Theoretical Concepts and Simulations for Materials Scientists Summer term 2009

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Exercises 2

1. Consider the Gauß function

$$G_{\eta}(x-x_0) = \frac{1}{\eta\sqrt{\pi}} e^{-\left(\frac{x-x_0}{\eta}\right)^2} \qquad \eta > 0$$

Sketch the Gauß function, determine its maximum, and calculate the width of the Gauß curve, which is defined by the distance between the two points $x_0 \pm \alpha$, where

$$G_{\eta}(x \pm \alpha - x_0) = \frac{1}{\eta \sqrt{\pi}} \frac{1}{e}.$$

Finally, calculate the integral

$$I = \int_{-\infty}^{+\infty} dx \, G_\eta(x - x_0) \,.$$

Consider especially all results for the limit $\eta \to 0$.

2. Consider the Lorentz function

$$L_{\eta}(x-x_0) = \frac{1}{\pi} \frac{\eta}{(x-x_0)^2 + \eta^2} \qquad \eta > 0.$$

Sketch the Lorentz function, determine its maximum, and calculate the width of the Lorentz curve, which is defined by the distance between the two points $x_0 \pm \alpha$, where the function assumes half of the maximum value. Finally, calculate the integral

$$I = \int_{-\infty}^{+\infty} dx \, L_{\eta}(x - x_0) \,.$$

Consider especially all results for the limit $\eta \to 0$.

- 3. In one dimension, Dirac's δ -distribution is specified by the requirements
 - (a)

$$\delta(x - x_0) = 0 \qquad \forall x \neq x_0$$

(b)

$$\int_{a}^{b} dx \,\delta(x - x_0) = \begin{cases} 1 & : a < x_0 < b \\ 0 & : \text{elsewhere} \end{cases}$$

Show that

(a)
$$\lim_{\eta \to 0} G_{\eta}(x - x_0) = \delta(x - x_0)$$
(b)

$$\lim_{\eta \to 0} L_{\eta}(x - x_0) = \delta(x - x_0)$$