

Square-integrable bases in the few-body Coulomb scattering problem

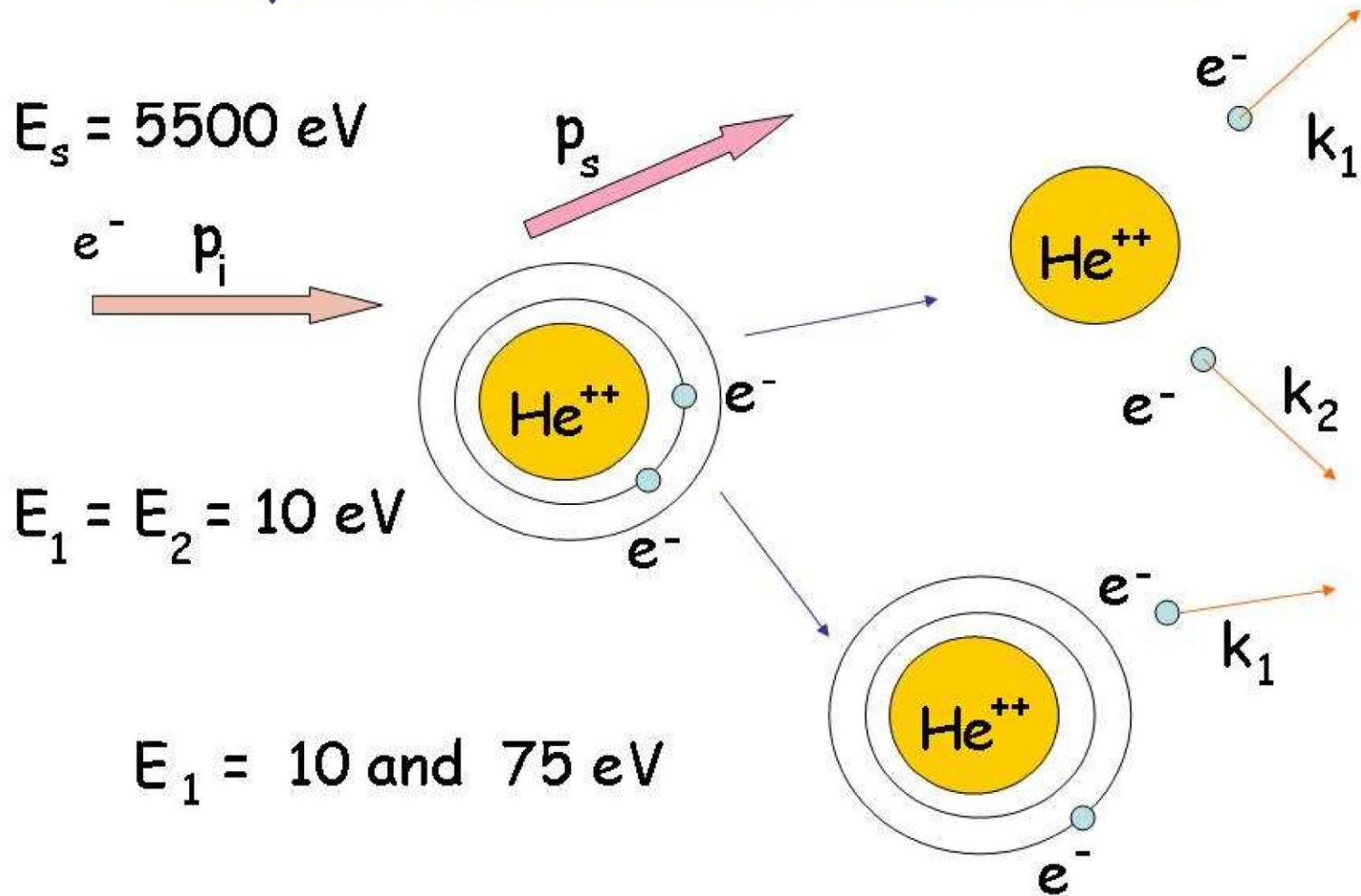
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Impact ionization of helium atom



Two-Electron Continuum (TEC)

- Convergent Close Coupling approach (CCC);
- Coulomb-Sturmian Separable Expansion method;
- J-Matrix method;
- R-Matrix method with Pseudo-States (RMPS);
- Exterior Complex Scaling approach (ECS)

TEC wave function is approximated by a product of two fixed charge Coulomb waves

$$\Psi_{C2} = N_1 e^{i\mathbf{k}_1 \cdot \mathbf{r}_1} F_1 \left[i \frac{Z}{k_1}, 1, -i (k_1 r_1 + \mathbf{k}_1 \cdot \mathbf{r}_1) \right] \\ \times N_2 e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} F_1 \left[i \frac{Z}{k_2}, 1, -i (k_2 r_2 + \mathbf{k}_2 \cdot \mathbf{r}_2) \right]$$

