# Convoluted Quasi Sturmian Basis in Coulomb Three-Body Problems

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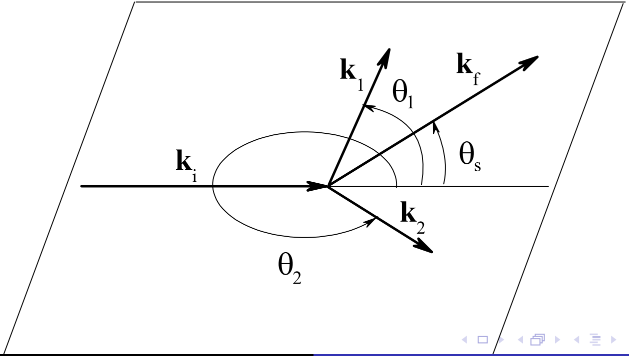
High-energy electron-impact double ionization of helium. The coplanar experimental data correspond to a fast scattered electron of $E_s = 5500$ eV; the energies of the ejected electrons are $E_1 = E_2 = 10$ eV, one electron being fixed at $\theta_1$ while the angle $\theta_2$ of the other electron varies.

A.Kheifets et. al. J. Phys. B **32**, 5047 (1999)



# Three-body system $(e^-, e^-, \mathrm{He}^{++}) = (1, 2, 3)$

$$\left[E - \hat{H}\right] \Phi_{sc}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \hat{W}_{fi}(\mathbf{r}_1, \mathbf{r}_2)\Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2). \quad (1)$$

$$E = \frac{k_1^2}{2} + \frac{k_2^2}{2}.$$

G.Gasaneo et. al. Phys. Rev. A **87**, 042707 (2013)

$$\hat{H} = -\frac{1}{2}\triangle_{r_1} - \frac{1}{2}\triangle_{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \quad (2)$$

$$\hat{W}_{fi}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{(2\pi)^3}\frac{4\pi}{q^2}(-2 + e^{i\mathbf{q}\cdot\mathbf{r}_1} + e^{i\mathbf{q}\cdot\mathbf{r}_2}), \quad (3)$$

$$\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f.$$

# Solution

## Expansion

$$\Phi_{sc}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{L,\ell,\lambda} \sum_{n,\nu=0}^{N-1} C_{n\nu}^{L(\ell\lambda)} \left| n\ell\nu\lambda; LM \right\rangle_Q , \tag{4}$$

## Basis

$$\left| n\ell\nu\lambda; LM \right\rangle_Q \equiv \frac{Q_{n\nu}^{\ell\lambda(+)}(E; r_1, r_2)}{r_1 r_2} \mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2). \tag{5}$$

## Spherical Harmonics

$$\mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \sum_{m\mu} (\ell m \lambda \mu \,|\, LM)\, Y_{\ell m}(\hat{\mathbf{r}}_1)\, Y_{\lambda\mu}(\hat{\mathbf{r}}_2). \tag{6}$$

# Radial Part

## Equation

$$\left[E - \hat{h}_1^{\ell} - \hat{h}_2^{\lambda}\right] Q_{n\nu}^{(\ell\lambda)(+)}(E; r_1, r_2) = \frac{\psi_n^{\ell}(r_1)\psi_\nu^{\lambda}(r_2)}{r_1 r_2}, \qquad (7)$$

## Radial Operators

$$\hat{h}^{\ell} = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{1}{2}\frac{\ell(\ell+1)}{r^2} - \frac{2}{r}, \qquad (8)$$

## Laguerre Basis Function

$$\psi_n^{\ell}(r) = \left[(n+1)_{2\ell+1}\right]^{-\frac{1}{2}} (2br)^{\ell+1} e^{-br} L_n^{2\ell+1}(2br). \qquad (9)$$

$b$ is the basis scale parameter.

# Convolution of Green's Functions

$$\hat{G}^{(\ell\lambda)(+)}(E) = \frac{1}{2\pi i}\int\limits_{\mathcal{C}_1} d\mathcal{E}\, \hat{G}^{\ell(+)}(\sqrt{2\mathcal{E}})\hat{G}^{\lambda(+)}(\sqrt{2(E-\mathcal{E})}). \quad (10)$$

$$\left[E - \hat{h}_1^{\ell} - \hat{h}_2^{\lambda}\right] G^{(\ell\lambda)(+)}(E; r_1, r_2; r_1', r_2') = \delta(r_1 - r_1')\delta(r_2 - r_2'). \quad (11)$$

