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Electron Correlations in the Framework of the Quasi Sturmians Approach

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Khabarovsk 19-23 Sep. 2016

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$(e, 3e)$

The Driven Equation

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

The Hamiltonian and Perturbation Operator

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \frac{1}{r_{12}}, \qquad (2)$$

$$\hat{H}_j = -\frac{1}{2}\triangle_{r_j} - \frac{2}{r_j}, \quad j = 1, 2. \qquad (3)$$

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

$$E = 20 \text{ eV}, \quad q = 0.24 \text{ a.u.}, \quad b = 0.6 \text{ a.u.}$$

Convoluted Quasi Sturmian functions

Basis Functions

$$\left|n_1\ell_1 n_2\ell_2; LM\right\rangle_Q \equiv \frac{Q_{n_1 n_2}^{\ell_1\ell_2(+)}(E; r_1, r_2)}{r_1 r_2}\mathcal{Y}_{LM}^{\ell_1\ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \qquad (5)$$

$$\mathcal{Y}_{LM}^{\ell_1\ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \sum_{m_1+m_2=M} (\ell_1 m_1 \ell_2 m_2 \,|\, LM)\, Y_{\ell_1 m_1}(\hat{\mathbf{r}}_1)\, Y_{\ell_2 m_2}(\hat{\mathbf{r}}_2). \qquad (6)$$

The Radial Equation

$$\left[E - \hat{h}_1^{\ell_1} - \hat{h}_2^{\ell_2}\right] Q_{n_1 n_2}^{\ell_1\ell_2(\pm)}(E; r_1, r_2) = \frac{\psi_{n_1}^{\ell_1}(r_1)\psi_{n_2}^{\ell_2}(r_2)}{r_1 r_2}, \qquad (7)$$

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

CQS Functions Asymptoic Behavior

The Leading Asymptotic Term

$$Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2) \simeq \sqrt{\frac{8}{\pi}}\, e^{i\frac{\pi}{4}} S_{n_1 \ell_1}(p_1) S_{n_2 \ell_2}(p_2) \times \frac{\exp\left\{ i\left[k\rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2) + \sigma_{\ell_1}(p_1) + \sigma_{\ell_2}(p_2) - \frac{\pi(\ell_1+\ell_2)}{2} \right]\right\}}{\sqrt{k\rho}}. \tag{9}$$

$$\tan(\alpha) = r_2/r_1, k = \sqrt{2E},$$

$$p_1 = k\cos(\alpha), p_2 = k\sin(\alpha),$$

$$\beta_1 = \frac{-2}{p_1}, \beta_2 = \frac{-2}{p_2},$$

$$e^{i\sigma_\ell(p)} = \frac{\Gamma(\ell + 1 + i\beta)/|}{\Gamma(\ell + 1 + i\beta)|}.$$

The Solution Representation

The Expansion

$$\Phi^{(+)}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{\ell_1,\,\ell_2=0}^{\infty}\ \sum_{n_1,\,n_2=0}^{\infty} C_{n_1n_2}^{L(\ell_1\ell_2)}\,|n_1\ell_1n_2\ell_2:LM\rangle_Q\,, \qquad (10)$$

The Asymptotic Behavior

$$\Phi^{(+)}(\mathbf{r}_1,\mathbf{r}_2)\simeq A(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\,\frac{\exp\{i\,[k\rho-\beta_1\ln(2p_1r_1)-\beta_2\ln(2p_2r_2)]\}}{\rho^{5/2}}, \qquad (11)$$

$$A(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)=\frac{2}{E\sin(2\alpha)}\sqrt{\frac{2}{\pi}}(2E)^{3/4}e^{\frac{i\pi}{4}}$$
$$\times\sum_{\ell_1\ell_2=0}^{\infty}\mathcal{Y}_{LM}^{\ell_1\ell_2}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\exp\left\{i\left[\sigma_{\ell_1}(p_1)+\sigma_{\ell_2}(p_2)-\frac{\pi(\ell_1+\ell_2)}{2}\right]\right\}$$
$$\times\sum_{n_1,n_2=0}^{\infty}C_{n_1n_2}^{L(\ell_1\ell_2)}S_{n_1\ell_1}(p_1)S_{n_2\ell_2}(p_2). \qquad (12)$$

