Resolutions of the Coulomb Operator. III. Reduced-Rank Schrödinger Equations Supplementary Information

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Higher integrals in the R=0 case

In cases where $R = 0$, the Gaussian product is concentric with $\phi_k(\boldsymbol{r})$ and the resulting unnormalized auxiliary integrals are

$$(\mu\nu|\phi_{nlm}) = \int x^a y^b z^c \exp(-\gamma^2 r^2)\phi_{nlm}(\boldsymbol{r})\, d\boldsymbol{r} \tag{1}$$

As in (4.31), Parseval's Theorem allows this to be recast as

$$(\mu\nu|\phi_{nlm}) = 4(\pi/\gamma^2)^{3/2} y_{lm}(a,b,c)\hat{F}_{nl}^{a+b+c}(\gamma) \tag{2}$$

where

$$y_{lm}(a,b,c) = \int_0^\pi \int_0^{2\pi} \sin^{1+a+b}\theta\ \cos^c\theta\ \cos^a\varphi\ \sin^b\varphi\ Y_{lm}(\theta,\varphi)\, d\varphi\, d\theta \tag{3}$$

is the angular part and $\hat{F}_{nl}^{l'}(\gamma)$, the binomial transform of $F_{kl}^{l'}(\gamma)$, is the radial part of the integration.

As shown in Table 1, the $F_{kl}^{l'}(\gamma)$ are linear combinations of

$$f_k^i(\gamma) \equiv \frac{(4\gamma)^{k+1}}{8\pi}\left(-\frac{1}{2\gamma}\right)^i \frac{\partial^i H_{-(k+1)}(\gamma)}{\partial\gamma^i} = \frac{(4\gamma)^{k+1}}{8\pi}\left(\frac{1}{\gamma}\right)^i (k+1)_i H_{-(k+i+1)}(\gamma) \tag{4}$$

where $l \le i \le l' = a+b+c$ and $(k+1)_i = (k+1)(k+2)...(k+i)$.

Because of the high symmetry of the system, most of the integrals (1) vanish. The exceptions are those in which the Gaussian product and the RO potential span the same irreducible representations of the spherical group. As a result, as mentioned in the main text, $\mathcal{L}$ is saturated at $2L$, leaving only $\mathcal{N}$ to be improved.

Table 1: F_{kl}^{L} as linear combinations of f_k^i

L	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$
0 (ss)	f_k^0				
1 (sp)		f_k^1			
2 (pp, sd)	$\frac{3}{2\gamma^2} f_k^0 - f_k^2$		f_k^2		
3 (pd)		$\frac{5}{2\gamma^2} f_k^1 - f_k^3$		f_k^3	
4 (dd)	$\frac{15}{(2\gamma^2)^2} f_k^0 - \frac{10}{2\gamma^2} f_k^2 + f_k^4$		$\frac{7}{2\gamma^2} f_k^2 - f_k^4$		f_k^4