

2) Gauss

$\langle \psi | \psi \rangle = 1$

$\psi(r) = N \cdot e^{-\beta r^2}$

$\Rightarrow N^{12} \cdot 4\pi \int_0^\infty dr r^2 \cdot e^{-2\beta r^2} = N^{12} \cdot 4\pi \left(\frac{1}{2}\right) \left(\frac{1}{2}\right) \left(\frac{1}{2}\right) \sqrt{\frac{\pi}{2\beta}} \beta^{-3/2} =$

$\underbrace{-\frac{1}{2} \cdot \frac{\partial}{\partial \beta} \int_0^\infty e^{-2\beta r^2} dr}_{\frac{1}{2} \cdot \sqrt{\frac{\pi}{2\beta}}}$

$= N^{12} \left(\frac{\pi}{2\beta}\right)^{3/2} = 1$

$\Rightarrow N = \left(\frac{2\beta}{\pi}\right)^{3/4}$

$\langle E_{pot} \rangle = \langle \psi | \frac{-z}{r} | \psi \rangle = -z N^{12} \cdot 4\pi \int_0^\infty dr r^2 e^{-\beta r^2} \cdot \frac{1}{r} e^{-\beta r^2} =$

$= -z N^{12} \cdot 4\pi \int_0^\infty dr \cdot r \cdot e^{-2\beta r^2} = -z N^{12} \cdot 4\pi \cdot \frac{1}{4\beta} \left[e^{-2\beta r^2} \right]_0^\infty = -z \sqrt{\frac{8\beta}{\pi}}$

$\langle E_{kin} \rangle = \langle \psi | -\frac{1}{2} \Delta | \psi \rangle = -\frac{1}{2} N^{12} \cdot 4\pi \int_0^\infty dr r^2 e^{-\beta r^2} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} e^{-\beta r^2} \right] =$

$= -\frac{1}{2} N^{12} \cdot 4\pi (-2\beta) \int_0^\infty dr e^{-\beta r^2} \left[3r^2 e^{-\beta r^2} + r^3 (-2\beta r) e^{-\beta r^2} \right] =$

$= -\frac{1}{2} N^{12} \cdot 4\pi (-2\beta) (-\frac{1}{2}) \left[3 \frac{\partial}{\partial \beta} \left(\frac{1}{2} \sqrt{\frac{\pi}{2\beta}} \right) + \beta \frac{\partial^2}{\partial \beta^2} \left(\frac{1}{2} \sqrt{\frac{\pi}{2\beta}} \right) \right] =$

$= -\frac{1}{2} \frac{2\beta}{\pi} \sqrt{\frac{2\beta}{\pi}} \cdot 4\pi \cdot \beta \cdot \left(-\frac{3}{4}\right) \sqrt{\frac{\pi}{2}} \cdot \beta^{-3/2} \cdot \left[1 - \frac{1}{2} \right] = \frac{3}{2} \beta$

$\Rightarrow \langle E \rangle = \frac{3}{2} \beta - z \sqrt{\frac{8\beta}{\pi}}$

$0 = \frac{\partial \langle E \rangle}{\partial \beta} = \frac{3}{2} - z \sqrt{\frac{8}{\pi}} \cdot \frac{1}{2} \cdot \frac{1}{\sqrt{\beta}} \Rightarrow \beta_0 = \frac{8 \cdot z^2}{9\pi}$

$\Rightarrow E_0 = \frac{3}{2} \cdot \frac{8 \cdot z^2}{9\pi} - z \cdot \frac{8 \cdot z}{3\pi} = -\frac{4 \cdot z^2}{3\pi}$ Also $z=1 \rightarrow E_0 = -0,424$

Mess: 3,4, ... 6 ab Gauss $\rightarrow E = -0,499 > \frac{1}{2}$