A long-range potential appears in the kernel of the corresponding Lippmann-Schwinger equation

J-matrix approach to electron-impact ionization of He

Schrödinger equation

$$\left[E + \frac{1}{2}\Delta_1 + \frac{1}{2}\Delta_2 + \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r_{12}} \right] \Psi^{(-)}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{r}_1, \mathbf{r}_2) = 0$$

$$\frac{Z}{r_i} = V_i^{(s)}(r_1, r_2) + V_i^{(l)}(r_1, r_2),$$

$$V_i^{(s)}(r_1, r_2) = \frac{Z}{r_i} \zeta(r_i, r_j), \quad V_i^{(l)}(r_1, r_2) = \frac{Z}{r_i} [1 - \zeta(r_i, r_j)]$$

$$\zeta(r_i, r_j) = 2 / \{1 + \exp[(r_i/a)^\nu / (1 + r_j/b)]\}.$$

$$\Omega_0 : r_1 \sim r_2 \rightarrow \infty, \quad \Omega_1 : r_1 \gg r_2 \text{ or } \Omega_2 : r_2 \gg r_1.$$

The final state wave function

$$\Psi^{(-)} = \frac{1}{\sqrt{2}} \left[\Psi_1^{(-)} + \Psi_2^{(-)} \right], \quad \Psi_2^{(-)} = g\hat{P}_{12}\Psi_1^{(-)}, \quad g = \pm 1$$

$$\left[E + \frac{1}{2}\Delta_1 + \frac{1}{2}\Delta_2 + \frac{Z-1}{r_1} + \frac{Z}{r_2} \right] \Psi_1^{(-)} = V(\mathbf{r}_1, \mathbf{r}_2)\Psi_1^{(-)} \quad (1)$$

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{r_{12}} - V_1^{(l)}(r_1, r_2) + \frac{Z-1}{r_1} - gV_2^{(s)}(r_1, r_2)\hat{P}_{12}. \quad (2)$$

$V(\mathbf{r}_1, \mathbf{r}_2)$ is short-range in the two-body scattering region Ω_1 ($r_1 \gg r_2$)

$$\hat{g}_1^{(-)}(E_1) = \left[E_1 + \frac{1}{2}\Delta_1 + \frac{Z-1}{r_1} \right]^{-1}$$

$$\hat{g}_2^{(-)}(E_2) = \left[E_2 + \frac{1}{2}\Delta_2 + \frac{Z}{r_2} \right]^{-1}$$

Lippmann-Schwinger type equation

$$\begin{aligned}\Psi_1^{(-)}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{r}_1, \mathbf{r}_2) &= [\varphi^{(-)}(\mathbf{k}_2, \mathbf{r}_2; Z) \varphi^{(-)}(\mathbf{k}_1, \mathbf{r}_1; Z - 1) \theta(k_1 - k_2) \\ &+ g\varphi^{(-)}(\mathbf{k}_1, \mathbf{r}_2; Z) \varphi^{(-)}(\mathbf{k}_2, \mathbf{r}_1; Z - 1) \theta(k_2 - k_1)] \quad (1') \\ &+ \int \int d\mathbf{r}'_1 d\mathbf{r}'_2 G^{(-)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; E) V(\mathbf{r}'_1, \mathbf{r}'_2) \Psi_1^{(-)}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{r}'_1, \mathbf{r}'_2).\end{aligned}$$

Green's Function

$$G^{(-)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; E) = \frac{1}{2\pi i} \int_c d\mathcal{E} g^{(-)}(\mathbf{r}_1, \mathbf{r}'_1; \mathcal{E} - i0; Z - 1) g^{(-)}(\mathbf{r}_2, \mathbf{r}'_2; E - \mathcal{E} - i0; Z).$$

Partial decomposition

$$\Psi_1^{(-)}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{r}_1, \mathbf{r}_2) = \frac{2}{\pi} \frac{1}{k_1 k_2} \sum_{\substack{L l_0 \lambda_0 \\ m_0 \mu_0}} (l_0 m_0 \lambda_0 \mu_0 | L M) i^{l_0 + \lambda_0} \\ \left[e^{-i(\sigma_{l_0}(k_1, Z-1) + \sigma_{\lambda_0}(k_2, Z))} \psi_{l_0 \lambda_0}^{LM}(\mathbf{r}_1, \mathbf{r}_2; k_1, k_2) Y_{l_0 m_0}^*(\widehat{\mathbf{k}}_1) Y_{\lambda_0 \mu_0}^*(\widehat{\mathbf{k}}_2) \theta(k_1 - k_2) + \right. \\ \left. g e^{-i(\sigma_{l_0}(k_2, Z-1) + \sigma_{\lambda_0}(k_1, Z))} \psi_{l_0 \lambda_0}^{LM}(\mathbf{r}_1, \mathbf{r}_2; k_2, k_1) Y_{l_0 m_0}^*(\widehat{\mathbf{k}}_2) Y_{\lambda_0 \mu_0}^*(\widehat{\mathbf{k}}_1) \theta(k_2 - k_1) \right].$$

