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最弱受约束电子势模型理论下使用双广义拉盖尔多项式计算氦原子基态能量

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Calculation of He Atom Ground-State Energy Using Double Generalized Laguerre Polynomial in the Weakest Bound Electron Potential Model Theory

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appendix 1

$$\left\langle \varphi_i(\mu)\left|\hat{h}(\mu)\right|\varphi_i(\mu)\right\rangle = \left\langle \varphi_i(\mu)\left|-\frac{1}{2}\nabla_\mu^2 - \frac{Z}{r_\mu}\right|\varphi_i(\mu)\right\rangle = \frac{z_i^{'2}}{2n_i^{'2}(2n_i^{'}-1)} - \frac{Zz_i^{'}}{n_i^{'2}}$$

$$\left\langle \varphi_i(\mu)\left|\hat{h}(\mu)\right|\varphi_j(\mu)\right\rangle = \left\langle \varphi_i(\mu)\left|-\frac{1}{2}\nabla_\mu^2 - \frac{Z}{r_\mu}\right|\varphi_j(\mu)\right\rangle$$
$$= [\Gamma(2l_i^{'}+3)\Gamma(2l_j^{'}+3)]^{-1/2}(\frac{2z_i^{'}}{n_i^{'}})^{l_i^{'}+3/2}(\frac{2z_j^{'}}{n_j^{'}})^{l_j^{'}+3/2}(\frac{z_i^{'}}{n_i^{'}}+\frac{z_j^{'}}{n_j^{'}})^{-l_i^{'}-l_j^{'}-1}\Gamma(l_i^{'}+l_j^{'}+1)$$
$$[-\frac{z_j^{'2}}{2n_j^{'2}}(l_i^{'}+l_j^{'}+2)(l_i^{'}+l_j^{'}+1)(\frac{z_i^{'}}{n_i^{'}}+\frac{z_j^{'}}{n_j^{'}})^{-2}+z_j^{'}(l_i^{'}+l_j^{'}+1)(\frac{z_i^{'}}{n_i^{'}}+\frac{z_j^{'}}{n_j^{'}})^{-1}-\frac{l_j^{'}(l_j^{'}+1)}{2}]$$
$$-Z[\Gamma(2l_i^{'}+3)\Gamma(2l_j^{'}+3)]^{-1/2}(\frac{2z_i^{'}}{n_i^{'}})^{l_i^{'}+3/2}(\frac{2z_j^{'}}{n_j^{'}})^{l_j^{'}+3/2}(\frac{z_i^{'}}{n_i^{'}}+\frac{z_j^{'}}{n_j^{'}})^{-l_i^{'}-l_j^{'}-2}\Gamma(l_i^{'}+l_j^{'}+2)$$

$$\left\langle \varphi_i(\mu)\varphi_i(\nu)\frac{1}{r_{\mu\nu}}\varphi_i(\mu)\varphi_i(\nu)\right\rangle$$
$$= \frac{z_i^{'}}{n_i^{'2}}\{1-2^{-4n_i^{'}}\Gamma(4n_i^{'}+1)[\Gamma(2n_i^{'}+1)]^{-2}\}$$

$$\left\langle \varphi_1(1)\varphi_1(2)\frac{1}{r_{12}}\varphi_2(1)\varphi_1(2)\right\rangle$$
$$= [\Gamma(2l_1^{'}+3)\Gamma(2l_2^{'}+3)]^{-1/2}(\frac{2z_2^{'}}{n_2^{'}})^{l_2^{'}+3/2}\{(\frac{2z_1^{'}}{n_1^{'}})^{l_1^{'}+5/2}(\frac{z_1^{'}}{n_1^{'}}+\frac{z_2^{'}}{n_2^{'}})^{-l_1^{'}-l_2^{'}-3}(2l_1^{'}+2)^{-1}\Gamma(l_1^{'}+l_2^{'}+3)$$
$$-(\frac{2z_1^{'}}{n_1^{'}})^{-l_2^{'}-1/2}[(2z_1^{'}n_2^{'})^{-1}(3z_1^{'}n_2^{'}+z_2^{'}n_1^{'})]^{-3l_1^{'}-l_2^{'}-4}[\Gamma(2l_1^{'}+3)]^{-1}\Gamma(3l_1^{'}+l_2^{'}+4)+(\frac{2z_1^{'}}{n_1^{'}})^{-l_2^{'}-1/2}$$
$$[\Gamma(2l_1^{'}+3)]^{-1}[\Gamma(2l_1^{'}+3)[(2z_1^{'}n_2^{'})^{-1}(z_1^{'}n_2^{'}+z_2^{'}n_1^{'})]^{-l_1^{'}-l_2^{'}-2}\Gamma(l_1^{'}+l_2^{'}+2)-\Gamma(2l_1^{'}+2)$$
$$[(2z_1^{'}n_2^{'})^{-1}(z_1^{'}n_2^{'}+z_2^{'}n_1^{'})]^{-l_1^{'}-l_2^{'}-3}\Gamma(l_1^{'}+l_2^{'}+3)-\int_0^\infty[(2l_1^{'}+2)-x]x^{l_1^{'}+l_2^{'}+1}e^{-\frac{z_1^{'}n_2^{'}+z_2^{'}n_1^{'}}{2z_1^{'}n_2^{'}}x}\Gamma(2l_1^{'}+2,x)dx]\}$$

