Supplementary material for: Nonadiabatic corrections to electric quadrupole transition rates in H_2

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ARTICLE HISTORY
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1. Electric quadrupole transition rate

We derive here the formula for the spontaneous electric quadrupole transition, starting from first principles. The Fermi's golden rule for the transition rate is

$$\frac{1}{\tau} = \frac{2\,\pi}{\hbar^2} \int d\nu_f \,\big|\langle f|H_I|u\rangle\big|^2\, \delta(\omega_f - \omega_u), \tag{1}$$

where the integral is over all final states f, which have the same energy as the initial state u.

In the long-wavelength approximation, the interaction Hamiltonian is

$$H_I = -\frac{1}{2}\, D^{ij}\, \nabla^j E^i(0)\,, \tag{2}$$

where D^{ij} is the quadrupole moment operator, and $E^i_{,j}$ is the derivative of the electric field. The quantum electromagnetic field is

$$\vec{A}(\vec{r}) = \int \frac{d^3k}{\sqrt{(2\,\pi)^3}} \sqrt{\frac{\hbar}{2\,\epsilon_0\,\omega}}\, \vec{\epsilon}_{k,\lambda} \left(a_{k,\lambda}\, e^{i\,\vec{k}\,\vec{r}} + a^+_{k,\lambda}\, e^{-i\,\vec{k}\,\vec{r}}\right), \tag{3}$$

$$\vec{E}(\vec{r}) = \int \frac{d^3k}{\sqrt{(2\,\pi)^3}}\, i \sqrt{\frac{\hbar\,\omega}{2\,\epsilon_0}}\, \vec{\epsilon}_{k,\lambda} \left(a_{k,\lambda}\, e^{i\,\vec{k}\,\vec{r}} - a^+_{k,\lambda}\, e^{-i\,\vec{k}\,\vec{r}}\right), \tag{4}$$

where

$$[a_{k,\lambda}\,,\, a^+_{k',\lambda'}] = \delta_{\lambda,\lambda'}\, \delta^3(\vec{k} - \vec{k}')\,. \tag{5}$$

Thus, the transition rate $A_{\rm E2} = 1/\tau$ with $\omega = k\,c$ is

$$A_{\rm E2} = \frac{2\,\pi}{\hbar^2} \int d^3k \sum_\lambda \left\langle \vec{k},\lambda; f\middle|\frac{1}{2}\, D^{ij}\, \nabla^j E^i(0)\middle|u;0\right\rangle^2 \delta(\omega - \omega_0)$$

$$
\begin{aligned}
&= \frac{2\,\pi}{4\,\hbar^2}\,\frac{\hbar\,\omega_0}{2\,\epsilon_0}\int \frac{d^3k}{(2\,\pi)^3}\sum_\lambda \left|\langle f|D^{ij}|u\rangle\,\epsilon^i_{k,\lambda}\,k^j\right|^2\delta(\omega-\omega_0)\\
&= \frac{2\,\pi}{4\,\hbar^2}\,\frac{\hbar\,\omega_0}{2\,\epsilon_0}\int \frac{d^3k}{(2\,\pi)^3}\,\langle u|D^{mn}|f\rangle\,\langle f|D^{ij}|u\rangle\sum_\lambda \epsilon^i_{k,\lambda}\,\epsilon^m_{k,\lambda}\,k^j\,k^n\,\delta(\omega-\omega_0)\\
&= \frac{\pi\,k_0}{4\,\hbar\,\epsilon_0}\int \frac{d^3k}{(2\,\pi)^3}\,\langle u|D^{mn}|f\rangle\,\langle f|D^{ij}|u\rangle\left(\delta^{im}-\frac{k^i\,k^m}{k^2}\right)k^j\,k^n\,\delta(k-k_0)\\
&= \frac{k^5\,e^2}{8\,\pi\,\hbar\,\epsilon_0}\,\langle u|d^{mn}|f\rangle\,\langle f|d^{ij}|u\rangle\int\frac{d\Omega}{4\,\pi}\left(\delta^{im}-n^i\,n^m\right)n^j\,n^n\,,
\end{aligned}
\tag{6}
$$

where $k = k_0$ from now on, $\vec{n} = \vec{k}/k$, and $D^{ij} = e\,d^{ij}$. The angular integrations are

$$
\int \frac{d\Omega}{4\,\pi}\,n^j\,n^n = \frac{\delta^{jn}}{3}\,, \tag{7}
$$

$$
\int \frac{d\Omega}{4\,\pi}\,n^i\,n^j\,n^m\,n^n = \frac{1}{15}\left(\delta^{ij}\,\delta^{mn}+\delta^{im}\,\delta^{jn}+\delta^{in}\,\delta^{jm}\right). \tag{8}
$$