Partial wave function

$$\psi_{l_0 \lambda_0}^{LM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{l, \lambda, n, \nu} C_{n\nu}^{L(l\lambda)}(E) \langle \mathbf{r}_1, \mathbf{r}_2 | n l \nu \lambda; LM \rangle,$$

$$\langle \mathbf{r}_1, \mathbf{r}_2 | n l \nu \lambda; LM \rangle = \frac{\phi_n^l(r_1)}{r_1} \frac{\phi_\nu^\lambda(r_2)}{r_2} \mathcal{Y}_{l\lambda}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2).$$

Sturmians

$$\phi_\nu^\lambda(r) = \left[\frac{(\nu - \lambda - 1)!}{(\nu + \lambda)!} \right]^{1/2} (2\kappa r)^{\lambda+1} e^{-\kappa r} L_{\nu-\lambda-1}^{2\lambda+1}(2\kappa r), \quad \nu \geq 1 + \lambda$$

$$\int_0^\infty \frac{dr}{r} \phi_\nu^\lambda(r) \phi_{\nu'}^\lambda(r) = \delta_{\nu, \nu'}$$

Coulomb partial spectral state

$$\varphi_l^\alpha(r; Z) = \sum_n \mathcal{S}_{nl}^\alpha(Z) \phi_n^l(r).$$

$$\mathcal{S}_{nl}(k; Z) = \left[\frac{(n+l)!}{(n-l-1)!} \right]^{1/2} 2^l \sin(\zeta)^{l+1} e^{-\pi t/2} \xi^{-it} \frac{|\Gamma(l+1-it)|}{(2l+1)!} \times (\xi)^{-(n-l-1)} {}_2F_1(-n+l+1, l+1-it; 2l+2; 1-\xi^2).$$

$$t = \frac{Z}{k}; \quad \xi = e^{i\zeta} = \frac{ik-\kappa}{ik+\kappa}.$$

Equation for coefficients

$$C_{n\nu}^{L(l\lambda)}(k_1, k_2) = \delta_{(l\lambda)(l_0\lambda_0)} \mathcal{S}_{nl_0}(k_1, Z-1) \mathcal{S}_{\nu\lambda_0}(k_2, Z) +$$

$$\sum_{n'\nu'n''\nu''}^N \left[\frac{1}{2\pi i} \int_{\mathcal{C}} d\mathcal{E} g_{nn'}^{(-)l}(\mathcal{E}, Z-1) g_{\nu\nu'}^{(-)\lambda}(E-\mathcal{E}, Z) \right]$$

$$\sum_{l''\lambda''} V_{n'\nu', n''\nu''}^{L(l\lambda)(l''\lambda'')} C_{n''\nu''}^{L(l''\lambda'')}(E).$$

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{r_{12}} - V_1^{(l)}(r_1, r_2) + \frac{Z-1}{r_1} - gV_2^{(s)}(r_1, r_2) \hat{P}_{12}.$$

Potential matrix elements

$$V_{n\nu, n'\nu'}^{L(l\lambda)(l'\lambda')} = \langle n l \nu \lambda; LM | V(\mathbf{r}_1, \mathbf{r}_2) | n' l' \nu' \lambda'; LM \rangle \quad (3)$$

Green's function matrix elements

$$g_{\nu\nu'}^{(\pm)\lambda}(E; Z) = -\frac{2}{p} \mathcal{S}_{\nu<\lambda}(p, Z) \mathcal{C}_{\nu>\lambda}^{(\pm)}(p, Z),$$

with $\nu_{<} = \min \{\nu, \nu'\}$; $\nu_{>} = \max \{\nu, \nu'\}$ and $p = \sqrt{2E}$.

$$\begin{aligned} \mathcal{C}_{nl}^{(\pm)}(p, Z) = & - \left[\frac{(n+l)!}{(n-l-1)!} \right]^{1/2} \frac{(n-l-1)! e^{\pi t/2} \xi^{it}}{(2 \sin \zeta)^l} \frac{\Gamma(l+1 \mp it)}{|\Gamma(l+1 \mp it)|} \times \\ & \times \frac{(\xi)^{\mp(n-l)}}{\Gamma(n+1 \mp it)} {}_2F_1(-l \mp it, n-l; n+1 \mp it; \xi^{\mp 2}). \end{aligned}$$

$$\mathcal{C}_{nl}^{(+)}(p, Z) = \mathcal{C}_{nl}^{(-)}(p, Z) + 2i\mathcal{S}_{nl}(p, Z).$$

