Erratum: Rates of convergence of the partial-wave expansion beyond the Kato cusp condition [Phys. Rev. A 88, 032511 (2013)]

Cong Wang

(Received 20 April 2015; published 22 June 2015)

DOI: 10.1103/PhysRevA.91.069904 PACS number(s): 31.15.ve, 31.15.xp, 31.15.xt, 99.10.Cd

(1) Under Eq. (5), "The first- and second-order energies" should be "The zeroth- and first-order energies".
(2) In Eq. (11), the upper limit of the summation should be "$N-n+2$", instead of "$N-n+1$".
(3) In Eq. (35), $(-1)^{\nu}$ should be $(-1)^{\frac{\nu+3}{2}}$.
(4) Under Eq. (36), $(-1)^{\nu}R_{\nu l}\geqslant 0$ should be $(-1)^{\frac{\nu+1}{2}}R_{\nu l}\geqslant 0$.
(5) In Eqs. (41) and (42), $O((l+1/2)^{-4})$ and $O((l+1/2)^{-2})$ contain polynomials of k, which cannot be taken outside the summation of k. The correct expressions for the right-hand sides of Eqs. (41) and (42) are

$$2(l+1/2)^{-1}\left[C'(l+a)^{-3}\sum_{k=0}^{(\nu+1)/2}C_{\nu lk}+O((l+1/2)^{-4})\sum_{k=0}^{(\nu+1)/2}kC_{\nu lk}+\cdots\right]\int_0^{\infty}r_>^{\nu+7}f(r_>,r_>)dr_>$$

and

$$2(l+1/2)^{-1}\left[(l+a)^{-1}\sum_{k=0}^{(\nu+1)/2}C_{\nu lk}+O((l+1/2)^{-2})\sum_{k=0}^{(\nu+1)/2}kC_{\nu lk}+\cdots\right]\int_0^{\infty}r_>^{\nu+5}f(r_>,r_>)dr_>,$$

respectively. Analyzing the l dependence for $\sum_k kC_{\nu lk},\sum_k k^2C_{\nu lk},\ldots$ is necessary.

The coefficient in the Sack expansion [1]

$$C_{\nu lk}=\frac{(-\nu/2)_l}{(1/2)_l}\frac{(l-\nu/2)_k(-1/2-\nu/2)_k}{(l+3/2)_k\qquad k!}$$

implies that the terms $\sum_k C_{\nu lk}$, $(l+1/2)^{-1}\sum_k kC_{\nu lk},\ldots$, and $(l+1/2)^{-1/2-\nu/2}\sum_k k^{1/2+\nu/2}C_{\nu lk}$ have the same order of inverse power of l, i.e., $(l+1/2)^{-1/2-\nu/2}$. This can be seen from

$$\frac{(l-\nu/2)_k}{(l+3/2)_k}=1+\frac{d_{10}+d_{11}k}{l+1/2}+\frac{d_{20}+d_{21}k+d_{22}k^2}{(l+1/2)^2}+\cdots,$$

$$\sum_{k=0}^{(\nu+1)/2}k^n\frac{(-1/2-\nu/2)_k}{k!}=(-1)^{1/2+\nu/2}(1/2+\nu/2)!S(n,1/2+\nu/2),$$

$$S(n,1/2+\nu/2)=\begin{cases}0, & n<1/2+\nu/2,\\ >0, & n\geqslant 1/2+\nu/2,\end{cases}$$

where d_{ij} is the expansion coefficient and $S(n,1/2+\nu/2)$ is the Stirling number of the second kind [2]. There is no incidental cancellation in summations of $\sum_k C_{\nu lk},\ldots,(l+1/2)^{-1/2-\nu/2}\sum_k k^{1/2+\nu/2}C_{\nu lk}$. Hence we conclude $R_{\nu+2l}R_{\nu' l}$ has $(l+a)^{-2}$ acceleration than $R_{\nu l}R_{\nu' l}$.

(6) Under Eq. (54), $O((l+a)^{-3})$ and $O((l+a)^{-1})$ should be $O((l+a)^{-4})$ and $O((l+a)^{-2})$, respectively.
(7) Above Eq. (55), "$n=0,1,2,\ldots,N+2$" should be "$n=0,1,2,\ldots,N+3$".
(8) Equations (55) and (56) should be

$$\int_{|r_1-r_2|}^{r_1+r_2}\left|\frac{\partial^{N+4}\psi}{\partial r_{12}^{N+4}}\right|^2dr_{12}<\infty,\qquad \int_0^{\infty}r_1^2dr_1\int_0^{\infty}r_2^2dr_2r_>^{2N+7}\int_{|r_1-r_2|}^{r_1+r_2}\left|\frac{\partial^{N+4}\psi}{\partial r_{12}^{N+4}}\right|^2dr_{12}<\infty.$$