Using $\alpha = e^2/(4\,\pi\,\epsilon_0\,\hbar\,c)$ the transition rate is

$$
A_{\mathrm{E2}} = \alpha\,c\,k^5\,\langle u|d^{ij}|f\rangle\,\langle f|d^{ij}|u\rangle\,\frac{1}{10} \tag{9}
$$

For a diatomic molecule the electric quadrupole operator can be written as

$$
d^{ij} = \left(n^i\,n^j - \frac{\delta^{ij}}{3}\right)D(R) \tag{10}
$$

thus

$$
A_{\mathrm{E2}} = \alpha\,c\,k^5\,\frac{1}{10}\,\langle\chi''|D(R)|\chi'\rangle^2\,\langle u|n^i\,n^j-\delta^{ij}/3|f\rangle\,\langle f|n^i\,n^j-\delta^{ij}/3|u\rangle \tag{11}
$$

where χ', χ'' are initial and final radial functions, respectively.

Angular momentum algebra

To calculate the rate for a specific angular momentum J', J'' of the initial and final state, respectively, we make use of the angular momentum algebra,

$$
(n^i_1\,n^j_1-\delta^{ij}/3)\,(n^i_2\,n^j_2-\delta^{ij}/3) = \frac{2}{3}\sum_m C^*_{2m}(\theta_1,\phi_1)\,C_{2m}(\theta_2,\phi_2) \tag{12}
$$

where

$$
C_{lm} = \sqrt{\frac{4\,\pi}{2\,l+1}}\,Y_{lm}(\theta,\phi). \tag{13}
$$

After averaging over initial M' and summing over final M'' the rate is

$$A_{\rm E2} = \frac{1}{15}\,\alpha\,c\,k^5\,\langle v''J''|D(R)|v'J'\rangle^2\,X(J'') \tag{14}$$

where

$$\begin{aligned} X(J'') &= \frac{1}{2\,J'+1}\sum_{M'}\sum_{M''}\sum_{q}|\langle J''M''|C_{2q}|J'M'\rangle|^2 \\ &= (2\,J''+1)\begin{pmatrix} J' & J'' & 2 \\ 0 & 0 & 0 \end{pmatrix}^2 \\ &= \begin{cases} \frac{3\,(J'+1)\,(J'+2)}{2\,(2\,J'+1)\,(2\,J'+3)} & \text{for } J''=J'+2\,, \\ \frac{J'\,(J'+1)}{(2\,J'-1)\,(2\,J'+3)} & \text{for } J''=J'\,, \\ \frac{3\,J'\,(J'-1)}{2\,(2\,J'-1)\,(2\,J'+1)} & \text{for } J''=J'-2\,, \end{cases} \end{aligned} \tag{15}$$

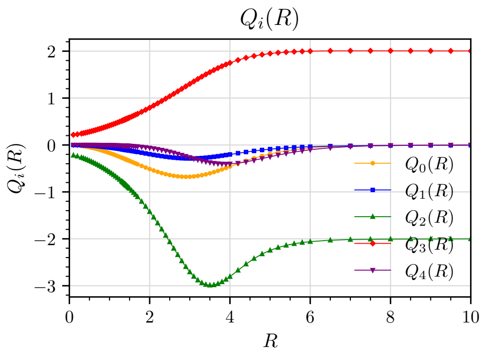
and where the sum over all possible J'' is equal to 1,