The five-fold differential cross-section of the (e, 3e) reaction

$$\frac{d^5\sigma}{d\Omega_s dE_1 d\Omega_1 dE_2 d\Omega_2} = \frac{4p_s k_1 k_2}{p_i Q^4} \times$$
$$| \langle \Psi^{(-)}(\mathbf{k}_1, \mathbf{k}_2) | \exp(i\mathbf{Q}\mathbf{r}_1) + \exp(i\mathbf{Q}\mathbf{r}_2) - 2|\Psi_0\rangle |^2 .$$

Here (E_i, \mathbf{p}_i) , (E_s, \mathbf{p}_s) , (E_1, \mathbf{k}_1) and (E_2, \mathbf{k}_2) are energies and momenta of, respectively, the fast incident, fast scattered, and two slow ejected electrons; $\mathbf{Q} = \mathbf{p}_i - \mathbf{p}_s$ is the (little) transferred momentum,

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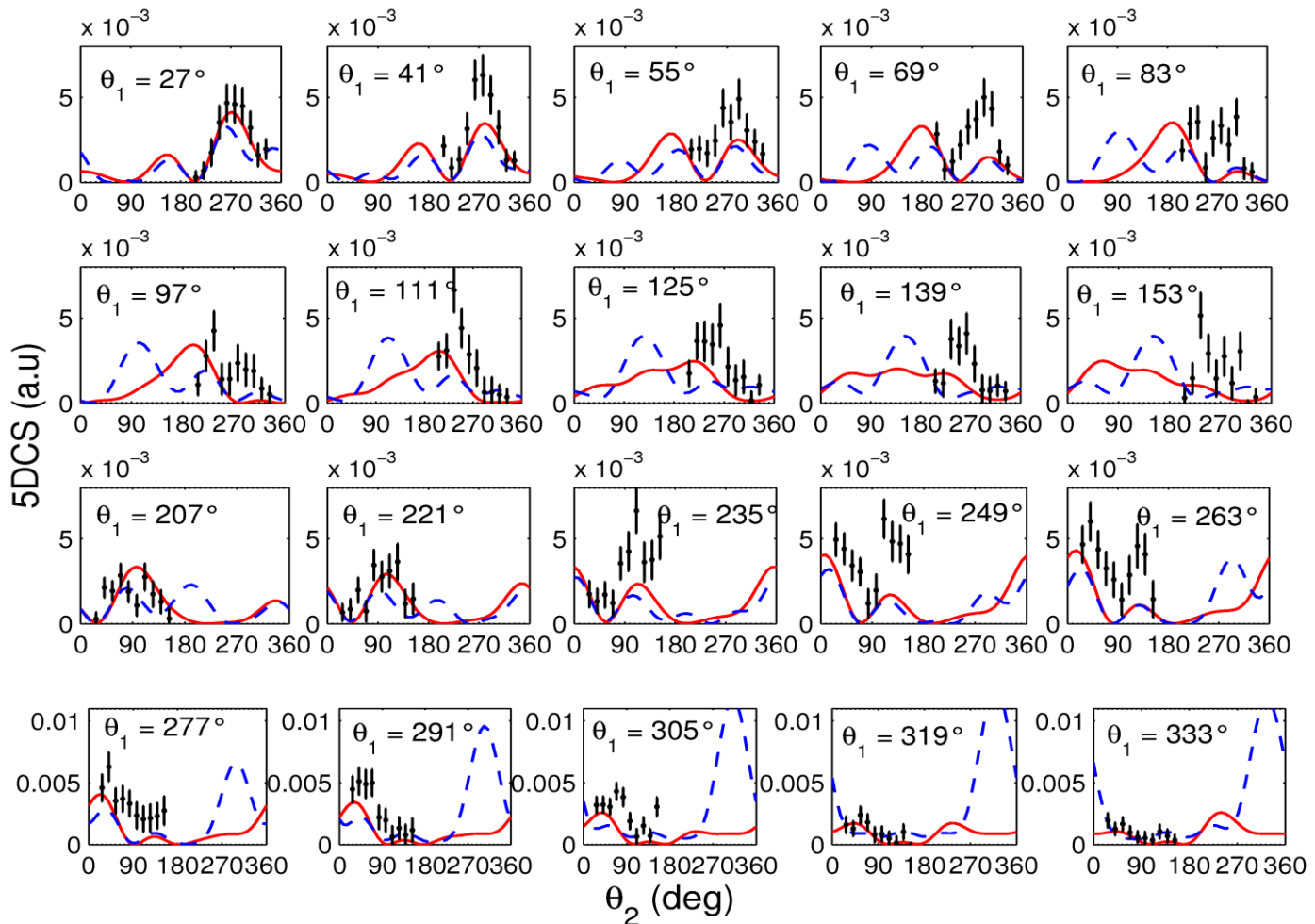
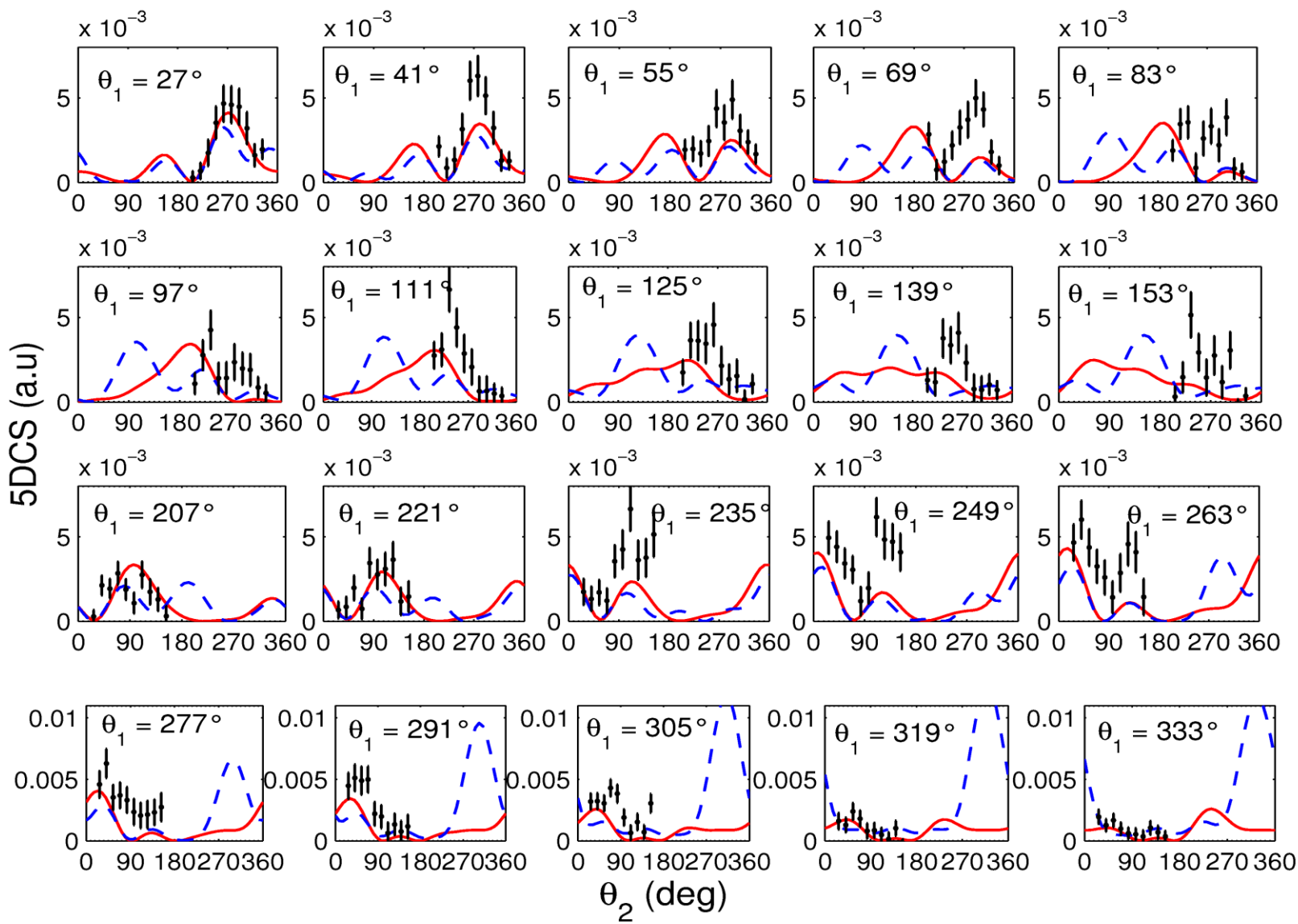


FIG. 1: (Color online) Fully five-fold differential cross section (5DCS) for electron impact double ionization reaction $He(e, 3e)He^{++}$. The incident energy is $E_0=5599$ eV and the energies of the slow ejected electrons are $E_1 = E_2 = 10$ eV. The scattering angle θ_s of the fast incident electron is fixed and equal to 0.45° while the angles of the ejected electrons are θ_1 and θ_2 . One of these angles, θ_1 is fixed and the other varies. The blue dashed line is our result obtained by means of a zero order calculation. The red solid line is the result obtained by solving the Lippmann-Schwinger equation (11) for the double continuum wave function. The solid dots with error-bars are the absolute experimental data of Lahmam-Bennani [4].



