Expansions

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1 Expansions

The potential and field of a charge distribution are:

$$\phi\left(\mathbf{r}\right) = \frac{kQ}{r}\ \mathrm{erf}\left\{\frac{r}{\sqrt{2}\sigma}\right\} \tag{1}$$

$$\mathbf{E}\left(\mathbf{r}\right) = kQ\left(\frac{\mathrm{erf}\left\{\frac{r}{\sqrt{2}\sigma}\right\}}{r^2} - \sqrt{\frac{2}{\pi}}\frac{\exp\left\{-\frac{r^2}{2\sigma^2}\right\}}{\sigma r}\right)\hat{\mathbf{r}} \tag{2}$$

Because r might become quite small if 2 particles are close, $\hat{\mathbf{r}}$ can cause problem. We thus replace it with $\hat{\mathbf{r}} = \mathbf{r}/\left|\mathbf{r}\right|$:

$$\mathbf{E}\left(\mathbf{r}\right) = kQ\left(\frac{\mathrm{erf}\left\{\frac{r}{\sqrt{2}\sigma}\right\}}{r^2} - \sqrt{\frac{2}{\pi}}\frac{\exp\left\{-\frac{r^2}{2\sigma^2}\right\}}{\sigma r}\right)\frac{\mathbf{r}}{r} \tag{3}$$

$$\mathbf{E}\left(\mathbf{r}\right) = kQ\left(\frac{\mathrm{erf}\left\{\frac{r}{\sqrt{2}\sigma}\right\}}{r^3} - \sqrt{\frac{2}{\pi}}\frac{\exp\left\{-\frac{r^2}{2\sigma^2}\right\}}{\sigma r^2}\right)\mathbf{r} \tag{4}$$

The value $\mathbf{r}$ is easy to calculate. For two particle p_0 and p_1, it is $\mathbf{r} = \mathbf{r}_0 - \mathbf{r}_1$.

Using $\hat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$ and $x = \frac{r}{\sqrt{2}\sigma}$, the previous equations are simplified to:

$$\begin{aligned}
\mathbf{E}(x) &= kQ\left(\frac{\operatorname{erf}\{x\}}{\left(\sqrt{2}\sigma x\right)^3} - \sqrt{\frac{2}{\pi}}\frac{\exp\{-x^2\}}{\sigma\left(\sqrt{2}\sigma x\right)^2}\right)\mathbf{r} \\
&= kQ\left(\frac{\operatorname{erf}\{x\}}{2^{3/2}\sigma^3 x^3} - \sqrt{\frac{2}{\pi}}\frac{\exp\{-x^2\}}{2\sigma^3 x^2}\right)\mathbf{r} \\
\mathbf{E}(x) &= \frac{kQ}{\sqrt{2}\sigma^3}\left(\frac{\operatorname{erf}\{x\}}{2x^3} - \frac{1}{\sqrt{\pi}}\frac{\exp\{-x^2\}}{x^2}\right)\mathbf{r} \\
\mathbf{E}(x) &= \frac{kQ}{\sqrt{2}\sigma^3}F(x)\,\mathbf{r} && (5) \\
\phi(x) &= \frac{kQ}{\sqrt{2}\sigma}\frac{\operatorname{erf}\{x\}}{x} && (6) \\
\phi(x) &= \frac{kQ}{\sqrt{2}\sigma}G(x) && (7)
\end{aligned}$$

where

$$\begin{aligned}
G(x) &= \frac{\operatorname{erf}\{x\}}{x} && (8) \\
F(x) &= \frac{\operatorname{erf}\{x\}}{2x^3} - \frac{1}{\sqrt{\pi}}\frac{\exp\{-x^2\}}{x^2} && (9)
\end{aligned}$$

A lookup table will be used for $F(x)$ and $G(x)$, and for $x < 1$, an expansion is performed. This is necessary since $F(x)$ is prone to floating point errors for $x \to 0$ $(0/0 - 1/0)$.

Wolfram Alpha gives the expansion. $G(x)$ now becomes[1]:

$$\begin{aligned}
\sqrt{\pi}G(x) \simeq 2 &- \frac{2x^2}{3} + \frac{x^4}{5} - \frac{x^6}{21} + \frac{x^8}{108} - \frac{x^{10}}{660} + \frac{x^{12}}{4680} - \frac{x^{14}}{37800} + \frac{x^{16}}{342720} - \frac{x^{18}}{3447360} + \frac{x^{20}}{38102400} \\
&- \frac{x^{22}}{459043200} + \frac{x^{24}}{5987520000} - \frac{x^{26}}{84064780800} + \frac{x^{28}}{1264085222400} - \frac{x^{30}}{20268952704000} \\
&+ \frac{x^{32}}{345226033152000} - \frac{x^{34}}{6224529991680000} + \frac{x^{36}}{118443913555968000} \\
&- \frac{x^{38}}{2372079457972224000} + \frac{x^{40}}{49874491167621120000} + O\left(x^{41}\right) && (10)
\end{aligned}$$

