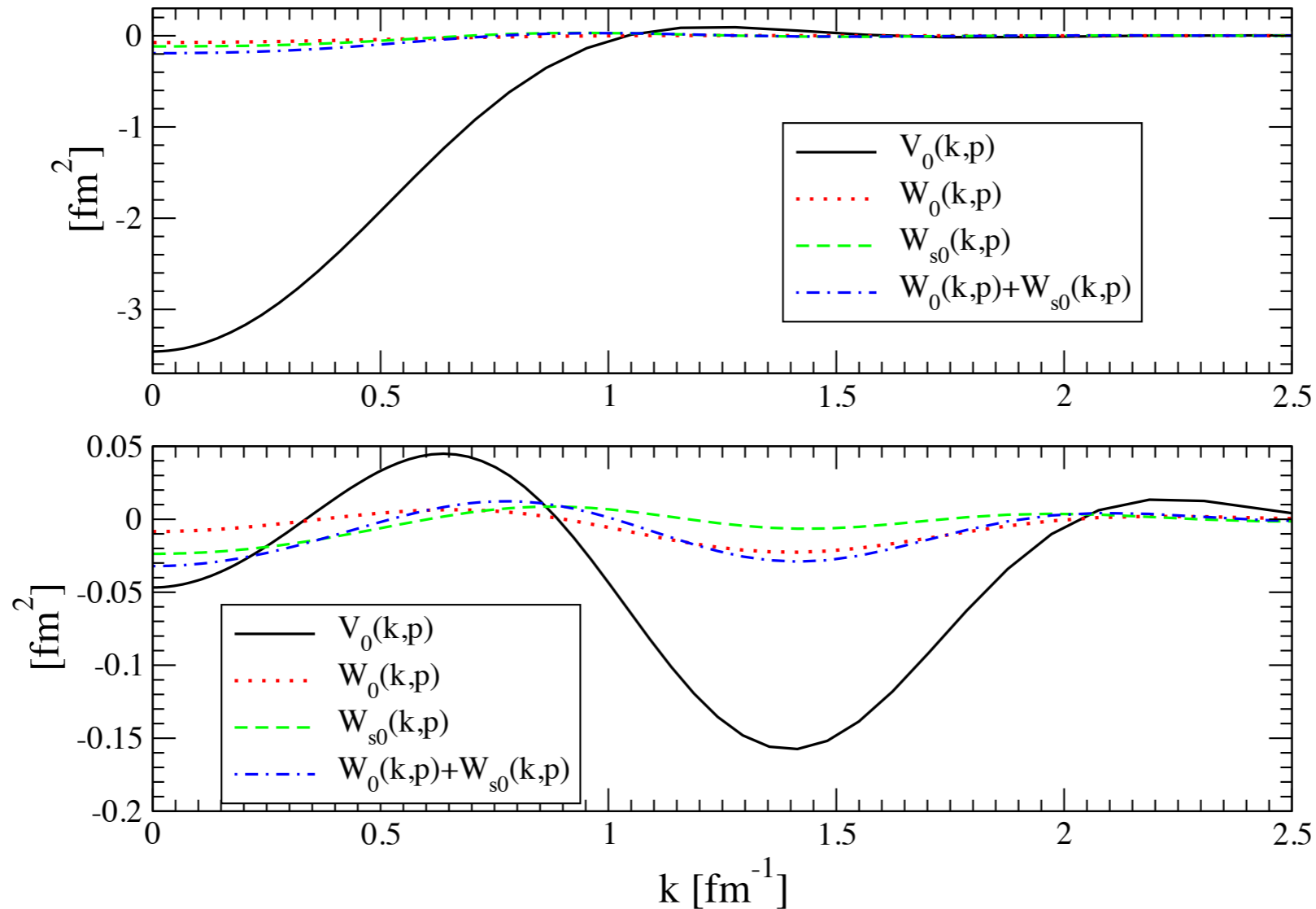


Figure 3: The real and imaginary parts to of the s-wave projected half-shell n+⁴⁸Ca optical potential as function of k for fixed momentum p , where $p^2 = 2\mu E_{c.m.}$. The top panel shoes $E_{c.m.} = 5$ MeV, the bottom panel $E_{c.m.} = 45$ MeV. The calculations use $R_r = r_r(A^{1/3} + 1)$.