$$X(J'+2)+X(J')+X(J'-2)=1\,. \tag{16}$$

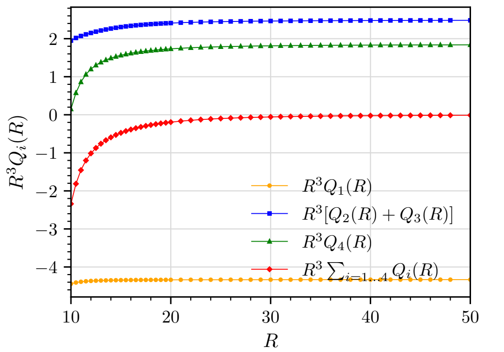
Finally, the transition rate is

$$A_{\rm E2} = (4\,\pi R_\infty c)\,\frac{1}{15}\,\alpha^5\,\Delta E_{\rm au}^5\,X\,\langle v''J''|D(R)|v'J'\rangle_{\rm au}^2\,. \tag{17}$$

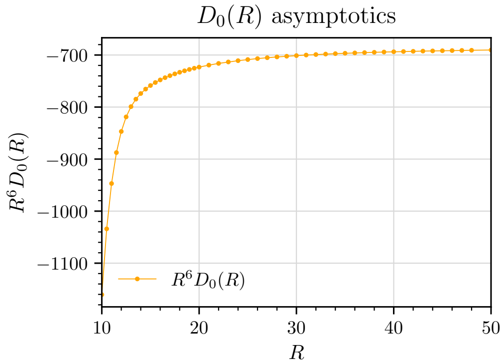
2. Detailed numerical results



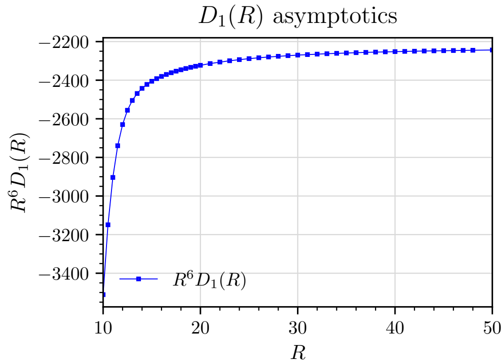
(a) $Q_0(R) = \frac{2}{3} D_0(R)$ and $Q_i(R)$ — components of $D_1(R)$. The constant values of $Q_2(R)$ and $Q_3(R)$ cancel at $R \to 0$ and $R \to \infty$.



(b) $Q_i(R)$ of $D_1(R)$ with $\sim R^{-3}$ tails: $R^3 Q_1(R) \to -4.33(2)$, $R^3(Q_2{+}Q_3) \to 2.50(2)$, $R^3 Q_4(R) \to 1.84(1)$; sum cancels (red).



(c) $R^6 D_0(R)$



(d) $R^6 D_1(R)$

Figure 1. R-behavior of $D_0(R)$, $D_1(R)$ and their components $Q_i(R)$.

Table 1. $Q_0(R) = \sum_a \langle (\vec{r}_a \cdot \vec{n})^2 - r_a^2/3 \rangle - R^2/3$, $Q_1(R) = -\frac{1}{2}\langle \phi_{\rm el}|(\vec{r}_{\rm el} \cdot \vec{n})^2 - \vec{r}_{\rm el}^{\,2}/3|\phi_{\rm el}\rangle$, $Q_2(R) = \langle \nabla_R^k \phi_{\Sigma^+}|\nabla_R^k \phi_{\rm el}\rangle$, $Q_3(R) = -2\,i/R^3\,\langle \vec{\phi}_\Pi|\vec{R} \times \vec{J}_{\rm el}|\phi_{\rm el}\rangle$, $Q_4(R) = \frac{1}{4}\langle \phi_{\Sigma^+}|(\sum_a \vec{p}_a)^2|\phi_{\rm el}\rangle$. Using single-sector JC ($y = x = 0, \alpha = u = w$, $R \le 10$ au, $\Omega = 15, 16$) and HL ($\alpha = -y = x = u = w = 1/2$, $R > 10$ au, $\Omega = 13, 14$) bases. $R_e = 1.4011$ au. Nonlinear parameter α is dimensionless, all other quantities in atomic units.

