

Expansions

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1 Expansions

The potential and field of a charge distribution are:

$$\phi(r) = \frac{kQ}{r} \operatorname{erf}\left\{\frac{r}{\sqrt{2}\sigma}\right\} \quad (1)$$

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

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

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

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

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:

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

$$\phi(x) = \frac{kQ}{\sqrt{2}\sigma} \frac{\operatorname{erf}\{x\}}{x}\tag{6}$$

$$\phi(x) = \frac{kQ}{\sqrt{2}\sigma} G(x)\tag{7}$$

where

$$G(x) = \frac{\operatorname{erf}\{x\}}{x}\tag{8}$$

$$F(x) = \frac{\operatorname{erf}\{x\}}{2x^3} - \frac{1}{\sqrt{\pi}} \frac{\exp\{-x^2\}}{x^2}\tag{9}$$

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 $x \rightarrow 0$ ($0/0 - 1/0$).

Wolfram Alpha gives the expansion. $G(x)$ now becomes¹:

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

¹<http://www.wolframalpha.com/input/?i=erf%28x%29%2F%28x%29>

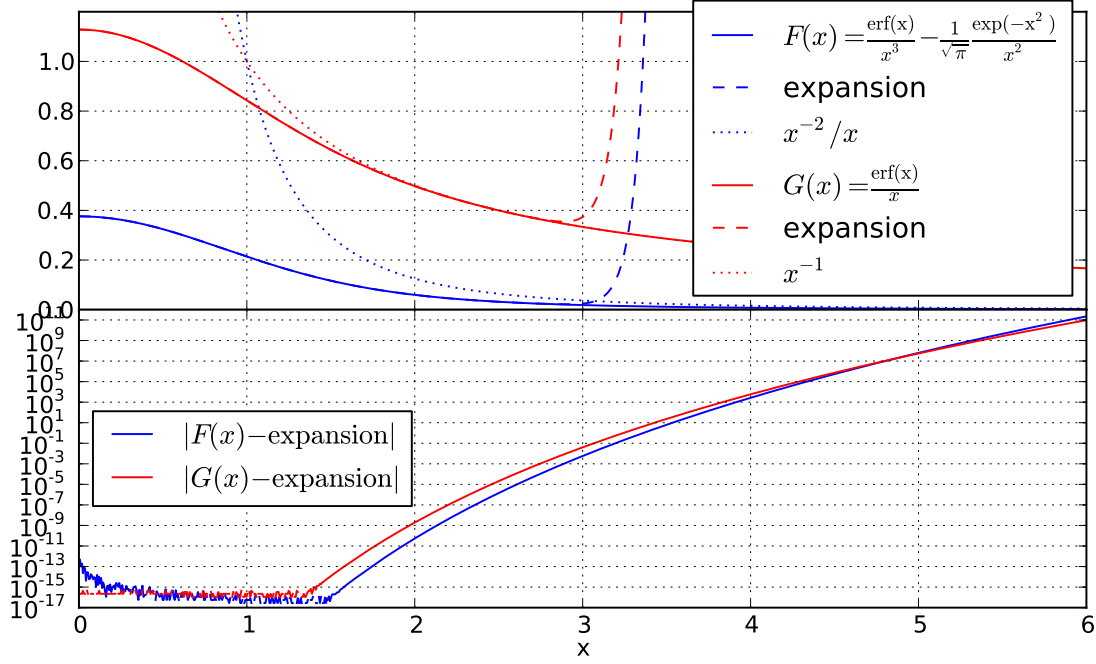


Figure 1: Expansions of $F(x)$ and $G(x)$

and $F(x)$ is²:

$$\begin{aligned}
\sqrt{\pi}F(x) \simeq & \frac{2}{3} - \frac{2x^2}{5} + \frac{x^4}{7} - \frac{x^6}{27} + \frac{x^8}{132} - \frac{x^{10}}{780} + \frac{x^{12}}{5400} - \frac{x^{14}}{42840} + \frac{x^{16}}{383040} - \frac{x^{18}}{3810240} + \frac{x^{20}}{41731200} \\
& - \frac{498960000}{x^{22}} + \frac{6466521600}{x^{24}} - \frac{90291801600}{x^{26}} + \frac{1351263513600}{x^{28}} - \frac{21576627072000}{x^{30}} \\
& + \frac{366148823040000}{x^{32}} - \frac{6580217419776000}{x^{34}} + \frac{124846287261696000}{x^{36}} \\
& - \frac{2493724558381056000}{x^{38}} + \frac{52307393175797760000}{x^{40}} \\
& - \frac{1149546198863462400000}{x^{42}} + \frac{264140171027737804800000}{x^{44}} + O(x^{45})
\end{aligned} \tag{11}$$

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

²http://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