The Two-Electron Continuum Representation

The Phase Factor

$$W_3(\mathbf{r}_1, \mathbf{r}_2) = -\frac{\rho}{k}\frac{1}{r_{12}} \ln\left(2k\rho\right). \tag{13}$$

The New Solution

$$\Phi^{(+)}\left(\mathbf{r}_1, \mathbf{r}_2\right) = e^{i\mathcal{W}(\mathbf{r}_1, \mathbf{r}_2)} \widetilde{\Phi}^{(+)}\left(\mathbf{r}_1, \mathbf{r}_2\right), \tag{14}$$

$$\mathcal{W}\left(\mathbf{r}_1, \mathbf{r}_2\right) \simeq W_3(\mathbf{r}_1, \mathbf{r}_2). \tag{15}$$

$$\widetilde{\Phi}^{(+)}\left(\mathbf{r}_1, \mathbf{r}_2\right) = \sum_{\ell_1, \ell_2=0}^{\infty} \sum_{n_1, n_2=0}^{\infty} \widetilde{C}_{n_1 n_2}^{L(\ell_1 \ell_2)} \left| n_1 \ell_1 n_2 \ell_2 : LM \right\rangle_Q . \tag{16}$$

The Two-Electron Continuum Representation

The New Equation

$$\left[E - \hat{H}_1 - \hat{H}_2 + \hat{\mathcal{L}}\right] \widetilde{\Phi}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = e^{-i\mathcal{W}(\mathbf{r}_1, \mathbf{r}_2)} \hat{W}_{fi} \Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2). \tag{17}$$

The 'Perturbation' Operator

$$\widehat{\mathcal{L}} = \widehat{\mathcal{U}} + \widehat{\mathcal{V}}, \tag{18}$$

$$\begin{aligned} \widehat{\mathcal{U}} = \frac{i}{2}\left[\triangle_{r_1}\mathcal{W} + \triangle_{r_2}\mathcal{W}\right] - \frac{1}{2}\left[\left(\nabla_{r_1}\mathcal{W}\right)^2 + \left(\nabla_{r_2}\mathcal{W}\right)^2\right] \\ +i\left[\frac{1}{r_1}\left(\nabla_{r_1}\mathcal{W}\right)\cdot\nabla_{\Omega_1} + \frac{1}{r_2}\left(\nabla_{r_2}\mathcal{W}\right)\cdot\nabla_{\Omega_2}\right], \end{aligned} \tag{19}$$

$$\widehat{\mathcal{V}} = i\left[\left(\nabla_{r_1}\mathcal{W}\right)\cdot\frac{\mathbf{r}_1}{r_1}\frac{\partial}{\partial r_1} + \left(\nabla_{r_2}\mathcal{W}\right)\cdot\frac{\mathbf{r}_2}{r_2}\frac{\partial}{\partial r_2}\right] - \frac{1}{r_{12}}. \tag{20}$$

The Two-Electron Continuum Representation

The 'Perturbation' Operator

$$\nabla_{r_1}\mathcal{W} \simeq -\frac{1}{k}\left\{\frac{\mathbf{r}_1}{r_{12}\rho}\left[1+\ln\left(2k\rho\right)\right] - \frac{\mathbf{r}_{12}}{r_{12}^3}\rho\ln\left(2k\rho\right)\right\}, \qquad (21)$$

$$\nabla_{r_2}\mathcal{W} \simeq -\frac{1}{k}\left\{\frac{\mathbf{r}_2}{r_{12}\rho}\left[1+\ln\left(2k\rho\right)\right] + \frac{\mathbf{r}_{12}}{r_{12}^3}\rho\ln\left(2k\rho\right)\right\}. \qquad (22)$$

Asymptotic Behavior

$$\frac{\partial}{\partial r_{1,2}}\left|n_1\ell_1 n_2\ell_2 : LM\right\rangle_Q \simeq ik\frac{r_{1,2}}{\rho}\left|n_1\ell_1 n_2\ell_2 : LM\right\rangle_Q . \qquad (23)$$