R	α	$Q^{(0)}(R)$	$Q_1(R)$	$Q_2(R)$	$Q_3(R)$	$Q_4(R)$
0.1	1.7000	−0.001967623(3)	−0.0005376311(5)	−0.220551(4)	0.216839(4)	0.0000360985(3)
0.2	1.6790	−0.007806294(10)	−0.002155510(5)	−0.240088(5)	0.227949(4)	0.00012155(4)
0.3	1.5374	−0.017367873(7)	−0.004864231(4)	−0.266631(2)	0.2432698(10)	0.00021047(2)
0.35	1.4533	−0.023487532(5)	−0.006631002(3)	−0.2819158(5)	0.2521172(4)	0.00024042(2)
0.4	1.3693	−0.030466375(3)	−0.008674122(2)	−0.2983707(2)	0.2616287(2)	0.000252051(7)
0.45	1.3180	−0.038278074(2)	−0.0109942791(10)	−0.3159175(2)	0.27173878(10)	0.000238711(6)
0.5	1.2667	−0.046895448(2)	−0.0135917943(8)	−0.33450472(6)	0.28239819(6)	0.000193605(4)
0.55	1.2425	−0.056290539(2)	−0.0164665738(7)	−0.35409949(4)	0.29356917(4)	0.000109751(4)
0.6	1.2183	−0.066434653(2)	−0.0196180660(6)	−0.37468238(3)	0.30522263(4)	−0.000020058(4)
0.65	1.1983	−0.077298381(2)	−0.0230452214(6)	−0.39624409(3)	0.31733598(3)	−0.000203278(3)
0.7	1.1783	−0.0888515970(10)	−0.0267464531(5)	−0.41878308(2)	0.32989159(2)	−0.000447650(3)
0.75	1.1493	−0.1010634581(8)	−0.0307195984(4)	−0.442303967(10)	0.34287563(2)	−0.000761224(3)
0.8	1.1203	−0.1139023861(7)	−0.0349618804(4)	−0.466816325(7)	0.356277283(10)	−0.001152387(2)
0.85	1.0990	−0.1273360510(6)	−0.0394698694(3)	−0.492333893(5)	0.370088043(8)	−0.001629889(2)
0.9	1.0776	−0.1413313498(5)	−0.0442394434(3)	−0.518873964(3)	0.384301276(6)	−0.002202863(2)
0.95	1.0607	−0.1558543824(5)	−0.0492657486(3)	−0.546456940(3)	0.398911828(5)	−0.002880850(2)
1.0	1.0437	−0.1708704260(4)	−0.0545431590(2)	−0.575106006(2)	0.413915732(4)	−0.003673822(2)
1.05	1.0306	−0.1863439101(4)	−0.0600652357(2)	−0.604846864(2)	0.429309976(4)	−0.0045921954(10)
1.1	1.0174	−0.2022383896(4)	−0.0658246859(2)	−0.6357075258(10)	0.445092310(3)	−0.0056468550(10)
1.15	1.0070	−0.2185165194(3)	−0.0718133217(2)	−0.6677181289(8)	0.461261094(3)	−0.0068491656(9)
1.2	0.9965	−0.2351400295(3)	−0.0780220196(2)	−0.7009107623(7)	0.477815161(3)	−0.0082109858(9)
1.25	0.9876	−0.2520697014(3)	−0.0844406802(2)	−0.7353192882(6)	0.494753714(2)	−0.0097446770(8)
1.3	0.9794	−0.2692653469(3)	−0.0910581891(2)	−0.7709791448(5)	0.512076222(2)	−0.0114631084(8)
1.32	0.9763	−0.2762088877(3)	−0.0937581810(2)	−0.7856016609(5)	0.519112651(2)	−0.0122051876(8)
1.34	0.9734	−0.2831857271(3)	−0.0964872273(2)	−0.8004326702(5)	0.526210438(2)	−0.0129798385(8)
1.36	0.9705	−0.2901931592(3)	−0.0992444727(2)	−0.8154746040(5)	0.533369570(2)	−0.0137879525(8)
1.38	0.9677	−0.2972284520(3)	−0.1020290335(2)	−0.8307299145(5)	0.540590032(2)	−0.0146304337(8)
1.39	0.9663	−0.3007556854(3)	−0.1034312733(2)	−0.8384383573(5)	0.544223257(2)	−0.0150648478(7)
1.4	0.9650	−0.3042888477(3)	−0.1048399974(2)	−0.8462010715(5)	0.547871810(2)	−0.0155081982(7)
R_e	0.9650	−0.3046778425(3)	−0.1049953479(2)	−0.8470582967(5)	0.548274087(2)	−0.0155575173(7)
1.41	0.9637	−0.3078275901(3)	−0.1062550874(2)	−0.8540183680(5)	0.551535689(2)	−0.0159606015(7)
1.42	0.9621	−0.3113715621(3)	−0.1076764227(2)	−0.8618905581(5)	0.555214892(2)	−0.0164221748(7)
1.44	0.9596	−0.3184737851(3)	−0.1105373382(2)	−0.8778008665(5)	0.562619260(2)	−0.0173733036(7)