on-shell t-matrix for Wood-Saxon Potential $U_{\text{nucl}}(q)$

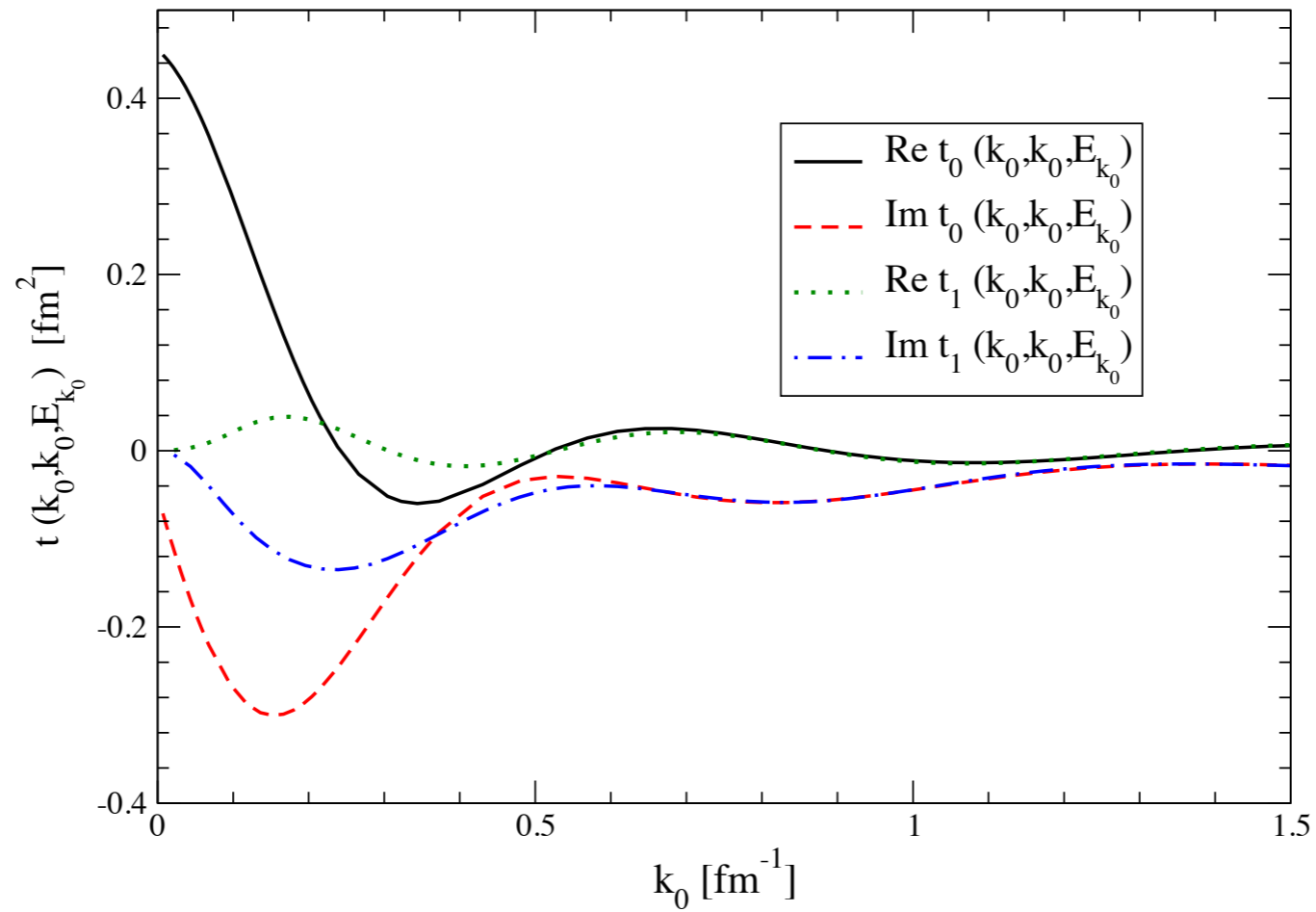


Figure 5: The real and imaginary parts to of the s-wave ($t_0(k_0, k_0, E_{k_0})$) and p-wave ($t_1(k_0, k_0, E_{k_0})$) projected on-shell shell t-matrix solved with the $n+^{48}\text{Ca}$ optical potential U_{nucl} as function of the on-shell momentum k_0 . The calculations use $R_r = r_r(A^{1/3} + 1)$.

p-space, r-space comparison: phase shifts

E_{lab} [MeV]	E_{cm} [MeV]	δ_0 [deg]		
		k – space	r – space	Neelam
5.00	4.897	-64.068	-64.071	-64.222
10.00	9.794	74.685	74.685	74.570
20.00	19.588	22.463	22.462	22.379
40.00	39.176	-38.026	-38.027	-38.084
50.00	48.970	-58.696	-58.697	-58.746

- k-space : code LH
- r-space : code CE
- Neelam : Fresco

p-space, r-space comparison: bound states

	n = 2	n = 1	n = 2	n = 1
	bound state code		Fresco	
l=0	15.7097	37.805	16.0284	37.9552
l=1	5.1160	28.295	5.4322	28.5426
l=2	17.691		18.03	
l=3	6.5228			

- bound state code : solves the equation

$$\psi_l(p) = \frac{1}{E_{b,l} - \frac{p^2}{2\mu}} \int dp' p'^2 v_l(p, p') \psi_l(p').$$

- returns wave function and binding energy
solved as linear system with dgeev from lapack

Unitary Pole Approximation (UPA)

- two body t-matrix

$$t = v + vgv$$

- spectral representation

$$1 = \sum_B |\Psi_B\rangle\langle\Psi_B| + \int d^3k |\Psi_k^{(+)}\rangle\langle\Psi_k^{(+)}|$$