The Temkin-Poet model case

The Solution

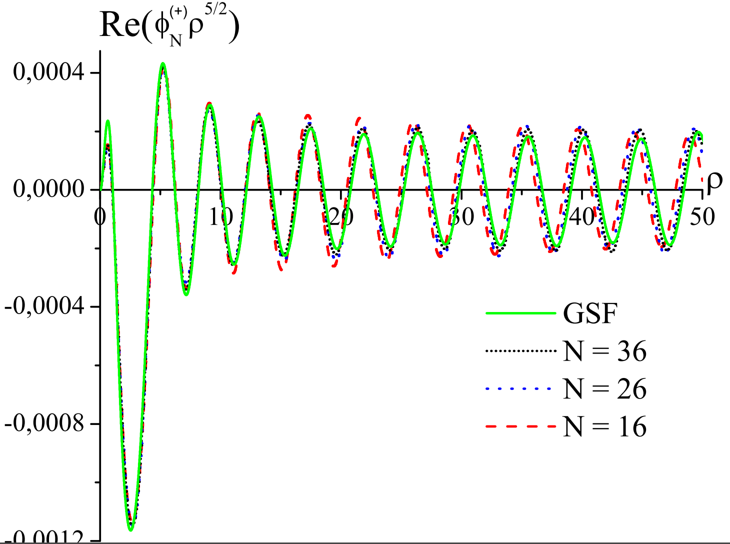
$$\Phi_N^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{n_1,\, n_2=0}^{N-1} C_{n_1 n_2} \, |n_1 0 n_2 0 : 0\rangle_Q \,. \tag{24}$$

$$\Phi_N^{(+)}(\mathbf{r}_1, \mathbf{r}_2) \simeq \frac{A_N}{4\pi\rho^{5/2}} \exp\left\{i\left[k\rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2)\right]\right\} \tag{25}$$

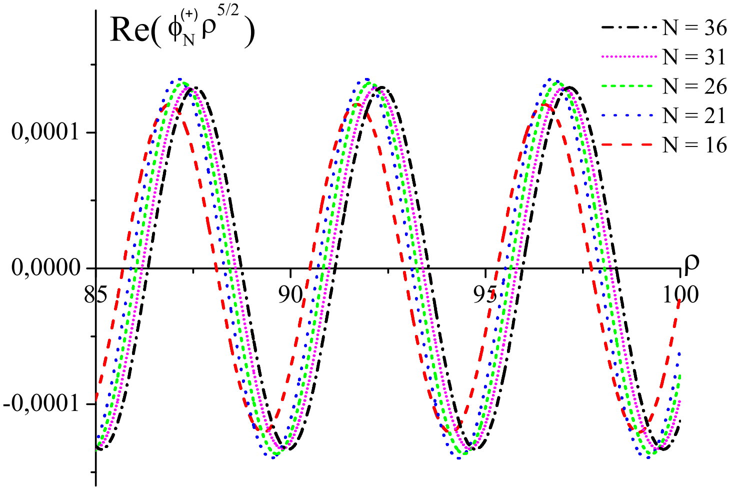
Asymptotic Behavior

$$A_N = \frac{2}{\sin(2\alpha)}\sqrt{\frac{8}{\pi}}\, e^{\frac{i\pi}{4}} k^{-1/2} \exp\left\{i\left[\sigma_0(p_1) + \sigma_0(p_2)\right]\right\} \times \sum_{n_1, n_2=0}^{N-1} C_{n_1 n_2} S_{n_1 0}(p_1) S_{n_2 0}(p_2). \tag{26}$$

The Temkin-Poet model case



The Temkin-Poet model case



The Two-Electron Continuum Representation

The Parametrization of the Phase

$$\mathcal{W}(r_1, r_2) = -\frac{s}{\sqrt{2E}}\frac{1}{u}\left(\ln(2\sqrt{2E}s) + c\right) + \frac{d}{u}, \tag{27}$$