[1] http://www.wolframalpha.com/input/?i=erf%28x%29%2Fx

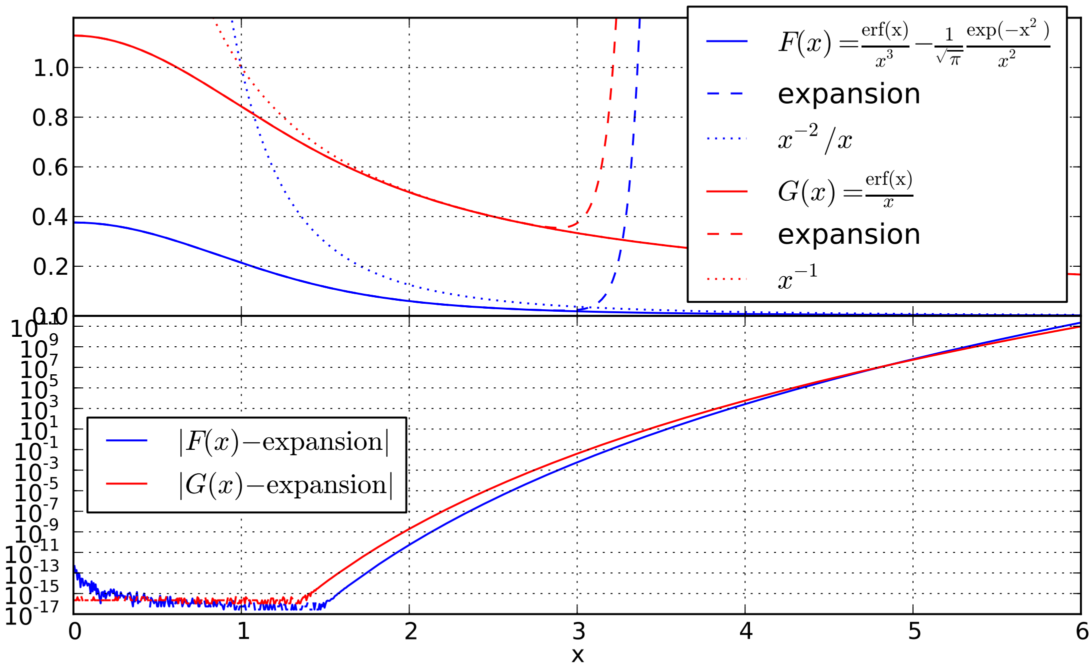

Figure 1: Expansions of $F(x)$ and $G(x)$

and $F(x)$ is[2]:

$$\begin{aligned}\sqrt{\pi}F(x) \simeq {} & \frac{2}{3} - \frac{2x^2}{5} + \frac{x^4}{7} - \frac{x^6}{27} + \frac{x^8}{132} - \frac{x^{10}}{780} + \frac{x^{12}}{5400} - \frac{x^{14}}{42840} + \frac{x^{16}}{383040} - \frac{x^{18}}{3810240} + \frac{x^{20}}{41731200} \\ & - \frac{x^{22}}{498960000} + \frac{x^{24}}{6466521600} - \frac{x^{26}}{90291801600} + \frac{x^{28}}{1351263513600} - \frac{x^{30}}{21576627072000} \\ & + \frac{x^{32}}{366148823040000} - \frac{x^{34}}{6580217419776000} + \frac{x^{36}}{124846287261696000} \\ & - \frac{x^{38}}{2493724558381056000} + \frac{x^{40}}{52307393175797760000} \\ & - \frac{x^{42}}{1149546198863462400000} + \frac{x^{44}}{26414017102773780480000} + O\left(x^{45}\right) \qquad (11)\end{aligned}$$

Figure 1 shows the expansions of $F(x)$ and $G(x)$ compared to the exact values. For $x < 1.5$, the error is less then the floating point noise.

[2]http://www.wolframalpha.com/input/?i=expansion+erf%28x%29%2F%282*x**3%29-1%2Fsqrt%28pi%29*exp%28-x**2%29%2F%28x**2%29

2 Expansions with r=log(a)

Let's define:

$$a = \ln (x) \tag{12}$$
$$\mathrm{e}^{a} = x \tag{13}$$

The two functions F and G becomes:

$$G(x) = \frac{\operatorname{erf}\{\mathrm{e}^{a}\}}{\mathrm{e}^{a}} \tag{14}$$
$$F(x) = \frac{\operatorname{erf}\{\mathrm{e}^{a}\}}{2(\mathrm{e}^{a})^{3}} - \frac{1}{\sqrt{\pi}} \frac{\exp\{-(\mathrm{e}^{a})^{2}\}}{(\mathrm{e}^{a})^{2}} \tag{15}$$
$$F(x) = \frac{\operatorname{erf}\{\mathrm{e}^{a}\}}{2\mathrm{e}^{3a}} - \frac{1}{\sqrt{\pi}} \frac{\exp\{-\mathrm{e}^{2a}\}}{\mathrm{e}^{2a}} \tag{16}$$

The expansions are:

$$G(x) \approx erf(1) + a(2/(esqrt(pi)) - erf(1)) + a^{2}((erf(1))/2 - 3/(esqrt(pi))) + a^{3}(1/(esqrt(pi)) - (erf(1)) \tag{17}$$