(9) In the first line of Eq. (57), "$i+j=N+2$" should be "$i+j=N+3$".
(10) Equation (63) was derived according to Kutzelnigg and Morgan's [3] claim, $\psi\to\frac{1}{2}r_{12}\Phi+O(r_{12}^3)$, $l\to\infty$. As suggested by the formal solution [4–6], the correct expression is $\psi\to\frac{1}{2}[1-\frac{1}{3}s\eta^2+O(\eta^4)]r_{12}\Phi+O(r_{12}^3)$, $l\to\infty$. Hence Eq. (63) and the following paragraph are invalid.
(11) The fourth paragraph below Eq. (64), "$\langle\chi|r_{12}^m(\hat{H}_0-E_0)|\Phi_m\rangle$ will be canceled by $\Phi_1=\Phi/2$ or is suppressed to $O(L^{-N-7})$, for $m=1$" should be "$\langle\chi|r_{12}^m(\hat{H}_0-E_0)|\Phi_m\rangle$ will be suppressed to $O(L^{-2N-6})$, for $m=1$".
(12) In the second line of Eq. (B42), the integral measure $r_<^2r_>^2dr_<dr_>$ was missing in the second square bracket.
(13) In Eq. (B53), it was attempted to obtain $\psi\to\frac{1}{2}r_{12}\Phi+O(r_{12}^3)$ from taking derivative of $r_<$ and performing integration by part. The derivation is valid at $O(r_<-r_>)^n$, $n=1$. It is not valid for $n>1$. Consider Eq. (B53) in the line of

Eqs. (A4)–(A7) in Ref. [3]. For $n = 1$

$$\begin{aligned}
&\int_0^\infty \int_0^{r_>} R_{-1l} R_{-1l} \frac{\partial}{\partial r_<}\left[\frac{\partial \psi(r_<,r_>,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_>,r_{12})}{\partial r_{12}}\right]_{\substack{r_<=r_>,\\ r_{12}=0}} r_<^2 r_>^2 dr_< dr_> \\
&= \frac{1}{2}\int_0^\infty \int_{r_<}^\infty R_{-1l} R_{-1l} \frac{\partial}{\partial r_<}\left[\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\right]_{r_{12}=0} r_<^2 r_>^2 dr_< dr_> \\
&= \frac{1}{2(2l-1)}\int_0^\infty \frac{\partial}{\partial r_<}\left[\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\right]_{r_{12}=0} r_<^3 dr_< \\
&= -\frac{3}{2(2l-1)}\int_0^\infty \left[\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\right]_{r_{12}=0} r_<^2 dr_< \\
&= -\frac{3}{8(2l-1)}\int_0^\infty \Phi(r_<,r_<)\Phi(r_<,r_<) r_<^2 dr_< \\
&= \frac{1}{8}\int_0^\infty \int_{r_>}^\infty R_{-1l} R_{-1l} \frac{\partial}{\partial r_<}[\Phi(r_<,r_<)\Phi(r_<,r_<)] r_<^2 r_>^2 dr_< dr_>.
\end{aligned}$$

Hence we can replace $\partial\psi/\partial r_{12}$ as Φ inside the derivative of $r_<$. However, for $n = 2$

$$\begin{aligned}
&\int_0^\infty \int_0^{r_>} R_{-1l} R_{-1l} \frac{\partial^2}{\partial r_<^2}\left[\frac{\partial \psi(r_<,r_>,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_>,r_{12})}{\partial r_{12}}\right]_{\substack{r_<=r_>,\\ r_{12}=0}} r_<^2 r_>^2 dr_< dr_> \\
&= \frac{1}{2}\int_0^\infty \int_0^{r_>} R_{-1l} R_{-1l} \left(\frac{\partial^2}{\partial r_<^2} - \frac{\partial^2}{\partial r_< \partial r_>}\right)\left[\frac{\partial \psi(r_<,r_>,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_>,r_{12})}{\partial r_{12}}\right]_{\substack{r_<=r_>,\\ r_{12}=0}} r_<^2 r_>^2 dr_< dr_> \\
&\quad + \frac{1}{4}\int_0^\infty \int_0^{r_>} R_{-1l} R_{-1l} \frac{\partial^2}{\partial r_<^2}\left[\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\frac{\partial \psi(r_<,r_<,r_{12})}{\partial r_{12}}\right]_{r_{12}=0} r_<^2 r_>^2 dr_< dr_>.
\end{aligned}$$

In general, the second line here is not zero. The correct linear r_{12} expression is the formal solution [4–6].

(14) In the last line of Eq. (C2), the argument of the hypergeometric function "$(n_2 + n_3 + n_4 + 2, n_3 + 1; n_2 + n_3 + n_4; -1)$" should be "$(n_2 + n_3 + n_4 + 2, n_3 + 1; n_2 + n_3 + 2; -1)$".

(15) In the Supplemental Material, Table I, one extra "1" was put after the point zero in all data with $L = 100, 1000, 10000$. For instance, "−1.17228781775312986866" should be "−1.7228781775312986866".

[1] R. A. Sack, J. Math. Phys. **5**, 245 (1964).
[2] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York, 1972).
[3] W. Kutzelnigg and J. D. Morgan III, J. Chem. Phys. **96**, 4484 (1992).
[4] R. J. White and W. B. Brown, Int. J. Quantum Chem. **1**, 61 (1967).
[5] W. B. Brown and R. J. White, Phys. Rev. Lett. **18**, 1037 (1967).
[6] W. B. Brown and R. J. White, Phys. Rev. Lett. **18**, 1178 (1967).