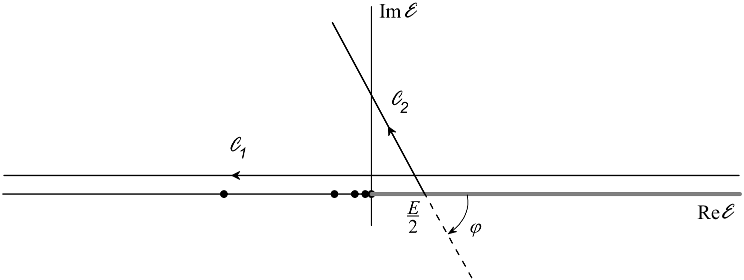
$$\left[\mathcal{E} - \hat{h}^{\ell}\right] G^{\ell(\pm)}(\sqrt{2\mathcal{E}}; r, r') = \delta(r - r'). \quad (12)$$

$$\begin{aligned} G^{\ell(\pm)}(k; r, r') = \pm\tfrac{1}{ik}\tfrac{\Gamma(\ell+1\pm i\alpha)}{(2\ell+1)!}\, &\mathcal{M}_{\mp i\alpha;\ell+1/2}(\mp 2ikr_<) \\ &\times\mathcal{W}_{\mp i\alpha;\ell+1/2}(\mp 2ikr_>), \end{aligned} \quad (13)$$

$$k = \sqrt{2\mathcal{E}},\ \alpha = \tfrac{\mu Z}{k} = \tfrac{-2}{k}.$$

# Path of Integration

R.Shakehaft, Phys. Rev. A **70**, 042704 (2004)



# Path of Integration II

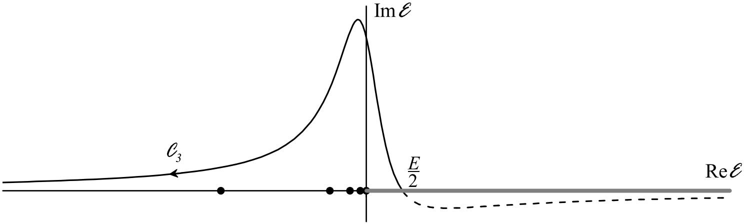



Figure: The contours $\mathcal{C}_3$.

# Convolution of Quasi Sturmians

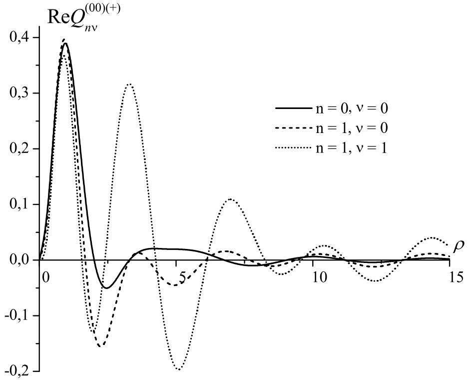
$$Q_{n\nu}^{(\ell\lambda)(+)}(E; r_1, r_2) = \frac{1}{2\pi i} \int\limits_{\mathcal{C}_3} d\mathcal{E}\, Q_n^{\ell(+)}(\sqrt{2\mathcal{E}}; r_1) Q_\nu^{\lambda(+)}(\sqrt{2(E-\mathcal{E})}; r_2). \tag{14}$$

$$Q_n^{\ell(\pm)}(k; r) = \int\limits_0^\infty dr'\, G^{\ell(\pm)}(k; r, r') \frac{1}{r'} \psi_n^\ell(r'). \tag{15}$$

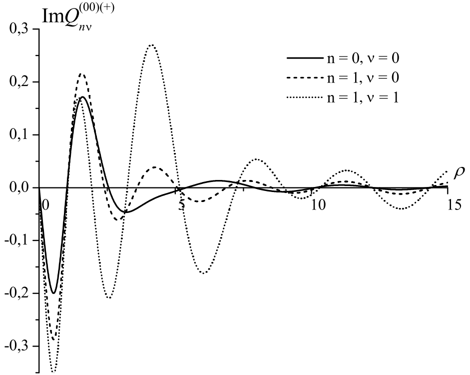
J.A.Del Punta et. al. J. Math. Phys. **55**, 052101 (2014)

$$Q_n^{\ell(\pm)}(k; r) = -\left[(n+1)_{2\ell+1}\right]^{-\frac{1}{2}} (2br)^{\ell+1} e^{-br} \frac{2}{(\lambda \mp ik)} \times \int\limits_0^1 dz\, (1-z)^{\ell \pm i\alpha} (1-\omega^{\pm 1} z)^{\ell \mp i\alpha} (1 - z - \omega^{\pm 1} z)^n \times \exp\left(z\,[b \pm ik]\, r\right) L_n^{2\ell+1}\left(\frac{(1-z)(1-\omega^{\pm 1} z)}{(1-z-\omega^{\pm 1} z)} 2br\right), \omega \equiv e^{i\xi} = \frac{b+ik}{b-ik}. \tag{16}$$