- leads to

$$\begin{aligned} \langle\mathbf{k}|t(z)|\mathbf{k}'\rangle &= \langle\mathbf{k}|v|\mathbf{k}'\rangle + \sum_B \frac{\langle\mathbf{k}|v|\Psi_B\rangle\langle\Psi_B|v|\mathbf{k}'\rangle}{z - E_b} \\ &\quad + \int d^3q \frac{\langle\mathbf{k}|v|\Psi_q^{(+)}\rangle\langle\Psi_q^{(+)}|v|\mathbf{k}'\rangle}{z - E_q} . \end{aligned}$$

- Hence for $z \rightarrow E_B \equiv -|E_B|$

$$t(z) \simeq \frac{v|\Psi_B\rangle\langle\Psi_B|v}{z + E_B} .$$

UPA

- Ansatz for separable potential

$$V \equiv v|\Psi_B\rangle\langle\Psi_B|v$$

- rank-1 t-matrix

$$t(z) = |h\rangle\tau(z)\langle h| = \frac{|h\rangle\langle h|}{\frac{1}{\lambda} - \langle h|g_0(z)|h\rangle},$$

- at the pole

$$\frac{1}{\lambda} = \langle\Psi_B|vg_0(-E_B)v|\Psi_B\rangle = \langle\Psi_B|v\frac{1}{z + E_B}v|\Psi_B\rangle = \langle\Psi_B|v|\Psi_B\rangle,$$

- t-matrix becomes

$$t(z) = \frac{v|\Psi_B\rangle\langle\Psi_B|v}{\langle\Psi_B|(v - vg_0(z)v)|\Psi_B\rangle}$$

- Explicitly

$$t_l(k', k, z) = \langle k'|v_l|\Psi_B^l\rangle \tau_l(z) \langle\Psi_B^l|v_l k\rangle = h_B^l(k')\tau_l(z)h_B^l(k)$$

- with

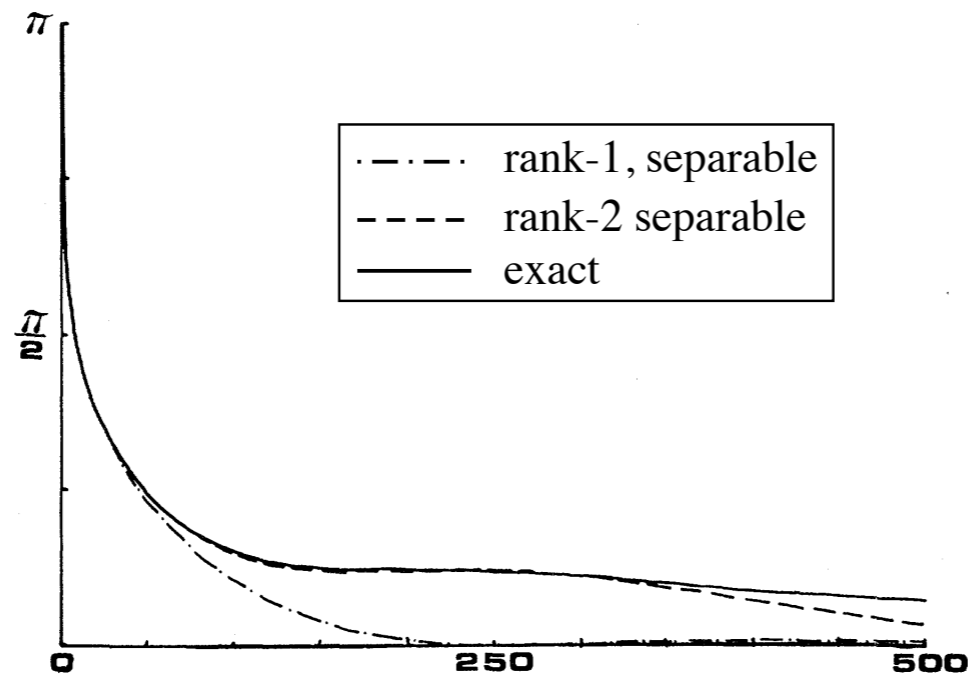
$$h_B^l(k) = \int dk' k'^2 v_l(k, k') \Psi_B^l(k')$$

$$\tau_l^{-1}(z) = \int dk k^2 \int dk' k'^2 \Psi_B^l(k) v_l(k, k') \Psi_B^l(k') - \int dk k^2 \frac{|h_B^l(k)|^2}{z - \frac{k^2}{2\mu} + i\epsilon}$$

Test case: D.J. Ernst, C.M. Shakin, R. M. Thaler and D. L. Weiss Phys. Rev. C8, 2056 (1973)