$$\left\langle \varphi_1(1)\varphi_1(2)\frac{1}{r_{12}}\varphi_2(1)\varphi_2(2)\right\rangle$$
$$=[\Gamma(2l_1^{'}+3)\Gamma(2l_2^{'}+3)]^{-1/2}(\frac{2z_1^{'}}{n_1^{'}})^{2l_1^{'}+3}(\frac{2z_2^{'}}{n_2^{'}})^{2l_2^{'}+3}(\frac{z_1^{'}}{n_1^{'}}+\frac{z_2^{'}}{n_2^{'}})^{-2l_1^{'}-2l_2^{'}-5}[\Gamma(l_1^{'}+l_2^{'}+2)\Gamma(l_1^{'}+l_2^{'}+3)$$
$$-2^{-2l_1^{'}-2l_2^{'}-3}\Gamma(2l_1^{'}+2l_2^{'}+4)]$$

$$\left\langle \varphi_2(1)\varphi_1(2)\frac{1}{r_{12}}\varphi_2(1)\varphi_1(2)\right\rangle$$
$$=\frac{z_2^{'}}{n_2^{'2}}-[\Gamma(2l_1^{'}+3)\Gamma(2l_2^{'}+3)]^{-1}(\frac{2z_2^{'}}{n_2^{'}})^{2l_2^{'}+3}\{(\frac{2z_1^{'}}{n_1^{'}})^{2l_1^{'}+2}(\frac{2z_1^{'}}{n_1^{'}}+\frac{2z_2^{'}}{n_2^{'}})^{-2l_1^{'}-2l_2^{'}-4}\Gamma(2l_1^{'}+2l_2^{'}+4)$$
$$-(\frac{2z_1^{'}}{n_1^{'}})^{-2l_2^{'}-2}\int_0^\infty[(2l_1^{'}+2)-x]x^{2l_2^{'}+1}e^{-\frac{z_2^{'}n_1^{'}}{z_1^{'}n_2^{'}}x}\Gamma(2l_1^{'}+2,x)dx\}$$

$$\left\langle \varphi_2(1)\varphi_1(2)\frac{1}{r_{12}}\varphi_2(1)\varphi_2(2)\right\rangle$$
$$=[\Gamma(2l_1^{'}+3)\Gamma(2l_2^{'}+3)]^{-1/2}(\frac{2z_1^{'}}{n_1^{'}})^{l_1^{'}+3/2}(\frac{2z_2^{'}}{n_2^{'}})^{l_2^{'}+3/2}(\frac{z_1^{'}}{n_1^{'}}+\frac{z_2^{'}}{n_2^{'}})^{-l_1^{'}-l_2^{'}-2}\Gamma(l_1^{'}+l_2^{'}+2)$$
$$+[\Gamma(2l_1^{'}+3)]^{-1/2}[\Gamma(2l_2^{'}+3)]^{-3/2}(\frac{2z_1^{'}}{n_1^{'}})^{l_1^{'}+3/2}(\frac{2z_2^{'}}{n_2^{'}})^{3l_2^{'}+9/2}(\frac{z_1^{'}}{n_1^{'}}+\frac{z_2^{'}}{n_2^{'}})^{-l_1^{'}-3l_2^{'}-5}$$
$$\{-[(z_1^{'}n_2^{'}+z_2^{'}n_1^{'})^{-1}(z_1^{'}n_2^{'}+3z_2^{'}n_1^{'})]^{-l_1^{'}-3l_2^{'}-4}\Gamma(l_1^{'}+3l_2^{'}+4)+(l_1^{'}+l_2^{'}+2)\Gamma(l_1^{'}+l_2^{'}+2)\Gamma(2l_2^{'}+2)$$
$$[(z_1^{'}n_2^{'}+z_2^{'}n_1^{'})^{-1}(2z_2^{'}n_1^{'})]^{-2l_2^{'}-2}-\Gamma(l_1^{'}+l_2^{'}+2)\Gamma(2l_2^{'}+3)[(z_1^{'}n_2^{'}+z_2^{'}n_1^{'})^{-1}(2z_2^{'}n_1^{'})]^{-2l_2^{'}-3}$$
$$-\int_0^\infty[(l_1^{'}+l_2^{'}+2)-x]x^{2l_2^{'}+1}e^{-\frac{2z_2^{'}n_1^{'}}{z_1^{'}n_2^{'}+z_2^{'}n_1^{'}}x}\Gamma(l_1^{'}+l_2^{'}+2,x)dx\}$$