- Convergence of the results with increasing N is not as satisfactory; there are abrupt (up to three times) kinks in the cross section in certain angular regions even for a small variation of N .
- Calculations show that, at $\theta_1 = \theta_2$, the cross section grows with increasing N , whereas here it should vanish.

This is an obvious deficiency of the theoretical scheme with a truncated potential.

Three particles of masses m_1, m_2, m_3 , charges Z_1, Z_2, Z_3 and momenta $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$

Hamiltonian

$$\hat{H} = -\frac{1}{2\mu_{12}}\Delta_{\mathbf{R}} - \frac{1}{2\mu_3}\Delta_{\mathbf{r}} + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}}, \quad (1)$$

Relative coordinates

$$\mathbf{r}_{ls} = \mathbf{r}_l - \mathbf{r}_s, \quad r_{ls} = |\mathbf{r}_{ls}|, \quad (2)$$

Jacobi coordinates

$$\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{r} = \mathbf{r}_3 - \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}. \quad (3)$$

Reduced masses

$$\mu_{12} = \frac{m_1m_2}{m_1 + m_2}, \quad \mu_3 = \frac{m_3(m_1 + m_2)}{m_1 + m_2 + m_3}. \quad (4)$$

Schrödinger equation

$$\hat{H}\Phi = E\Phi$$

Energy $E > 0$

$$E = \frac{1}{2\mu_{12}} \mathbf{K}^2 + \frac{1}{2\mu_3} \mathbf{k}^2,$$

Wave function

$$\Phi = e^{i(\mathbf{K}\cdot\mathbf{R}+\mathbf{k}\cdot\mathbf{r})}\Psi$$

Reduced wave function

$$\left[-\frac{1}{2\mu_{12}} \Delta_{\mathbf{R}} - \frac{1}{2\mu_3} \Delta_{\mathbf{r}} - \frac{i}{\mu_{12}} \mathbf{K} \cdot \nabla_{\mathbf{R}} - \frac{i}{\mu_3} \mathbf{k} \cdot \nabla_{\mathbf{r}} + \frac{Z_1 Z_2}{r_{12}} + \frac{Z_2 Z_3}{r_{23}} + \frac{Z_1 Z_3}{r_{13}} \right] \Psi = 0 \quad (5)$$

Generalized parabolic coordinates

$$\xi_1 = r_{23} + \hat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23}, \quad \eta_1 = r_{23} - \hat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23},$$

$$\xi_2 = r_{13} + \hat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13}, \quad \eta_2 = r_{13} - \hat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13},$$

$$\xi_3 = r_{12} + \hat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12}, \quad \eta_3 = r_{12} - \hat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12},$$

$\mathbf{k}_{ls} = \frac{\mathbf{k}_l m_s - \mathbf{k}_s m_l}{m_l + m_s}$ is the relative momentum, $\hat{\mathbf{k}}_{ls} = \frac{\mathbf{k}_{ls}}{k_{ls}}$ and $k_{ls} = |\mathbf{k}_{ls}|_7$

$$[D_0 + D_1] \Psi = 0. \quad (5')$$

D_0 contains the leading term of the kinetic energy and the total potential energy:

$$\hat{D}_0 = \sum_{j=1}^3 \frac{1}{\mu_{ls}(\xi_j + \eta_j)} \left[\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls} \right],$$

for $j \neq l, s$ and $l < s$,

$$\hat{h}_{\xi_j} = -2 \left(\frac{\partial}{\partial \xi_j} \xi_j \frac{\partial}{\partial \xi_j} + ik_{ls} \xi_j \frac{\partial}{\partial \xi_j} \right),$$

$$\hat{h}_{\eta_j} = -2 \left(\frac{\partial}{\partial \eta_j} \eta_j \frac{\partial}{\partial \eta_j} - ik_{ls} \eta_j \frac{\partial}{\partial \eta_j} \right).$$

$$t_{ls} = \frac{Z_l Z_s \mu_{ls}}{k_{ls}} \quad \text{and} \quad \mu_{ls} = \frac{m_l m_s}{m_l + m_s}.$$

D_1 is the non-orthogonal part of the kinetic energy operator.