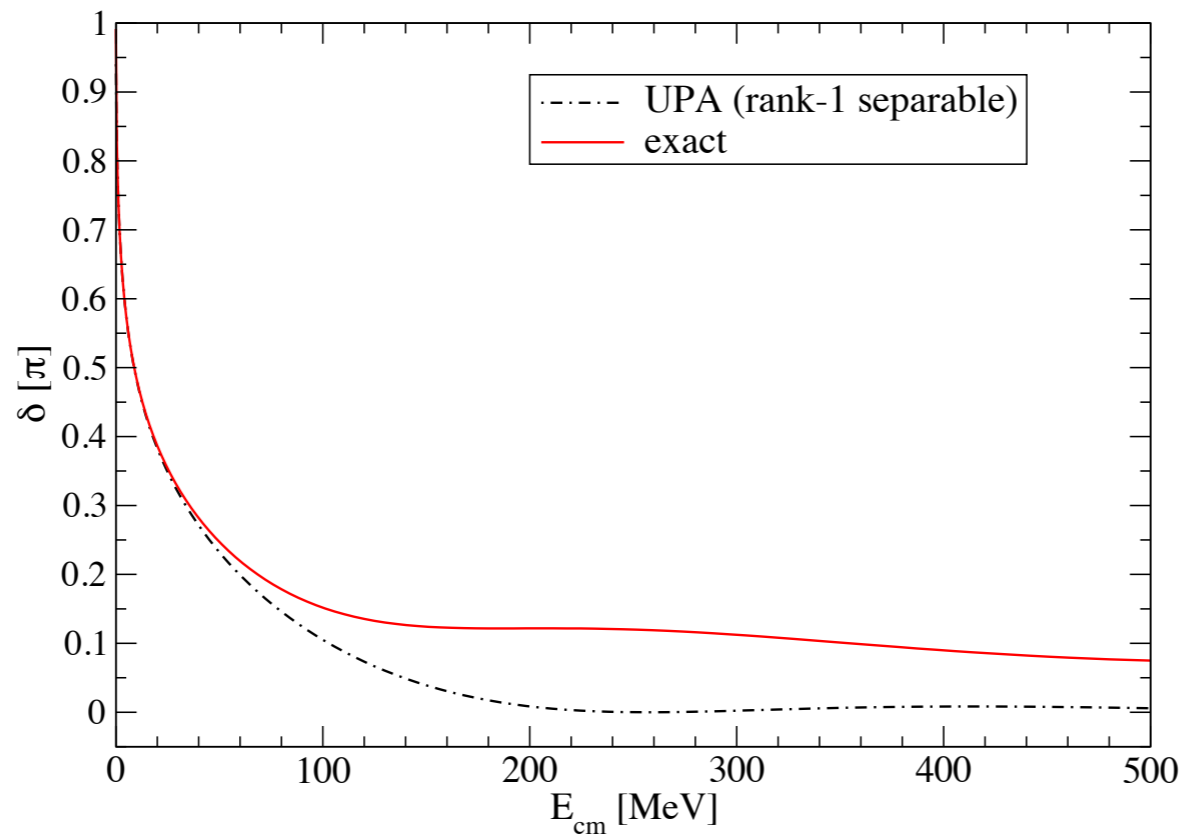
"deuteron" phase shifts
potential: squarewell: $V_0=38.5$, $R=1.93$

● ESTW



r-space

● LH



Extension to positive energies (EST)

- Original hamiltonian

$$H = H_0 + V$$

- construct $\mathcal{V} = |v\rangle\lambda\langle v|$ such that at some energy, E_k , the separable hamiltonian is identical to the original one

- for separable potential

$$|\Phi_{k_E}^{(+)}\rangle = |k_E\rangle + \frac{\lambda\langle v|k_E\rangle g_0(E)|v\rangle}{1 - \lambda\langle v|g_0(E_k)|v\rangle}$$

- for the original potential

$$|\Psi_{k_E}^{(+)}\rangle = |k_E\rangle + g_0(E_{k_E})V|\Psi_{k_E}^{(+)}\rangle.$$

- taking $|v\rangle \equiv V|\Psi_{k_E}^{(+)}\rangle$

then
$$\frac{1}{\lambda} = \langle \Psi_{k_E}^{(+)} | V | \Psi_{k_E}^{(+)} \rangle,$$

$$\mathcal{V} = \frac{V|\Psi_{k_E}^{(+)}\rangle\langle\Psi_{k_E}^{(+)}|V}{\langle\Psi_{k_E}^{(+)}|V|\Psi_{k_E}^{(+)}\rangle} \equiv |h_k\rangle\lambda\langle h_k|,$$

D. J. Ernst, C. M. Shakin and R. M. Thaler, Phys. Rev. C **8**, 46 (1973).

- **t-matrix**

$$\langle k'|t(z)|k\rangle \equiv \langle k'|h_k\rangle\tau(z)\langle h_k|k\rangle \equiv \langle k'|h_k\rangle \left[\frac{1}{\lambda} - \langle h_k|g_0(z)|h_k\rangle \right]^{-1} \langle h_k|k\rangle.$$

$$\begin{aligned} \langle p'|t(E)|p\rangle &= \frac{\langle p'|V|\Psi_{k_E}^{(+)}\rangle\langle\Psi_{k_E}^{(+)}|V|p\rangle}{\langle\langle\Psi_{k_E}^{(+)}|V - Vg_0(E)V|\Psi_{k_E}^{(+)}\rangle\rangle} \\ t(p', p, E) &= \frac{t_{k_E}^*(p)t_{k_E}(p')}{\langle\Psi_{k_E}^{(+)}|V - Vg_0(E)V|\Psi_{k_E}^{(+)}\rangle}, \end{aligned}$$