appendix 2

$$E=\left(c_1^2+c_2^2+\frac{2^{4+d_1+d_2}c_1c_2(\frac{z_1^{'}}{1+d_1})^{\frac{3}{2}+d_1}(\frac{z_2^{'}}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2})^{-3-d_1-d_2}\Gamma(3+d_1+d_2)}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}\right)^{-2}$$

$$[\left\{2c_1^4+2c_1^2c_2^2+4c_1^3c_2\frac{(\frac{2z_1^{'}}{1+d_1})^{\frac{3}{2}+d_1}(\frac{2z_2^{'}}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2})^{-3-d_1-d_2}\Gamma(3+d_1+d_2)}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}\right\}$$

$$\left\{-\frac{Zz_1^{'}}{(1+d_1)^2}+\frac{1}{2(1+2d_1)}\frac{z_1^{'2}}{(1+d_1)^2}\right\}+$$

$$\left\{4c_1^3c_2+4c_1c_2^3+8c_1^2c_2^2\frac{(\frac{2z_1^{'}}{1+d_1})^{\frac{3}{2}+d_1}(\frac{2z_2^{'}}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2})^{-3-d_1-d_2}\Gamma(3+d_1+d_2)}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}\right\}$$

$$\left\{\frac{(\frac{2z_1^{'}}{1+d_1})^{\frac{3}{2}+d_1}(\frac{2z_2^{'}}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2})^{-1-d_1-d_2}\Gamma(1+d_1+d_2)}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}\right.$$

$$\left[-\frac{1}{2}d_2(1+d_2)-\frac{z_2^{'2}}{2(1+d_2)^2}\left(1+d_1+d_2\right)\left(2+d_1+d_2\right)\left(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2}\right)^{-2}+\left(1+d_1+d_2\right)z_2^{'}\left(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2}\right)^{-1}\right]$$

$$\left.-2\frac{(\frac{2z_1^{'}}{1+d_1})^{\frac{3}{2}+d_1}(\frac{2z_2^{'}}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2})^{-2-d_1-d_2}\Gamma(2+d_1+d_2)}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}\right\}+\left[-\frac{Zz_2^{'}}{(1+d_2)^2}+\frac{1}{2(1+2d_2)}\frac{z_2^{'2}}{(1+d_2)^2}\right]$$

$$\left[2c_1^2c_2^2+2c_2^4+4c_1c_2^3\frac{(\frac{2z_1^{'}}{1+d_1})^{\frac{3}{2}+d_1}(\frac{2z_2^{'}}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1^{'}}{1+d_1}+\frac{z_2^{'}}{1+d_2})^{-3-d_1-d_2}\Gamma(3+d_1+d_2)}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}\right]+$$

$$c_1^4\left\{\frac{z_1^{'}}{(1+d_1)^2}\left(1-\frac{2^{-4(1+d_1)}\Gamma(5+4d_1)}{\Gamma(3+2d_1)^2}\right)\right\}+$$

$$4c_1^3c_2\left\{\frac{(\frac{2z_1'}{1+d_1})^{\frac{5}{2}+d_1}(\frac{2z_2'}{1+d_2})^{\frac{3}{2}+d_2}(\frac{z_1'}{1+d_1}+\frac{z_2'}{1+d_2})^{-3-d_1-d_2}\Gamma(3+d_1+d_2)}{(2+2d_1)\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}-\right.$$

$$\frac{(\frac{2z_1'}{1+d_1})^{-\frac{1}{2}-d_2}(\frac{2z_2'}{1+d_2})^{\frac{3}{2}+d_2}(\frac{3(1+d_2)z_1'+(1+d_1)z_2'}{2(1+d_2)z_1'})^{-4-3d_1-d_2}\Gamma(4+3d_1+d_2)}{\Gamma[3+2d_1]\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}+$$

$$\frac{1}{\sqrt{\Gamma(3+2d_1)\Gamma(3+2d_2)}}(\frac{2z_1'}{1+d_1})^{-\frac{1}{2}-d_2}(\frac{2z_2'}{1+d_2})^{\frac{3}{2}+d_2}\left[(\frac{(1+d_2)z_1'+(1+d_1)z_2'}{2(1+d_2)z_1'})^{-2-d_1-d_2}\Gamma(2+d_1+d_2)-\right.$$

$$\frac{\left(\frac{(1+d_2)z_1'+(1+d_1)z_2'}{2(1+d_2)z_1'}\right)^{-3-d_1-d_2}\Gamma\left(3+d_1+d_2\right)}{2+2d_1}-$$