# Real Parts of CQS



# Imaginary Parts of CQS



# Asymptotic Forms

## One-Particle Quasi Sturmian Function

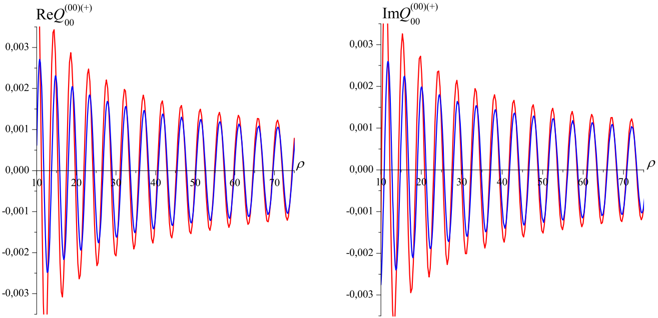
$$Q_n^{\ell(\pm)}(k;r) \underset{r\to\infty}{\sim} -\frac{2}{k}\,S_{n\ell}(k)\,e^{\pm i\left\{kr-\alpha\ln(2kr)-\frac{\pi\ell}{2}+\sigma_\ell\right\}}. \qquad (17)$$

## Two-Particle Quasi Sturmian Function

$$Q_{n\nu}^{(\ell\lambda)(+)} \sim \frac{1}{E}\sqrt{\frac{2}{\pi}}S_{n\ell}(p_1)S_{\nu\lambda}(p_2)(2E)^{3/4}e^{\frac{i\pi}{4}} \times \frac{\exp\left\{i\left[\sqrt{2E}\rho+\sigma_\ell+\sigma_\lambda-\frac{\pi(\ell+\lambda)}{2}-\alpha_1\ln(2p_1r_1)-\alpha_2\ln(2p_2r_2)\right]\right\}}{\sqrt{\rho}}. \qquad (18)$$

$$\rho=\sqrt{r_1^2+r_2^2},\ \tan\phi=r_2/r_1,$$
$$p_1=\sqrt{2E}\cos\phi,\ p_2=\sqrt{2E}\sin\phi,$$
$$\alpha_1=\frac{-2}{p_1},\ \alpha_2=\frac{-2}{p_2}.$$

The real and imaginary parts of the CQS function $Q_{00}^{(00)(+)}$ on the diagonal $r_1 = r_2 = \rho/\sqrt{2}$ (red lines). The real and imaginary components of the corresponding asymptotic representation (18) (blue lines).



# Solution

## Solution Asymptotic Behavior

$$\Phi_{sc}^{(+)}(\mathbf{r}_1,\mathbf{r}_2) \approx \frac{2}{E\sin(2\phi)}\sqrt{\frac{2}{\pi}}(2E)^{3/4}$$
$$\times e^{\frac{i\pi}{4}}\frac{\exp\left\{i\left[\sqrt{2E}\rho-\alpha_1\ln(2p_1r_1)-\alpha_2\ln(2p_2r_2)\right]\right\}}{\rho^{5/2}}$$
$$\times\sum_{\ell\lambda L}\left(\left[\sum_{n,\nu=0}^{N-1}C_{n\nu}^{L(\ell\lambda)}S_{n\ell}(p_1)S_{\nu\lambda}(p_2)\right]\right.$$
$$\left.\times\exp\left\{i\left[\sigma_\ell(p_1)+\sigma_\lambda(p_2)-\frac{\pi(\ell+\lambda)}{2}\right]\right\}\mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\right). \quad (19)$$

# Green's Function

S. P. Merkuriev and L. D. Faddeev, Quantum Scattering Theory for Several Particle Systems

## Green's Function Asymptotic Behavior

$$G^{(+)}(E;\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}'_1,\mathbf{r}'_2) \approx \frac{(2E)^{3/4}e^{\frac{i\pi}{4}}}{(2\pi)^{5/2}} \times \frac{\exp\left\{i\left[\sqrt{2E}\rho+W_0(\mathbf{r}_1,\mathbf{r}_2)\right]\right\}}{\rho^{5/2}}\Psi^{(-)*}_{\mathbf{k}'_1,\mathbf{k}'_2}(\mathbf{r}'_1,\mathbf{r}'_2), \quad (20)$$