- **explicitly**

$$\begin{aligned} \tau(E)^{-1} &= t^*(k_E, k_E, E_{k_E}) \\ &+ 2\mu \left[\mathcal{P} \int dp p^2 \frac{|t(p, k_E, E_{k_E})|^2}{k_E^2 - p^2} - \mathcal{P} \int dp p^2 \frac{|t(p, k_E, E_{k_E})|^2}{k_0^2 - p^2} \right] \\ &+ i\pi\mu \left[k_0 |t(k_0, k_E, E_{k_E})|^2 - k_E |t(k_E, k_E, E_{k_E})|^2 \right] \end{aligned}$$

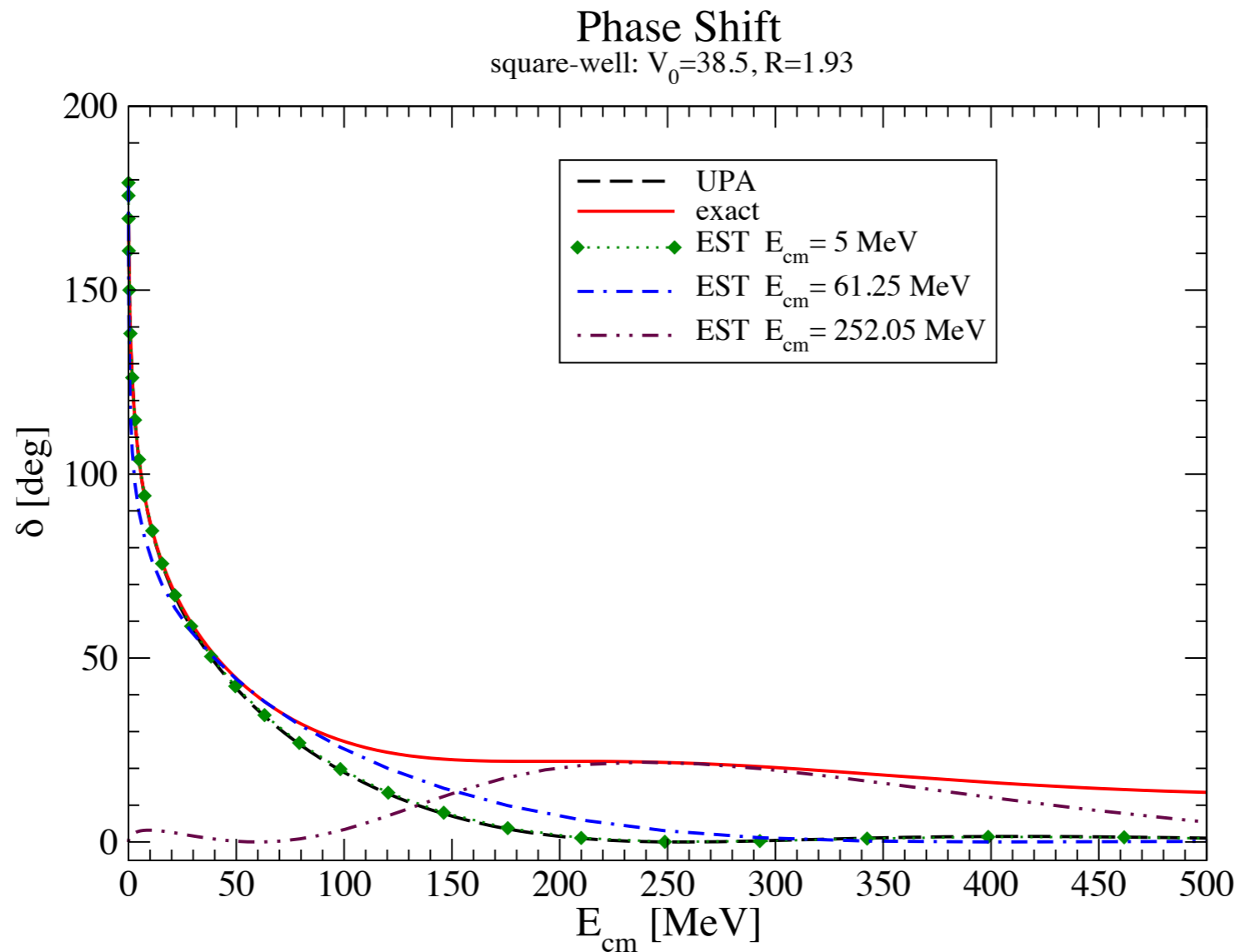
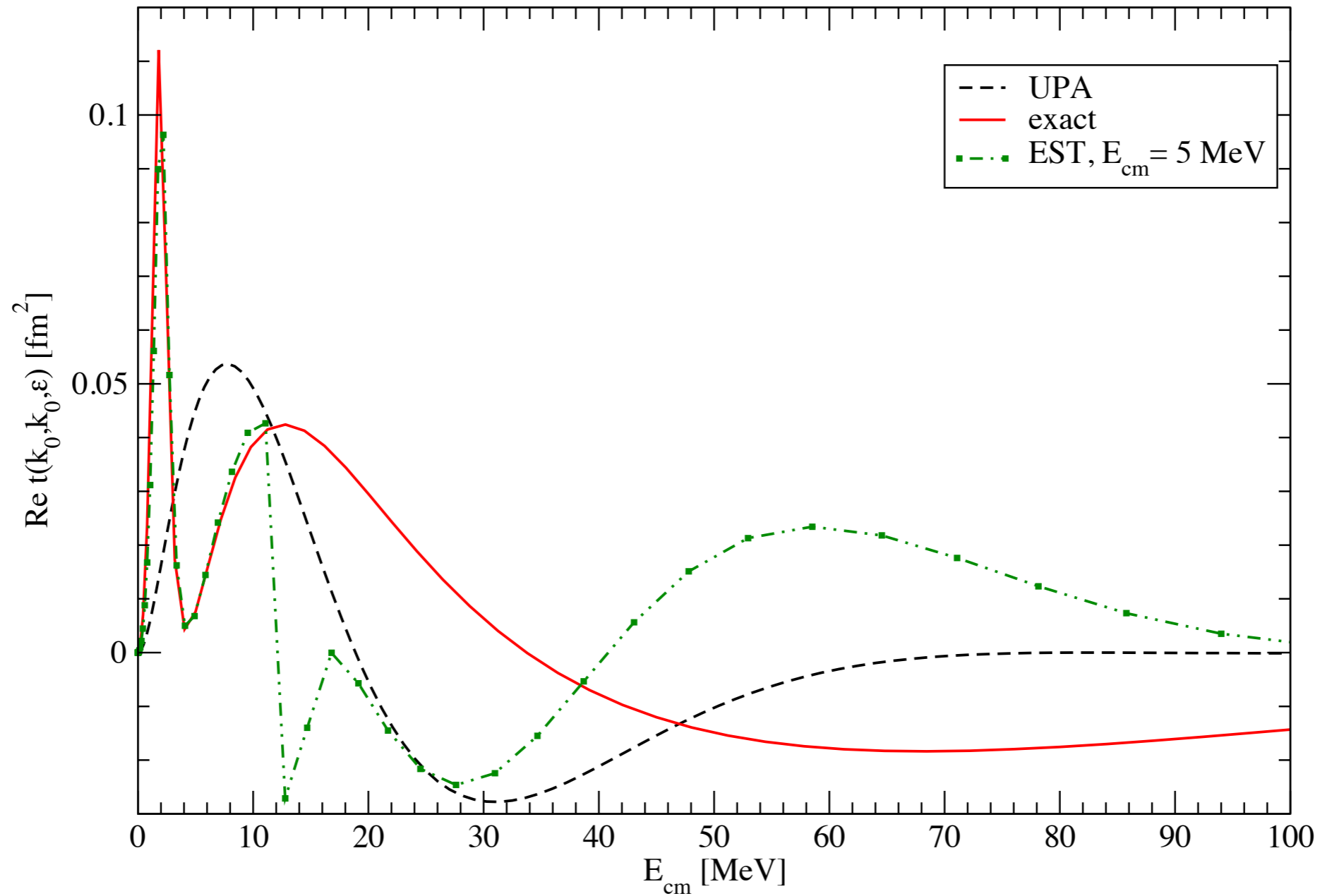