$$u = a + r_>,\ s = \sqrt{a + \rho^2}.$$

$$a = 2.5, \quad c = -2.364, \quad d = -0.75. \tag{28}$$

The Two-Electron Continuum Representation

The New Solution

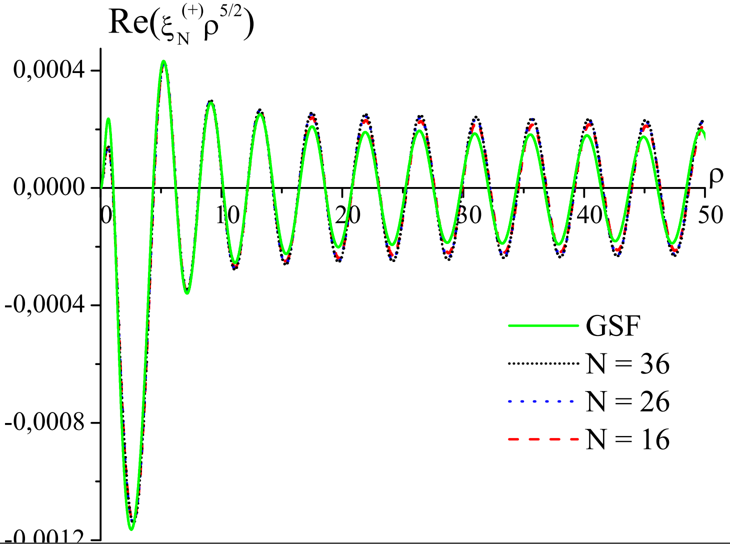
$$\widetilde{\Phi}_N^{(+)}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{n_1,\,n_2=0}^{N-1} \widetilde{C}_{n_1 n_2}\, |n_1 0 n_2 0 : 0\rangle_Q \,. \tag{29}$$

$$\widetilde{\Phi}_N^{(+)}(\mathbf{r}_1,\mathbf{r}_2) \simeq \frac{\widetilde{A}_N}{4\pi\rho^{5/2}} \exp\left\{i\left[k\rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2)\right]\right\} \tag{30}$$

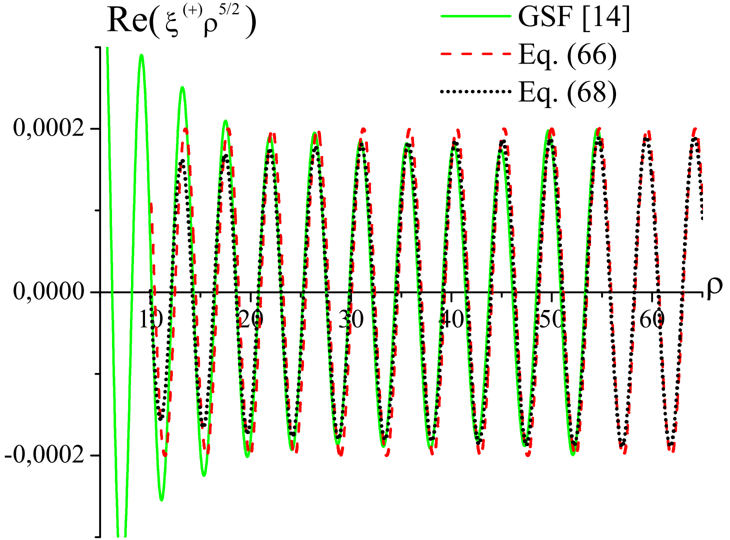
Asymptotic Behavior

$$\widetilde{A}_N = \frac{2}{\sin(2\alpha)}\sqrt{\frac{8}{\pi}}\, e^{\frac{i\pi}{4}} k^{-1/2} \exp\left\{i\left[\sigma_0(p_1)+\sigma_0(p_2)\right]\right\} \times \sum_{n_1,n_2=0}^{N-1} \widetilde{C}_{n_1 n_2} S_{n_1 0}(p_1) S_{n_2 0}(p_2). \tag{31}$$