The Coulomb phase $W_0$

$$W_0(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\rho}{\sqrt{2E}}\left(\frac{-2}{r_1}+\frac{-2}{r_2}+\frac{1}{r_{12}}\right)\ln 2\sqrt{2E}\rho. \quad (21)$$

$$\mathbf{k}'_1 = p_1\hat{\mathbf{r}}_1,\ \mathbf{k}'_2 = p_2\hat{\mathbf{r}}_2.$$

# Solution II

## Solution Asymptotic Behavior

$$\Phi_{sc}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) \approx \frac{(2E)^{3/4} e^{\frac{i\pi}{4}}}{(2\pi)^{5/2}} \frac{\exp\left\{i\left[\sqrt{2E}\rho + W_0(\mathbf{r}_1, \mathbf{r}_2)\right]\right\}}{\rho^{5/2}} T_{\mathbf{k}_1', \mathbf{k}_2'}, \tag{22}$$

## Transition Amplitude

$$T_{\mathbf{k}_1', \mathbf{k}_2'} = \left\langle \Psi_{\mathbf{k}_1', \mathbf{k}_2'}^{(-)} \middle| \hat{W}_{fi} \middle| \Phi^{(0)} \right\rangle . \tag{23}$$

# Cross Section

## Transition Amplitude

$$
\begin{aligned}
T_{\mathbf{k}'_1,\mathbf{k}'_2} &= \frac{(4\pi)^2}{E\sin(2\phi)} \\
\times \exp\{-i\,[W_0(\mathbf{r}_1,\mathbf{r}_2) &+ \alpha_1 \ln(2p_1 r_1) + \alpha_2 \ln(2p_2 r_2)]\} \\
\times \sum_{\ell\lambda L} \Bigg( \Bigg[ \sum_{n,\nu=0}^{N-1} & C_{n\nu}^{L(\ell\lambda)} S_{n\ell}(p_1) S_{\nu\lambda}(p_2) \Bigg] \\
\times \exp\left\{ i \left[ \sigma_\ell(p_1) + \sigma_\lambda(p_2) - \frac{\pi(\ell+\lambda)}{2} \right] \right\} & \mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2) \Bigg) .
\end{aligned}
\tag{24}
$$

## Differential Cross Section

$$
\frac{d^5\sigma}{d\Omega_1 d\Omega_2 d\Omega_f dE_1 dE_2} = \frac{1}{(2\pi)^2} \frac{k_f k_1 k_2}{k_i} \left| T_{\mathbf{k}'_1,\mathbf{k}'_2} \right|^2 . \tag{25}
$$

# Matrix Equation

## Equation for $C_{n'\nu'}^{L(\ell'\lambda')}$

$$\sum_{\substack{L,\ell',\lambda'\\ n',\nu'}} C_{n'\nu'}^{L(\ell'\lambda')} \Big[ \big| \, n'\widetilde{\ell'\nu'\lambda'; LM} \big\rangle_L + \hat{V}_3^C \, |n'\ell'\nu'\lambda'; LM\rangle_Q \Big] = \hat{W}_{fi} \, \big|\Phi^{(0)}\big\rangle \,, \tag{26}$$

$$\big| \, n\widetilde{\ell\nu\lambda; LM} \, \big\rangle_L \equiv \frac{\psi_n^{\ell}(r_1)\psi_\nu^{\lambda}(r_2)}{r_1^2 r_2^2} \mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2). \tag{27}$$

$$|n\ell\nu\lambda; LM\rangle_L \equiv r_1 r_2 \big| \, n\widetilde{\ell\nu\lambda; LM} \, \big\rangle_L \,, \tag{28}$$

$$_L\langle n\ell\nu\lambda; LM| \, n'\widetilde{\ell'\nu'\lambda'; LM} \, \big\rangle_L = \delta_{n,n'}\delta_{\nu,\nu'}\delta_{\ell,\ell'}\delta_{\lambda,\lambda'}. \tag{29}$$

# Matrix Equation II

$$\sum_{L,\ell',\lambda'} \sum_{n',\nu'=0}^{N-1} \left[\delta_{n,n'}\delta_{\nu,\nu'}\delta_{\ell,\ell'}\delta_{\lambda,\lambda'} - U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'}\right] C^{L(\ell'\lambda')}_{n'\nu'} = R^{L(\ell\lambda)}_{n\nu}. \tag{30}$$

$$R^{L(\ell\lambda)}_{n\nu} = {}_L\langle n\ell\nu\lambda; LM|\hat{W}_{fi}\left|\Phi^{(0)}\right\rangle. \tag{31}$$