Figure 9: The s-wave for a square well potential with parameters adjusted such that the deuteron binding energy of -2.225 MeV is reproduced. The solid line gives the calculation with the square well potential while the dashed line shows the calculation with the rank-1 UPA approximation. The dotted, double-dash-dotted, and double-dot-dashed lines are calculated with EST rank-1 separable potentials constructed at the energies indicated in the figure.

n-⁴⁸Ca on-shell t-matrix
Wood-Saxon : $l=2$, $V_0=48.85$ MeV, $R_0=1.25A^{1/3}$ fm, $a=0.65$ fm



Next: Extension to rank-2 potential

- generalized separable potential

$$V = \sum_{i,j} v |\Psi_i\rangle \langle \Psi_i| M |\Psi_j\rangle \langle \Psi_j| v$$

- constraint

$$\delta_{ik} = \sum_j \langle \Psi_i | M | \Psi_j \rangle \langle \Psi_j | v | \Psi_k \rangle = \sum_j \langle \Psi_i | v | \Psi_j \rangle \langle \Psi_j | M | \Psi_k \rangle.$$

for rank-2

$$\sum_{j=1}^2 M_{ij} \langle \alpha_j | v | \alpha_k \rangle = \delta_{ik}.$$

- form factor

$$\mathbf{h}(p) = \begin{pmatrix} h_B(p) \\ t(p, k_E, E_{k_E}) \end{pmatrix} = \langle p | V | \begin{pmatrix} |\Psi_B\rangle \\ |\Phi_{k_E}^{(+)}\rangle \end{pmatrix} \equiv \langle p | V | \begin{pmatrix} |\alpha_1\rangle \\ |\alpha_2\rangle \end{pmatrix}.$$

- M-matrix elements

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \cdot \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

with $A_{ij} \equiv \langle \alpha_j | v | \alpha_i \rangle$

D. J. Ernst, C. M. Shakin and R. M. Thaler, Phys. Rev. C **8**, 46 (1973).

- diagonalize \mathbf{M}

$$\hat{\mathbf{M}} \equiv \mathbf{U}\mathbf{M}\mathbf{U}^{-1}$$

- eigenvectors

$$|\hat{\alpha}_i\rangle = \sum_j U_{ij}|\alpha_j\rangle$$

- coupling strengths

$$\hat{\lambda}_i = \langle \hat{\alpha}_i | \hat{\mathbf{M}} | \hat{\alpha}_i \rangle$$