The Temkin-Poet model case



The Temkin-Poet model case



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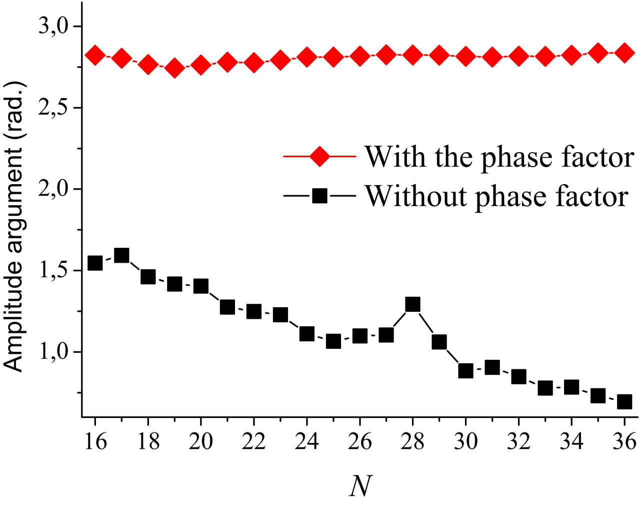
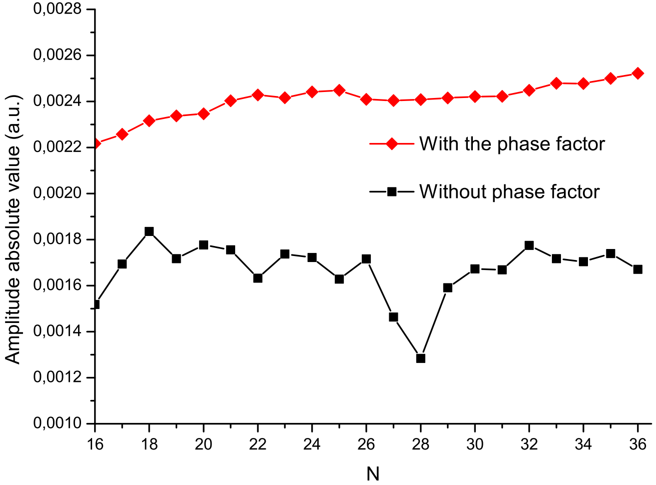


The Temkin-Poet model case



The Two-Channel Case

The Multipole Expansion

$$\mathcal{Y}_{00}^{00}, \mathcal{Y}_{00}^{11}$$

$$V_{12} = \sum_{\ell=0}^{2} \left(\frac{r_<^{\ell}}{r_>^{\ell+1}} \right) P_\ell(x), \tag{32}$$

$$x = \frac{r_1^2 + r_2^2 - r_{12}^2}{2 r_1 r_2}. \tag{33}$$

The Two-Channel Case

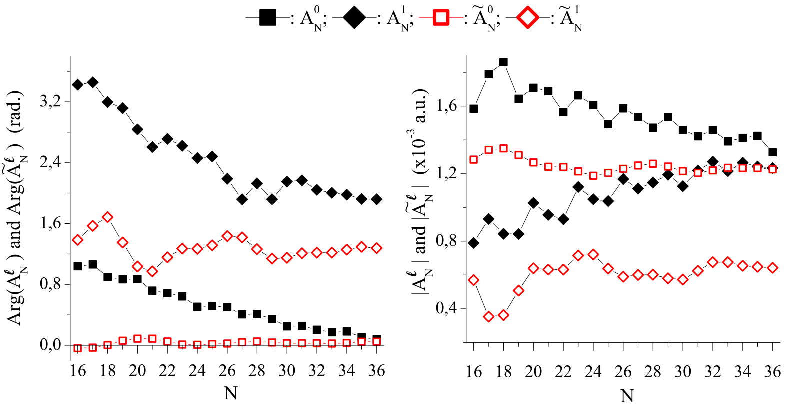
The Solution

$$\Phi_N^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\ell=0,1} \sum_{n_1,\, n_2=0}^{N-1} C^{\ell}_{n_1 n_2} \, |n_1 \ell n_2 \ell : 0\rangle_Q \,. \quad (34)$$

$$\Phi_N^{(+)}(\mathbf{r}_1, \mathbf{r}_2) \simeq \frac{1}{\rho^{5/2}} \exp\left\{i \left[k\rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2)\right]\right\} \sum_{\ell=0,1} A^{\ell}_N \mathcal{Y}^{\ell\ell}_{00}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \quad (35)$$

$$A^{\ell}_N = \frac{2}{\sin(2\alpha)} \sqrt{\frac{8}{\pi}}\, e^{\frac{i\pi}{4}} k^{-1/2} \exp\left\{i \left[\sigma_\ell(p_1) + \sigma_\ell(p_2) - \pi\ell\right]\right\} \times \sum_{n_1, n_2=0}^{N-1} C^{\ell}_{n_1 n_2} S_{n_1 \ell}(p_1) S_{n_2 \ell}(p_2). \quad (36)$$