$$\left.\left.\frac{1}{\Gamma\left(3+2d_1\right)}\int_0^\infty e^{\frac{x(-(1+d_2)z_1'-(1+d_1)z_2')}{2(1+d_2)z_1'}}\left(2+2d_1-x\right)x^{1+d_1+d_2}\Gamma(2+2d_1,x)dx\right]\right\}+$$

$$4c_1^2c_2^2\left\{\frac{1}{\Gamma[3+2d_1]\Gamma[3+2d_2]}(\frac{2z_1'}{1+d_1})^{3+2d_1}(\frac{2z_2'}{1+d_2})^{3+2d_2}(\frac{z_1'}{1+d_1}+\frac{z_2'}{1+d_2})^{-5-2d_1-2d_2}\right.$$

$$\left.\left[\Gamma\left(2+d_1+d_2\right)\Gamma\left(3+d_1+d_2\right)-2^{-3-2d_1-2d_2}\Gamma\left(4+2d_1+2d_2\right)\right]\right\}+$$

$$2c_1^2c_2^2\left\{\frac{z_2'}{(1+d_2)^2}-\frac{(\frac{2z_1'}{1+d_1})^{2+2d_1}(\frac{2z_2'}{1+d_2})^{3+2d_2}(\frac{2z_1'}{1+d_1}+\frac{2z_2'}{1+d_2})^{-4-2d_1-2d_2}\Gamma(4+2d_1+2d_2)}{\Gamma\left(3+2d_1\right)\Gamma\left(3+2d_2\right)}-\right.$$

$$\frac{1}{\Gamma\left(3+2d_1\right)\Gamma\left(3+2d_2\right)}\left(\frac{2z_1'}{1+d_1}\right)^{-2-2d_2}\left(\frac{2z_2'}{1+d_2}\right)^{3+2d_2}$$

$$\left.\int_0^\infty e^{-\frac{(1+d_1)xz_2'}{(1+d_2)z_1'}}\left(2+2d_1-x\right)x^{1+2d_2}\Gamma\left(2+2d_1,x\right)\right\}+$$

$$4c_1c_2{}^3\left\{\frac{\left(\frac{2z_1'}{1+d_1}\right)^{\frac{3}{2}+d_1}\left(\frac{2z_2'}{1+d_2}\right)^{\frac{3}{2}+d_2}\left(\frac{z_1'}{1+d_1}+\frac{z_2'}{1+d_2}\right)^{-2-d_1-d_2}\Gamma\left(2+d_1+d_2\right)}{\sqrt{\Gamma\left(3+2d_1\right)\Gamma\left(3+2d_2\right)}}+\right.$$

$$\frac{1}{\Gamma\left(3+2d_1\right)\sqrt{\Gamma\left(3+2d_1\right)\Gamma\left(3+2d_2\right)}}\left(\frac{2z_1'}{1+d_1}\right)^{\frac{3}{2}+d_1}\left(\frac{2z_2'}{1+d_2}\right)^{\frac{9}{2}+3d_2}$$

$$\left(\frac{z_1'}{1+d_1}+\frac{z_2'}{1+d_2}\right)^{-5-d_1-3d_2}[$$

$$\left(2+d_1+d_2\right)\left(\frac{2\left(1+d_1\right)z_2'}{\left(1+d_2\right)z_1'+\left(1+d_1\right)z_2'}\right)^{-2-2d_2}\Gamma\left(2+d_1+d_2\right)\Gamma\left(2+2d_2\right)-$$

$$\left(\frac{2\left(1+d_1\right)z_2'}{\left(1+d_2\right)z_1'+\left(1+d_1\right)z_2'}\right)^{-3-2d_2}\Gamma\left(2+d_1+d_2\right)\Gamma\left(3+2d_2\right)-$$

$$\left(\frac{\left(1+d_2\right)z_1'+3\left(1+d_1\right)z_2'}{\left(1+d_2\right)z_1'+\left(1+d_1\right)z_2'}\right)^{-4-d_1-3d_2}\Gamma\left(4+d_1+3d_2\right)-$$

$$\left.\left.\int_0^\infty e^{-\frac{2\left(1+d_1\right)xz_2'}{\left(1+d_2\right)z_1'+\left(1+d_1\right)z_2'}}\left(2+d_1+d_2-x\right)x^{1+2d_2}\Gamma\left(2+d_1+d_2,x\right)dx\right]\right\}+$$

$$c_2{}^4\left\{\frac{z_2'}{\left(1+d_2\right)^2}\left(1-2^{-4\left(1+d_2\right)}\frac{\Gamma\left(5+4d_2\right)}{\Gamma\left(3+2d_2\right)^2}\right)\right\}\Bigg]$$