- rank-2 separable potential (Neelam and CE)

$$v_l(p', p) = h_{l,1}(p')\lambda_{11}h_{l,1}(p) + h_{l,2}(p')\lambda_{22}h_{l,2}(p)$$

- t-matrix

$$t_l(p', p, E) = \sum_{i,j=1}^2 h_{l,i}(p')\tau_{ij}(E)h_{l,j}(p)$$

with

$$\tau_{ij}(E) = (\lambda - B(E))_{ij}^{-1},$$

where

$$B_{ij}(E) \equiv \int dp'' p''^2 \frac{h_i(p'')h_j(p'')}{E - p''^2/2\mu}$$

OR Calculate t-matrix without diagonalizing \mathbf{M}

Half-Shell $n\text{-}^{48}\text{Ca}$ potential (CH89) -- p-wave

top: $E_{\text{cm}} = 5 \text{ MeV}$, bottom: $E_{\text{cm}} = 45 \text{ MeV}$ ---- $p^2 = 2\mu E_{\text{cm}}$

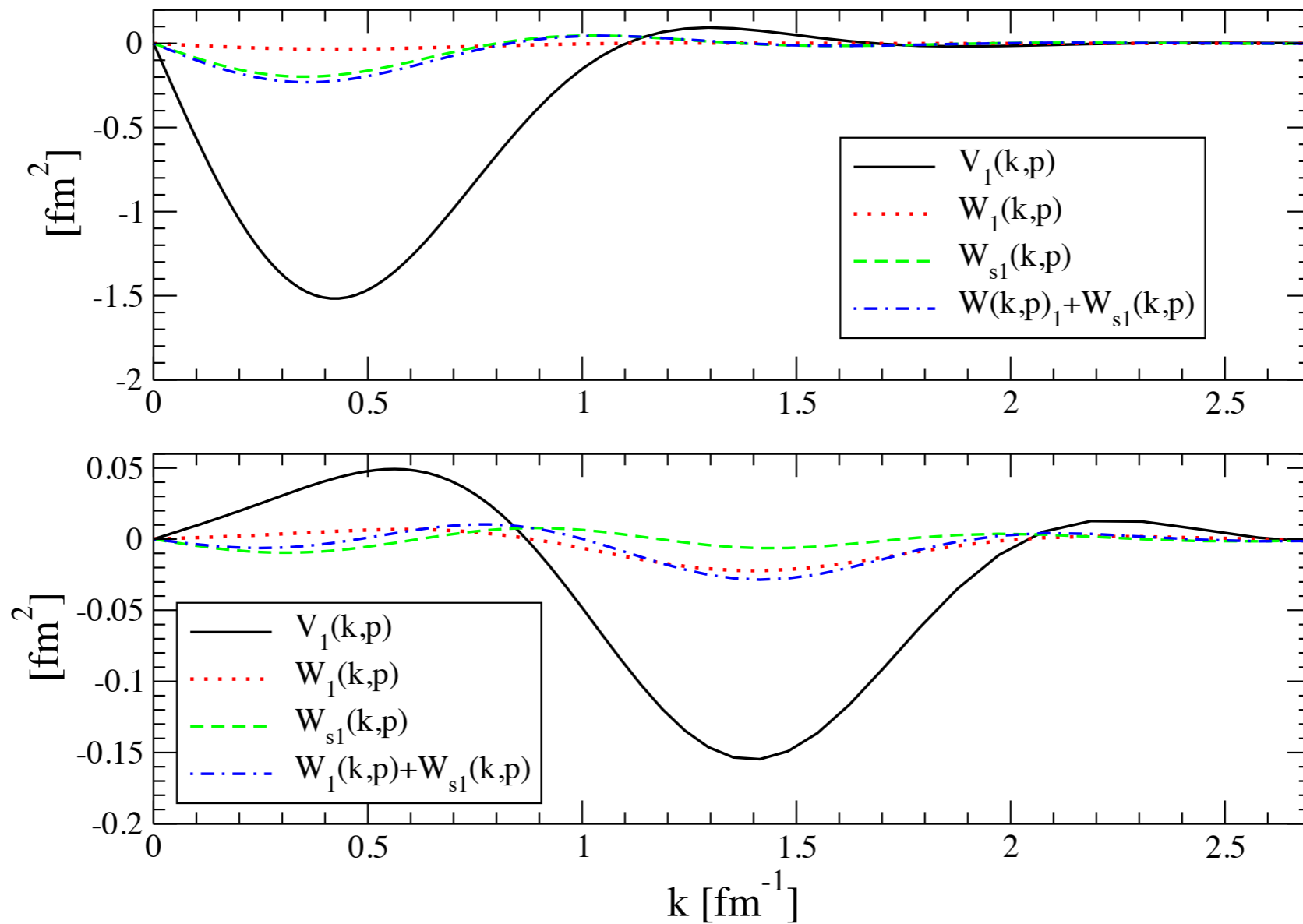


Figure 4: The real and imaginary parts to of the p-wave projected half-shell $n+^{48}\text{Ca}$ optical potential as function of k for fixed momentum p , where $p^2 = 2\mu E_{c.m.}$. The top panel shoes $E_{c.m.} = 5 \text{ MeV}$, the bottom panel $E_{c.m.} = 45 \text{ MeV}$. The calculations use $R_r = r_r(A^{1/3} + 1)$.