In the case of $(e^-, e^-, He^{++}) = (123)$ system with $m_3 = \infty$,

$$\hat{D}_1 = \sum_{j=1}^2 (-1)^{j+1} \left[\mathbf{u}_j^- \cdot \mathbf{u}_3^- \frac{\partial^2}{\partial \xi_j \partial \xi_3} + \mathbf{u}_j^- \cdot \mathbf{u}_3^+ \frac{\partial^2}{\partial \xi_j \partial \eta_3} \right. \\ \left. + \mathbf{u}_j^+ \cdot \mathbf{u}_3^- \frac{\partial^2}{\partial \eta_j \partial \xi_3} + \mathbf{u}_j^+ \cdot \mathbf{u}_3^+ \frac{\partial^2}{\partial \eta_j \partial \eta_3} \right],$$

$$\mathbf{u}_j^\pm = \hat{\mathbf{r}}_{ls} \mp \hat{\mathbf{k}}_{ls}.$$

C3 wave function

$$\hat{D}_0 \Psi_{C3} = 0,$$

$$\Psi_{C3} = \prod_{j=1}^3 {}_1F_1(it_{ls}, 1; -ik_{ls}\xi_j).$$

Two-dimensional Coulomb Green's function

$$\hat{G}^{(\pm)} = [\mathfrak{h} + C]^{-1}.$$

$$\mathfrak{h} = \frac{1}{\mu(\xi + \eta)} \left[\hat{h}_\xi + \hat{h}_\eta + 2kt \right].$$

$$G^{(\pm)}(t, \mathcal{E}; \xi, \eta, \xi', \eta') = \mp \frac{i\gamma}{4} e^{\frac{i}{2}k(\xi' - \xi + \eta - \eta')} \mu(\xi' + \eta') \int_0^\infty dz \sinh(z) \left[\coth\left(\frac{z}{2}\right) \right]^{\mp 2i\tau} \\ \times e^{\pm i\frac{\gamma}{2}(\xi + \xi' + \eta + \eta') \cosh(z)} I_0\left(\mp i\gamma\sqrt{\xi\xi'} \sinh(z)\right) I_0\left(\mp i\gamma\sqrt{\eta\eta'} \sinh(z)\right),$$

$$C = \frac{1}{\mu} \left(\frac{k^2}{2} - \mathcal{E} \right), \quad \mathcal{E} = \frac{\gamma^2}{2}, \quad \tau = \frac{k}{\gamma} t$$

Six-dimensional Green's function

$$\hat{\mathcal{G}} = \hat{D}_0^{-1},$$

$$\hat{D}_0 = \hat{\mathfrak{h}}_1 + \hat{\mathfrak{h}}_2 + \hat{\mathfrak{h}}_3.$$

$$\begin{aligned} \mathcal{G}^{(+)}(X, X') &= \frac{1}{\mu_{23} \mu_{13}} \int_{\mathcal{C}_1} \int_{\mathcal{C}_2} d\mathcal{E}_1 d\mathcal{E}_2 G^{(+)}(t_{23}, \mathcal{E}_1; X_1, X'_1) \\ &\quad \times G^{(+)}(t_{13}, \mathcal{E}_2; X_2, X'_2) G^{(+)}(t_{12}, \mathcal{E}_3; X_3, X'_3), \end{aligned}$$

