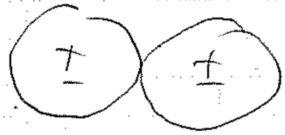
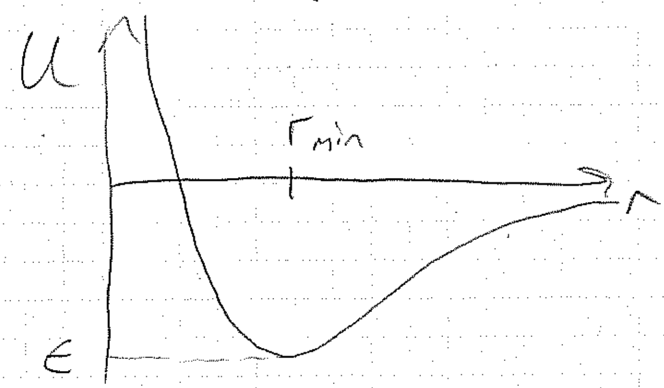
Example Lennard Jones Potential



- collision of neutral atoms.
- such as He atoms in an ideal gas.
- electron clouds repel and atoms become polarized

$$U(r) = \epsilon\left(\left(\frac{r_{min}}{r}\right)^{12} - 2\left(\frac{r_{min}}{r}\right)^{6}\right)$$

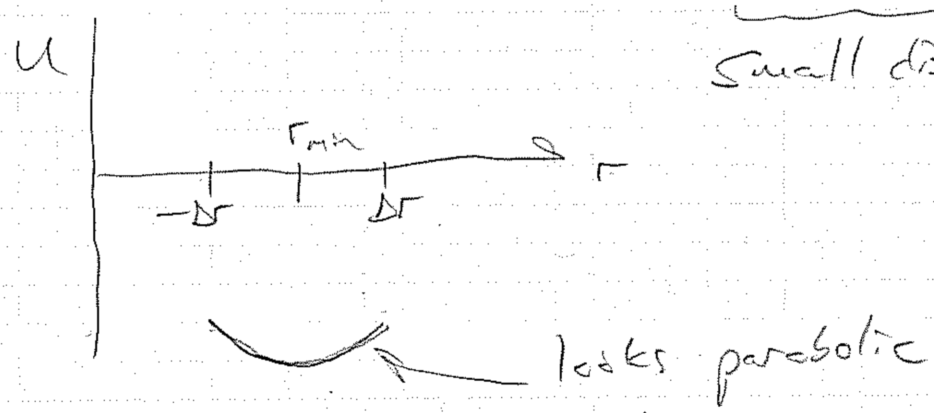


- Show that for small displacement, U is approximately a harmonic oscillator.
- Find $F(r)$

Binomial Approximation

$$(1+x)^n \approx 1+nx \quad \text{if} \quad x \ll 1$$

Suppose $r = r_{min} + \Delta r$ where $\underbrace{\Delta r \ll r_{min}}_{\text{small displacement!}}$.



$$U = \epsilon\left(\left(\frac{r_{min}}{r}\right)^{12} - 2\left(\frac{r_{min}}{r}\right)^{6}\right)$$

$$= \epsilon\left(\frac{r_{min}}{r}\right)^{6}\left(\left(\frac{r_{min}}{r}\right)^{6} - 2\right)$$

$$\frac{r_{min}}{r} = \frac{r_{min}}{r_{min}+\Delta r} = \frac{1}{1+\frac{\Delta r}{r_{min}}} = \left(1+\frac{\Delta r}{r_{min}}\right)^{-1}$$

So at $r = r_{min} + \Delta r$

$$U = \epsilon\left(1+\frac{\Delta r}{r_{min}}\right)^{-6}\left(\left(1+\frac{\Delta r}{r_{min}}\right)^{-6} - 2\right)$$

$$\approx \epsilon\left(1-\frac{6\Delta r}{r_{min}}\right)\left(1-\frac{6\Delta r}{r_{min}} - 2\right)$$

$$\approx \epsilon\left(1-\frac{6\Delta r}{r_{min}}\right)\left(-1-\frac{6\Delta r}{r_{min}}\right)$$

$$\approx -\epsilon\left(1-\frac{6\Delta r}{r_{min}}\right)\left(1+\frac{6\Delta r}{r_{min}}\right)$$

$$\approx -\epsilon\left(1-\frac{36\Delta r^2}{r_{min}^2}\right)$$

$$U \approx -\epsilon\left(1 - 36\frac{\Delta r^2}{r_{min}^2}\right)$$

$$\approx -\epsilon + \underbrace{\frac{36\epsilon}{r_{min}^2}}\Delta r^2$$

quadratic like a spring.

$$F_r = -\frac{\partial U}{\partial r}$$

$$= -\epsilon\left(r_{mm}^{12}(-12)r^{-13} - 2r_{mm}^{6}(-6)r^{-7}\right)$$

$$= -\epsilon\left(\left(\frac{r_{mm}}{r}\right)^{12}\left(\frac{-12}{r}\right) - 2\left(\frac{r_{mm}}{r}\right)^{6}\left(\frac{-6}{r}\right)\right)$$

$$= +\epsilon\left(\frac{12}{r}\left(\frac{r_{mm}}{r}\right)^{12} - \frac{12}{r}\left(\frac{r_{mm}}{r}\right)^{6}\right)$$

$$\boxed{F_r = \frac{\epsilon 12}{r}\left(\left(\frac{r_{mm}}{r}\right)^{12} - \left(\frac{r_{mm}}{r}\right)^{6}\right)}$$

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