Convergence of the bipolar expansion for the Coulomb potential

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The bipolar expansion for the Coulomb potential,

$$\frac{1}{|\mathbf{r_1} - \mathbf{R} - \mathbf{r_2}|} \;=\; \sum c_{l_1 l_2 l_3}^{m_1 m_2}\, Y_{l_1}^{m_1}(\theta_1, \phi_1)\; Y_{l_2}^{m_2}(\theta_2, \phi_2)\; Y_{l_3}^{-m_1-m_2}(\theta_3, \phi_3)\, v_{l_1, l_2, l_3}(r_1, r_2, R),$$

is a four-region expansion: in three of the regions, one distance is dominant ($R > r_1 + r_2$, $r_1 > r_2 + R$, or $r_2 > r_1 + R$); in the fourth, the radii satisfy the triangle inequality, ($r_1 + r_2 > R > |r_1 - r_2|$), and associated charge densities would be interpenetrating. The radial function $v_{l_1, l_2, l_3}(r_1, r_2, R)$ has a different functional form in each region. (See, for instance, Ref. [1].)

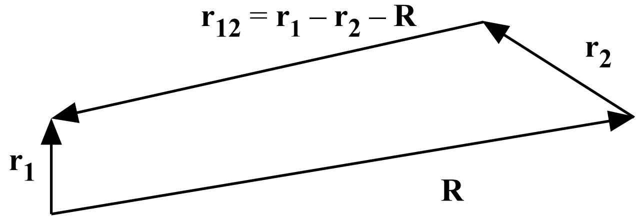

Figure 1: $\mathbf{r_1}$, $\mathbf{r_2}$, and $\mathbf{R}$, drawn for the case $R > r_1 + r_2$.

When any one distance is dominant, for example $R > r_1 + r_2$, then the bipolar expansion converges absolutely by comparison with the series

$$\frac{1}{R - r_1 - r_2} \;=\; \sum_{l_1=0}^{\infty} \sum_{l_1=0}^{\infty} \binom{l_1 + l_2}{l_1} r_1^{l_1} r_2^{l_2} R^{-l_1 - l_2 - 1}$$

For the interpenetrating region, it has only recently been shown numerically that the convergence is conditional[2]: there are terms whose magnitudes decrease like $1/(l_1 + l_2)$, e.g., like the harmonic series. This study discusses both analytics of the interpenetrating series and numerical consequences.

[1] Kay, K. G., Todd, H. D., and Silverstone, H. J. *J. Chem. Phys.*, 51(6):2363–2367, 1969.

[2] Silverstone, H. J., "On the convergence of the interpenetrating bipolar expansion for the Coulomb potential" *Advances in Quantum Chemistry: Molecular Electronic Structure Theory* 67 (in press, 2013).