The Two-Channel case



The Two-Channel Case

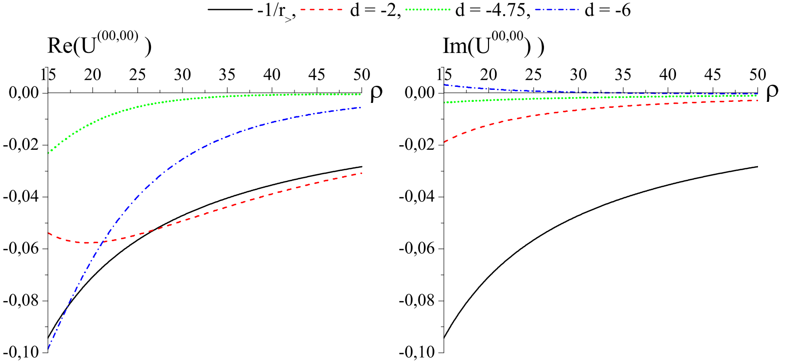
The Parametrization of the Phase

$$\mathcal{W}(\mathbf{r}_1, \mathbf{r}_2) = -\frac{s}{k}\left[\ln(2ks) + d\right]\left(\frac{1}{u} + \frac{r_1 r_2}{u^3} P_1(x) + \frac{(r_1 r_2)^2}{u^5} P_2(x)\right), \tag{37}$$

$$u = \sqrt{a^2 + r_>^2}, \quad s = \sqrt{a + \rho^2}, \tag{38}$$

$$a = 5, \quad d = -4.75. \tag{39}$$

The Two-Channel case



The Two-Electron Continuum Representation

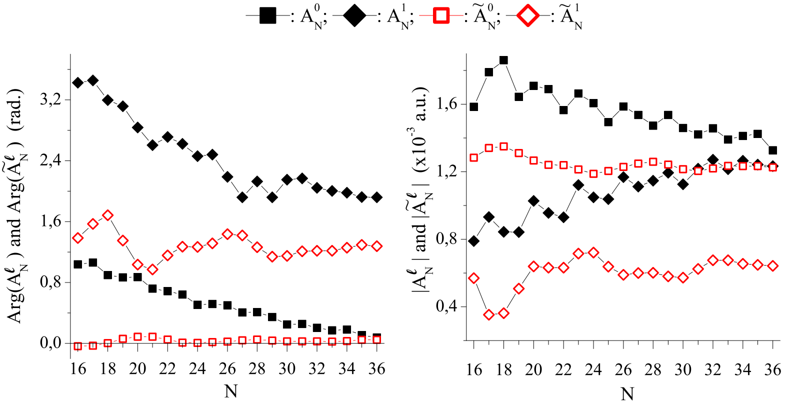
The New Solution

$$\widetilde{\Phi}_N^{(+)}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{\ell=0,1}\sum_{n_1,\,n_2=0}^{N-1} \widetilde{C}^{\ell}_{n_1 n_2}\,|n_1\ell n_2\ell : 0\rangle_Q\,. \qquad (40)$$

$$\widetilde{\Phi}_N^{(+)}(\mathbf{r}_1,\mathbf{r}_2) \simeq \frac{1}{\rho^{5/2}}\exp\{i\,[k\rho - \beta_1\ln(2p_1r_1) - \beta_2\ln(2p_2r_2)]\} \sum_{\ell=0,1}\widetilde{A}^{\ell}_N\mathcal{Y}^{\ell\ell}_{00}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2), \qquad (41)$$

$$\widetilde{A}^{\ell}_N = \frac{2}{\sin(2\alpha)}\sqrt{\frac{8}{\pi}}\,e^{\frac{i\pi}{4}}\,k^{-1/2}\exp\{i\,[\sigma_\ell(p_1)+\sigma_\ell(p_2)-\pi\ell]\} \times \sum_{n_1,n_2=0}^{N-1}\widetilde{C}^{\ell}_{n_1 n_2}S_{n_1\ell}(p_1)S_{n_2\ell}(p_2). \qquad (42)$$

The Two-Channel case



Summary

- The phase factor method is extended to include higher partial waves
- This approach is based upon the extraction from the three-body continuum wave function the logarithmic phase factor, corresponding to the Coulomb electron-electron interaction, and expansion of the new wave function in terms of the so-called Convoluted Quasi Sturmians (CQS). Due to the asymptotic behavior of CQS they constitute a suitable set of basis functions for the continuum wave function representation in the entire space
- The use of an appropriate phase form provides a considerable improvement of the rate of convergence