1.46	0.9570	−0.3255926803(3)	−0.1134217434(2)	−0.8939344933(5)	0.570084899(2)	−0.0183625367(7)
1.48	0.9546	−0.3327253851(3)	−0.1163286074(2)	−0.9102939343(5)	0.577611787(2)	−0.0193908373(7)
1.5	0.9524	−0.3398690110(3)	−0.1192568694(2)	−0.9268816792(5)	0.585199904(2)	−0.0204591794(7)
1.55	0.9466	−0.3577566634(3)	−0.1266639052(2)	−0.9693660835(5)	0.604437872(2)	−0.0233116993(7)
1.6	0.9409	−0.3756480357(3)	−0.1341798887(2)	−1.0133308866(5)	0.6240577539(10)	−0.0264362929(7)
1.65	0.9360	−0.3934958832(3)	−0.1417857295(2)	−1.0588127107(6)	0.6440587139(10)	−0.0298489155(7)
1.7	0.9311	−0.4112519924(3)	−0.1494611292(2)	−1.1058458972(6)	0.6644395791(9)	−0.0335657637(7)
1.8	0.9218	−0.4462915383(3)	−0.1649334114(2)	−1.2046862413(7)	0.7063341658(8)	−0.0419775182(7)
1.9	0.9132	−0.4803633838(3)	−0.1804106351(2)	−1.3100394357(8)	0.7497222606(8)	−0.0518016635(7)
2.0	0.9051	−0.5130527287(3)	−0.1956888631(2)	−1.4219756330(9)	0.7945736713(8)	−0.0631634192(7)
2.1	0.8975	−0.5439369085(3)	−0.2105483388(2)	−1.5403903886(10)	0.8408440359(7)	−0.0761762036(7)
2.2	0.8900	−0.5725904941(3)	−0.2247566212(2)	−1.664936137(2)	0.8884712721(7)	−0.0909326440(7)
2.3	0.8829	−0.5985920667(3)	−0.2380729945(2)	−1.794945313(2)	0.9373717771(7)	−0.1074934351(7)
2.4	0.8759	−0.6215328267(3)	−0.2502542553(3)	−1.929351346(2)	0.9874365285(7)	−0.1258742207(7)
2.5	0.8690	−0.6410270804(3)	−0.2610618882(3)	−2.066617833(2)	1.0385273249(7)	−0.1460310558(7)
2.6	0.8623	−0.6567244739(3)	−0.2702705065(3)	−2.204690419(2)	1.0904735053(7)	−0.1678454914(8)
2.7	0.8556	−0.6683236018(2)	−0.2776772612(3)	−2.340989142(2)	1.1430695770(7)	−0.1911108794(8)
2.8	0.8489	−0.6755863355(2)	−0.2831117245(3)	−2.472459657(2)	1.1960742477(7)	−0.2155220170(8)
2.9	0.8422	−0.6783519068(2)	−0.2864455524(3)	−2.5956980023(10)	1.2492113733(6)	−0.2406705948(8)
3.0	0.8355	−0.6765495164(2)	−0.2876010713(3)	−2.7071541490(9)	1.3021732696(6)	−0.2660488961(8)
3.1	0.8286	−0.6702080653(2)	−0.2865578558(3)	−2.8034046861(8)	1.3546266779(6)	−0.2910636624(8)
3.2	0.8219	−0.65946161642(9)	−0.2833564101(3)	−2.8814670114(7)	1.4062214161(5)	−0.3150609046(8)
3.3	0.8147	−0.64454942242(6)	−0.2780982705(3)	−2.9391109916(6)	1.4566014158(5)	−0.3373607886(8)
3.4	0.8077	−0.62580982628(4)	−0.2709421893(3)	−2.9751151531(5)	1.5054174782(4)	−0.3572998315(8)
3.5	0.8004	−0.603668002410(4)	−0.2620965179(3)	−2.9894178898(5)	1.5523407705(4)	−0.3742759427(7)
3.6	0.7931	−0.57861825589(3)	−0.2518083808(3)	−2.9831312404(5)	1.5970758745(3)	−0.3877908204(7)
3.7	0.7852	−0.55120229333(5)	−0.2403506469(3)	−2.9584118697(4)	1.6393721811(2)	−0.3974842207(7)
3.8	0.7773	−0.52198537799(8)	−0.2280079590(3)	−2.9182132369(4)	1.6790325828(2)	−0.4031557483(6)
3.9	0.7692	−0.49153248297(10)	−0.2150631351(3)	−2.8659656712(4)	1.71591875660(10)	−0.4047718258(6)
4.0	0.7605	−0.4603864290(2)	−0.2017851030(3)	−2.8052408030(4)	1.74995275707(6)	−0.4024578843(5)
4.2	0.7432	−0.3979701336(2)	−0.1751804343(3)	−2.6716274308(4)	1.80943975219(2)	−0.3872058067(4)
4.4	0.7248	−0.3380570232(2)	−0.1497710691(3)	−2.5393026299(3)	1.85793560053(6)	−0.3606247965(3)