half-shell t-matrix for wood-saxon $U_{\text{nucl}}(q)$

top: $E_{\text{cm}} = 5$ MeV bottom: $E_{\text{cm}} = 45$ MeV

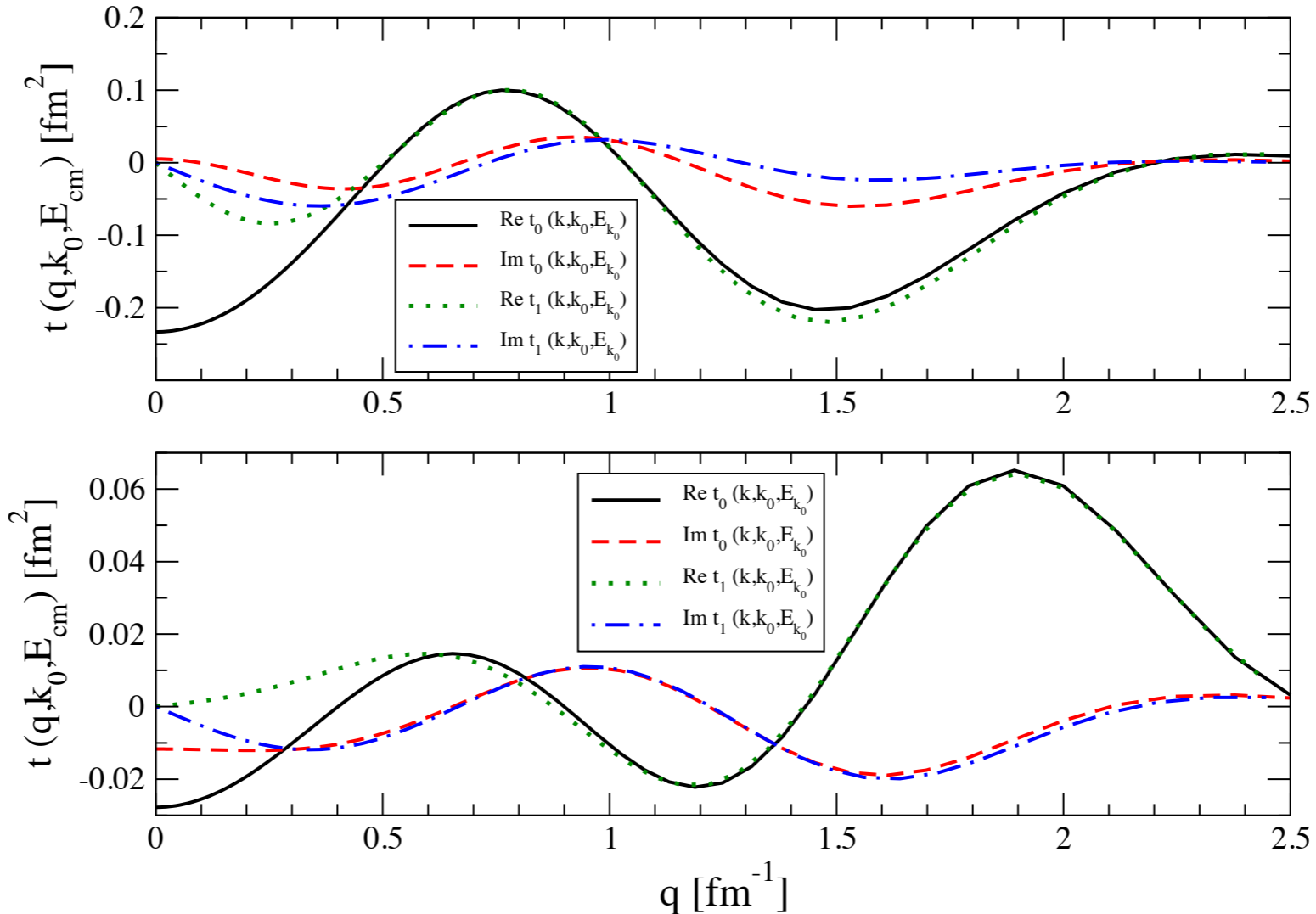


Figure 6: The real and imaginary parts to of the s-wave ($t_0(q, k_0, E_{k_0})$) and p-wave ($t_1(q, k_0, E_{k_0})$) projected half-shell t-matrix solved with the $n+^{48}\text{Ca}$ optical potential U_{nucl} as function of q for fixed momentum k_0 , where $k_0^2 = 2\mu E_{\text{c.m.}}$. The top panel shoes $E_{\text{c.m.}} = 5$ MeV, the bottom panel $E_{\text{c.m.}} = 45$ MeV. The calculations use $R_r = r_r(A^{1/3} + 1)$.

