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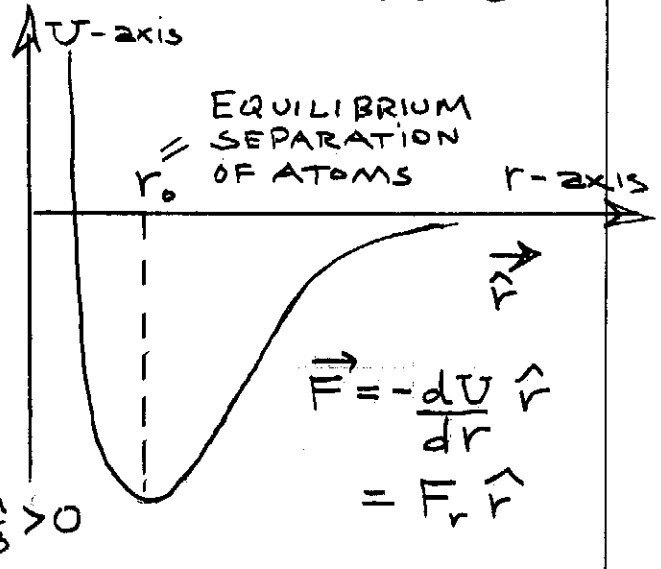
sec. 8-6 Reading a Potential Energy Curve

••38 The potential energy of a diatomic molecule (a two-atom system like H_2 or O_2) is given by

$$U = \frac{A}{r^{12}} - \frac{B}{r^6},$$

where r is the separation of the two atoms of the molecule and A and B are positive constants. This potential energy is associated with the force that binds the two atoms together. (a) Find the *equilibrium separation*—that is, the distance between the atoms at which the force on each atom is zero. Is the force repulsive (the atoms are pushed apart) or attractive (they are pulled together) if their separation is (b) smaller and (c) larger than the equilibrium separation?

THE LENNARD-JONES POTENTIAL FOR THE DIATOMIC MOLECULE



$\vec{F} = -\frac{dU}{dr}\hat{r} = F_r \hat{r}$

FOR SMALL $r << r_{equilibrium} \equiv r_0$

$U \sim \frac{A}{r^{12}}$ WHICH GOES TO $+\infty$ AS $r \to 0$ (SINCE $B/r^6 << A/r^{12}$)

THE FORCE $F = -\frac{dU}{dr} = -\frac{-12A}{r^{13}} > 0$

$= -$SLOPE $=$ POSITIVE

$\Rightarrow$ ATOMS ARE REPULSIVE TO EACH OTHER AND WANT TO INCREASE THEIR SEPARATION $= r$ (and RETURN TO EQUILIBRIUM)

FOR LARGE $r >> r_0 =$ EQUILIBRIUM SEPARATION

$U \sim -\frac{B}{r^6}$ SINCE $\frac{A}{r^{12}}$ IS MUCH SMALLER $\left(\text{i.e. } \frac{B}{r^6} >> \frac{A}{r^{12}}\right)$

THE FORCE: $F = -\frac{dU}{dr} = ---\frac{6B}{r^7} < 0$

OR $-$SLOPE $=$ NEGATIVE $\Rightarrow$ FORCE IS IN $-\hat{r}$ DIRECTION

$\Rightarrow$ ATOMS ARE ATTRACTED TO EACH OTHER AND WANT TO DECREASE THEIR SEPARATION $= r$ (AND RETURN TO EQUILIBRIUM)

EQUILIBRIUM: $F = -\left.\frac{dU}{dr}\right|_{r=r_0} \equiv 0$ IS IN THE REGION WHERE BOTH TERMS / ARE IMPORTANT; ATTRACTION & REPULSION

ALSO MINIMUM FOR U

$F = \left(--\frac{12A}{r^{13}} - --\frac{6B}{r^7}\right)\Big|_{r=r_0} = 0 \Rightarrow \frac{6B}{r_0^7} = \frac{12A}{r_0^{13}}$

$\Rightarrow r_0^6 = 2\frac{A}{B} \Rightarrow r_0 = (2A/B)^{1/6}$ EQUILIBRIUM SEPARATION

OF ATOMS OCCURS WHERE THERE IS 0 NET BY ONE ON THE OTHER. THIS IS WHERE THERE IS A MINIMUM OF THE POTENTIAL ENERGY FUNCTION