Table 1. (continued)

R	α	$Q^{(0)}(R)$	$Q_1(R)$	$Q_2(R)$	$Q_3(R)$	$Q_4(R)$
4.6	0.7057	−0.2829269230(2)	−0.1265823608(3)	−2.4214706388(2)	1.89648455854(8)	−0.3266378000(2)
4.8	0.6856	−0.2338578990(2)	−0.1061354647(3)	−2.32349318854(8)	1.92645889578(8)	−0.28899038987(9)
5.0	0.6653	−0.1913148077(2)	−0.0885653233(3)	−2.245559261384(7)	1.94932299928(8)	−0.25073025029(2)
5.2	0.6448	−0.1551866745(2)	−0.0737522640(3)	−2.18527476597(7)	1.96646989915(8)	−0.21403202507(4)
5.4	0.6243	−0.1250063798(2)	−0.0614342982(3)	−2.13941814898(10)	1.97913038768(7)	−0.18025194143(7)
5.6	0.6043	−0.1001228809(2)	−0.0512887177(3)	−2.1048668952(2)	1.98833796473(7)	−0.15008976851(8)
5.8	0.5857	−0.0798212915(2)	−0.0429844040(3)	−2.0789662755(2)	1.99492945218(6)	−0.12377317371(8)
6.0	0.5705	−0.0633984915(2)	−0.0362114176(2)	−2.0596014782(2)	1.99956458739(5)	−0.10122062579(7)
6.5	0.5631	−0.03523729936(10)	−0.0242732607(2)	−2.03004328882(4)	2.00564580210(3)	−0.05935734181(2)
7.0	0.5483	−0.01942265132(6)	−0.01705305479(8)	−2.01586181279(5)	2.007485677919(9)	−0.03350365051(5)
7.5	0.5350	−0.01071667411(4)	−0.01256361842(5)	−2.0090507868(2)	2.007540776661(2)	−0.0182205766(2)
8.0	0.5305	−0.00597573699(2)	−0.00965698897(3)	−2.0057272937(4)	2.006928682731(5)	−0.0094765925(4)
8.5	0.5300	−0.00340106800(2)	−0.00768496278(2)	−2.0040303179(5)	2.00613328030(2)	−0.0046073056(5)
9.0	0.5301	−0.001994989991(7)	−0.00628254793(2)	−2.0030872750(5)	2.00534978279(2)	−0.0019625620(5)
9.5	0.5302	−0.001215839150(7)	−0.00524184984(2)	−2.00249969182(5)	2.00464663129(4)	−0.000563725073(7)
10.0	0.5000	−0.00077365858(5)	−0.00444163471(8)	−2.00208963536(3)	2.00403922544(3)	0.0001513657(2)
10.5	0.5000	−0.00051441175(4)	−0.00380877235(6)	−2.00177815561(3)	2.00352255074(3)	0.00049776051(9)
11.0	0.5000	−0.00035634526(3)	−0.00329728647(4)	−2.00152920409(2)	2.00308510428(2)	0.00064862608(7)
11.5	0.5000	−0.00025579173(2)	−0.00287694618(3)	−2.00132485423(2)	2.002714510001(10)	0.00069770221(6)
12.0	0.5000	−0.000189088440(10)	−0.00252698135(3)	−2.00115483236(2)	2.002399545393(6)	0.00069513284(5)
12.5	0.5000	−0.000143117560(7)	−0.00223254784(2)	−2.00101227838(2)	2.002130682239(4)	0.00066748804(4)
13.0	0.5000	−0.000110381026(5)	−0.001982679342(10)	−2.000892078027(9)	2.001900055967(2)	0.00062872648(4)
13.5	0.5000	−0.000086432849(4)	−0.001769055669(7)	−2.000790197595(6)	2.001701248360(2)	0.00058610604(3)