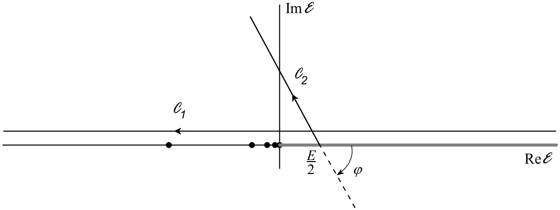
$$U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} = {}_L\langle n\ell\nu\lambda; LM|\frac{1}{r_{12}}\left|n'\ell'\nu'\lambda'; LM\right\rangle_Q \tag{32}$$

$$\begin{aligned} U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} &= {}_L\langle n\ell\nu\lambda; LM|\tfrac{1}{r_{12}}\hat{G}^{(\ell'\lambda')(+)}\left|n'\ell'\widetilde{\nu'\lambda'; LM}\right\rangle_L \\ &= \sum_{n''\nu''=0}^{N-1} {}_L\langle n\ell\nu\lambda; LM|\tfrac{1}{r_{12}}|n''\ell'\nu''\lambda'; LM\rangle_L \\ &\times {}_L\left\langle n''\ell'\widetilde{\nu''\lambda'; LM}\right|\hat{G}^{(\ell'\lambda')(+)}\left|n'\ell'\widetilde{\nu'\lambda'; LM}\right\rangle_L. \end{aligned} \tag{33}$$

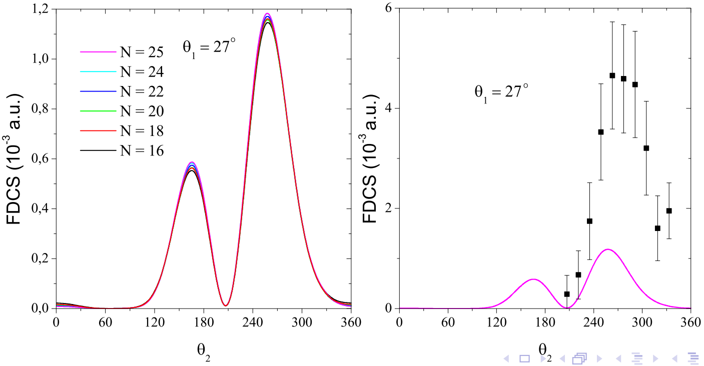
# Matrix Elements of The Green's Function

$$G^{(\ell\lambda)(+)}_{n\nu,n'\nu'} = {}_L\left\langle n\widetilde{\ell\nu\lambda; LM}\middle|\hat{G}^{(\ell\lambda)(+)}\middle|n'\widetilde{\ell\nu'\lambda; LM}\right\rangle_L \qquad (34)$$

$$G^{(\ell\lambda)(+)}_{n\nu,n'\nu'} = \frac{1}{2\pi i}\int\limits_{\mathcal{C}_2} d\mathcal{E}\, G^{\ell(+)}_{nn'}(\sqrt{2\mathcal{E}})G^{\lambda(+)}_{\nu\nu'}(\sqrt{2(E-\mathcal{E})}). \qquad (35)$$



Convergence of the differential cross section for the He($e$, 3$e$)He$^{++}$ reaction as $N$ increases.The coplanar experimental data correspond to a fast scattered electron of $E_s = 5500$ eV; the energies of the ejected electrons are $E_1 = E_2 = 10$ eV, one electron being fixed at $\theta_1 = 27^0$ while the angle $\theta_2$ of the other electron varies.



# Summary

- Two-particle basis functions are proposed which, by analogy with the Green's function of two non-interacting hydrogenic atomic systems, are expressed as a convolution integral of two one-particle QS functions.
- The asymptotic limit for these basis functions in the region $\Omega_0$ is expressed in closed form as a six-dimensional outgoing spherical wave which allows one to obtain an explicit closed-form result for the transition amplitude.
- It is very surprising, in view of the fact that the equation is non-compact on the basis set, the convergence is achieved in our calculations.

- Outlook

$$\widetilde{Q}_{n\nu}^{(\ell\lambda)(+)}(E; r_1, r_2) = e^{iW_3(\mathbf{r}_1, \mathbf{r}_2)} Q_{n\nu}^{(\ell\lambda)(+)}(E; r_1, r_2), \quad (36)$$

$$W_3(\mathbf{r}_1, \mathbf{r}_2) = -\frac{\rho}{\sqrt{2E}} \frac{1}{r_{12}} \ln 2\sqrt{2E}\rho. \quad (37)$$

Thanks for attention!