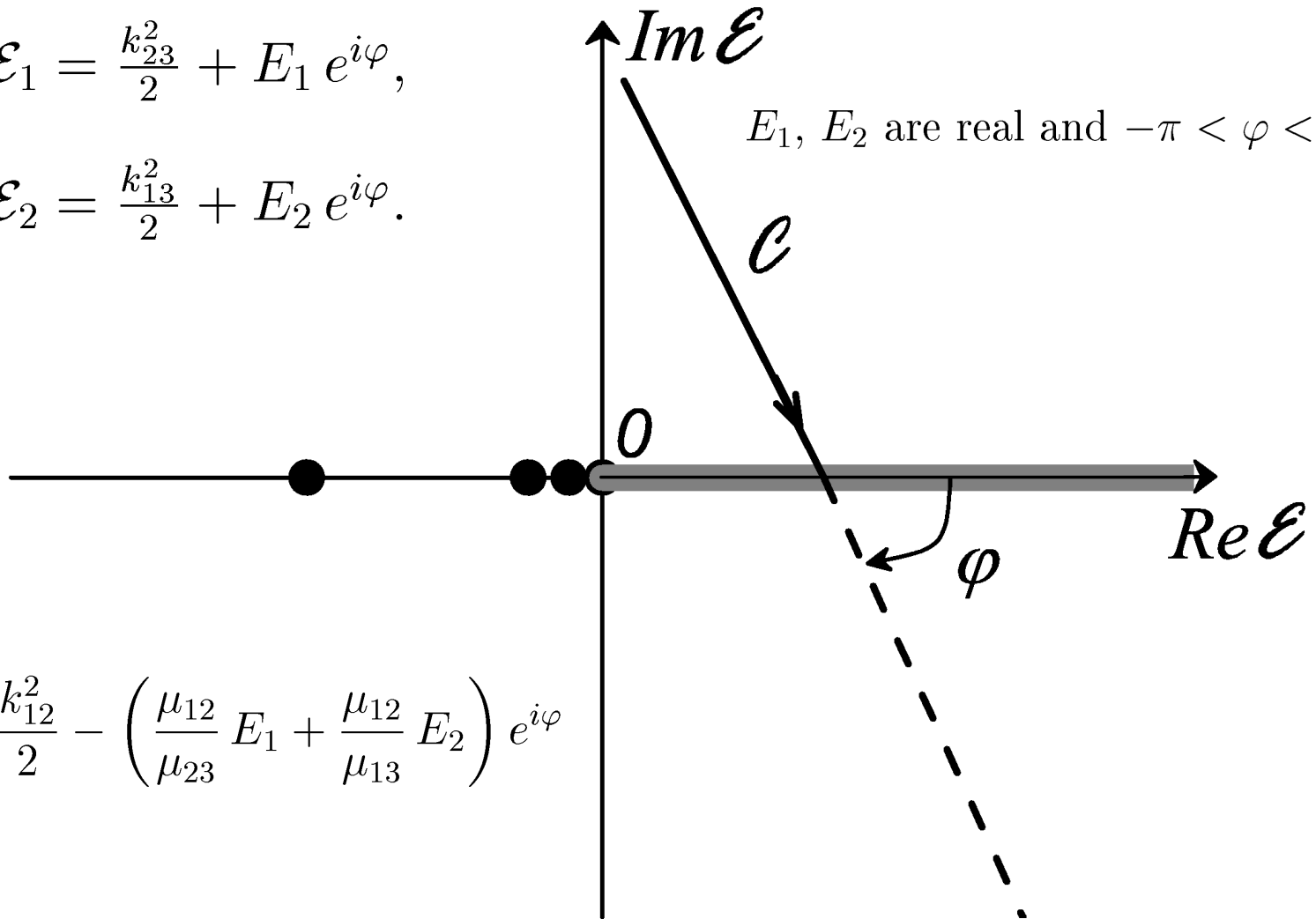
$$X = \{X_1, X_2, X_3\}, \quad X_j = \{\xi_j, \eta_j\}, \quad j = 1, 2, 3.$$

Path of integration

$$\mathcal{E}_1 = \frac{k_{23}^2}{2} + E_1 e^{i\varphi},$$

$$\mathcal{E}_2 = \frac{k_{13}^2}{2} + E_2 e^{i\varphi}.$$

E_1, E_2 are real and $-\pi < \varphi < 0$.



$$\mathcal{E}_3 = \frac{k_{12}^2}{2} - \left(\frac{\mu_{12}}{\mu_{23}} E_1 + \frac{\mu_{12}}{\mu_{13}} E_2 \right) e^{i\varphi}$$

Lippmann-Schwinger type equation

$$\Psi = \Psi_{C3} - \hat{\mathcal{G}}\hat{D}_1\Psi.$$

The kernel of $\hat{\mathcal{G}}\hat{D}_1$ is non-compact

Square integrable parabolic basis functions

$$|\mathfrak{N}\rangle = \prod_{j=1}^3 \phi_{n_j m_j}(\xi_j, \eta_j),$$

$$\phi_{n_j m_j}(\xi_j, \eta_j) = \psi_{n_j}(\xi_j) \psi_{m_j}(\eta_j),$$

$$\psi_n(x) = \sqrt{2b_j} e^{-b_j x} L_n(2b_j x).$$

$$\Psi = \Psi_{C3} - \sum_{j=1}^3 \sum_{n_j=0}^{N_j-1} \sum_{m_j=0}^{M_j-1} [\underline{C}]_{\mathfrak{N}} \hat{\mathcal{G}} |\mathfrak{N}\rangle \quad (6)$$

Wave function

$$\Psi = \Psi_{sc} + \Psi_{C3}$$

$$\Psi_{sc} \sim \sum a_{\mathfrak{n}} f_{\mathfrak{n}}, \quad (6')$$

Quasi Sturmians $\{f_{\mathfrak{n}}\}$

$$f_{\mathfrak{n}} = \hat{\mathcal{G}} |\mathfrak{n}\rangle$$

Driven equation

$$\left[\hat{D}_0 + \hat{D}_1 \right] \Psi_{sc} = -\hat{D}_1 \Psi_{C3}$$

- We expect that the resulting Sturmian functions to provide a basis of expansion for this kind of three-body Coulomb problem.

Thanks for attention!