14.0	0.5000	−0.000068529520(3)	−0.001585230565(5)	−2.000703387411(4)	2.0015290371430(6)	0.00054333660(2)
14.5	0.5000	−0.000054909459(2)	−0.001426126617(3)	−2.000629015635(3)	2.0013791675873(4)	0.00050225099(2)
15.0	0.5000	−0.000044399263(2)	−0.001287691560(2)	−2.000564950406(2)	2.0012481611432(2)	0.000463688948(9)
15.5	0.5000	−0.0000361919193(7)	−0.001166656207(2)	−2.000509465075(3)	2.00113316088668(8)	0.000427965548(7)
16.0	0.5000	−0.0000297173746(5)	−0.0010603589906(8)	−2.000461159531(3)	2.00103180867949(4)	0.000395120977(6)
16.5	0.5000	−0.0000245640726(3)	−0.0009666158482(5)	−2.000418895326(3)	2.00094214809297(2)	0.000365054722(5)
17.0	0.5000	−0.0000204295575(2)	−0.0008836219422(3)	−2.000381743044(3)	2.00086254772184(2)	0.000337598322(5)
17.5	0.5000	−0.00001708828194(9)	−0.0008098763214(2)	−2.000348940188(3)	2.000791640456261(7)	0.000312555051(4)
18.0	0.5000	−0.00001436997851(6)	−0.00074412347436(9)	−2.000319857803(3)	2.000728275201897(5)	0.000289721550(4)
18.5	0.5000	−0.00001214475239(3)	−0.00068530752270(6)	−2.000293974157(3)	2.000671478316788(4)	0.000268899451(3)
19.0	0.5000	−0.00001031258881(2)	−0.00063253600713(4)	−2.000270854006(3)	2.000620422655556(4)	0.000249901359(3)
19.5	0.5000	−0.000008795838746(9)	−0.00058505103452(3)	−2.000250132247(3)	2.000574402593992(3)	0.000232553632(3)
20.0	0.5000	−0.000007533759936(5)	−0.00054220612930(2)	−2.000231500973(3)	2.000532813777115(3)	0.000216697329(3)
21.0	0.5000	−0.000005592128231(2)	−0.00046829906954(2)	−2.000199504583(3)	2.000460922778439(3)	0.000188895648(3)
22.0	0.5000	−0.0000042109449171(4)	−0.000407243200031(9)	−2.000173202770(2)	2.000401383256083(3)	0.000165503433(2)
23.0	0.5000	−0.0000032124361611(2)	−0.000356360699981(7)	−2.000151369465(2)	2.000351656721260(2)	0.000145718733(2)
24.0	0.5000	−0.00000247991979088(5)	−0.000313616847844(7)	−2.000133085500(2)	2.000309804899576(2)	0.000128896743(2)
25.0	0.5000	−0.00000193530946005(4)	−0.000277446662120(6)	−2.000117651754(2)	2.000274330737534(2)	0.000114519128(2)
26.0	0.5000	−0.00000152541821356(3)	−0.000246633009547(5)	−2.0001045295090(9)	2.000244065696308(2)	0.0001021683200(9)
27.0	0.5000	−0.00000121343066776(2)	−0.000220219590512(5)	−2.0000932987429(8)	2.000218088735741(2)	0.0000915067307(8)
28.0	0.5000	−0.00000097348439669(2)	−0.000197447954389(4)	−2.0000836284620(7)	2.000195667321900(2)	0.0000822602529(7)
29.0	0.5000	−0.00000078716245275(2)	−0.000177711323972(4)	−2.0000752552788(6)	2.000176213954392(2)	0.0000742052654(6)
30.0	0.5000	−0.00000064118396110(1)	−0.000160520342875(4)	−2.0000679677258(5)	2.000159253772464(1)	0.0000671584319(5)
31.0	0.5000	−0.00000052585948050(3)	−0.000145477389339(9)	−2.0000615946217(10)	2.000144400165470(3)	0.0000609686923(10)
32.0	0.5000	−0.00000043404274873(3)	−0.000132257118553(9)	−2.0000559963416(9)	2.000131336231673(3)	0.0000555109609(9)
33.0	0.5000	−0.00000036040962886(2)	−0.000120591583835(8)	−2.0000510581990(9)	2.000119800555210(3)	0.0000506811571(9)
34.0	0.5000	−0.00000030095585309(2)	−0.000110258758884(7)	−2.0000466853737(8)	2.000109576202840(2)	0.0000463922660(8)
35.0	0.5000	−0.00000025264304325(2)	−0.000101073610573(7)	−2.0000427989922(7)	2.000100482143740(2)	0.0000425712053(7)
36.0	0.5000	−0.00000021314647970(2)	−0.000092881101811(6)	−2.0000393330719(7)	2.000092366508615(2)	0.0000391563227(7)
37.0	0.5000	−0.000000180673511282(9)	−0.000085550667307(6)	−2.0000362321188(6)	2.000085101256434(2)	0.0000360953851(6)
38.0	0.5000	−0.000000153831550612(8)	−0.000078971822339(5)	−2.0000334492264(6)	2.000078577926771(2)	0.0000333439580(6)
39.0	0.5000	−0.000000131531235905(7)	−0.000073050649606(5)	−2.0000309445592(5)	2.000072704235456(2)	0.0000308640918(5)
40.0	0.5000	−0.000000112914777041(6)	−0.000067706971432(5)	−2.0000286841362(5)	2.000067401329878(2)	0.0000286232527(5)
41.0	0.5000	−0.00000009730250345(2)	−0.00006287206048(2)	−2.000026638849(2)	2.000062601563609(4)	0.000026593448(2)
42.0	0.5000	−0.00000008415268196(2)	−0.00005848677629(2)	−2.000024783661(2)	2.000058246682442(4)	0.000024750509(2)
43.0	0.5000	−0.00000007303108889(2)	−0.00005450004051(2)	−2.000023096962(1)	2.000054286338229(3)	0.0000230734976(10)
44.0	0.5000	−0.00000006358780838(2)	−0.00005086758319(2)	−2.000021560025(1)	2.000050676865407(3)	0.0000215442170(10)
45.0	0.5000	−0.00000005553942367(2)	−0.00004755090699(2)	−2.0000201565734(9)	2.000047380269118(3)	0.0000201468044(9)
46.0	0.5000	−0.00000004865526197(2)	−0.000044516427673(10)	−2.0000188724095(9)	2.000044363384642(3)	0.0000188673899(8)
47.0	0.5000	−0.000000042746706392(9)	−0.000041734757848(9)	−2.0000176951126(8)	2.000041597176218(3)	0.0000176938118(8)
48.0	0.5000	−0.000000037658843526(8)	−0.000039180107555(9)	−2.0000166137839(7)	2.000039056149774(3)	0.0000166153777(7)
50.0	0.5000	−0.000000029456062098(6)	−0.000034663750907(8)	−2.0000147017986(7)	2.000034562489611(2)	0.0000147073323(7)