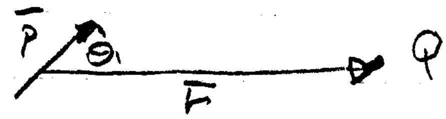
POTENTIAL ENERGY OF A DIPOLE p AND CHARGE Q

as $V(r,\theta,\varphi) = \dfrac{\bar{p}\cdot\hat{r}}{4\pi\varepsilon_0 r^2} = \dfrac{p\cos\theta}{4\pi\varepsilon_0 r^2}$



THE POTENTIAL ENERGY IS

$$U(r,\theta,\varphi) = \frac{Qp\cos\theta}{4\pi\varepsilon_0 r^2}$$

SUPPOSE DIPOLE IS FREE TO ROTATE, WHAT IS AVE POTENTIAL ENERGY?

LET r BE FIXED

IF ENERGY OF DIPOLE POINTING IN θ,φ IS $U(r,\theta,\varphi)$ THEN PROBABILITY OF THIS STATE AT TEMPERATURE T IS (SEE BOLTZMANN LINK)

$$P(r,\theta,\varphi)\sin\theta\, d\theta\, d\varphi = \frac{e^{-U(r,\theta,\varphi)/kT}\sin\theta\, d\theta\, d\varphi}{\int e^{-U(r,\theta,\varphi)/kT}\sin\theta\, d\theta\, d\varphi}$$

NOTE $\int P(r,\theta,\varphi)\sin\theta\, d\theta\, d\varphi = 1$

So $$P(r,\theta,\varphi)\sin\theta\, d\theta\, d\varphi = \frac{e^{-\frac{a\cos\theta}{kT}}\sin\theta\, d\theta}{\int e^{-\frac{a\cos\theta}{kT}}\sin\theta\, d\theta}$$

WHERE $a \equiv Qp/4\pi\varepsilon_0 r^2$

AVE $u(r,\theta,\varphi) \equiv \langle u(r,\theta,\varphi)\rangle = \int u(r,\theta,\varphi)\, P(r,\theta,\varphi) \sin\theta\, d\theta\, d\varphi$

$$= \frac{\int a\cos\theta\, e^{-a\cos\theta/kT} \sin\theta\, d\theta\, d\varphi}{\int e^{-a\cos\theta/kT} \sin\theta\, d\theta\, d\varphi}$$

$$= (kT)^2 \frac{d}{d\,kT} \ln \int e^{-a\cos\theta/kT} \sin\theta\, d\theta\, d\varphi$$

$$\equiv (kT)^2 \frac{d}{d\,kT} \ln Z(kT)$$

THE INTEGRAL IS IMMEDIATE

$$Z = \frac{2\pi kT}{a} e^{-\frac{a\cos\theta}{kT}} \Big|_0^{\pi} = \frac{2\pi kT}{a}\left(e^{\frac{a}{kT}} - e^{-\frac{a}{kT}}\right)$$

$$Z = \frac{4\pi kT}{a} \sinh \frac{a}{kT}$$

$$\ln Z = \ln \frac{4\pi kT}{a} + \ln \sinh \frac{a}{kT}$$

$$\langle u\rangle = (kT)^2 \frac{d}{d\,kT} \ln Z$$

$$\langle u\rangle = -kT\left[\frac{a}{kT} \coth a/kT - 1\right] = \bar{u}(r)$$

LIMITS $\quad a = \dfrac{Qp}{4\pi\varepsilon_0 r^2} \gg kT$ (i.e. <u>LOW</u> TEMPERATURE)

$\dfrac{a}{kT} \gg 1 \;,\; \coth\dfrac{a}{kT} \to 1$

So $\bar{u}(r) \approx -a = -\dfrac{Qp}{4\pi\varepsilon_0 r^2}$ THE LOWEST ENERGY STATE

GOES LIKE $1/r^2$ $\qquad \overleftarrow{\bar{p}} \qquad +Q$

IF $\dfrac{a}{kT} \ll 1$ (HIGH TEMPERATURE)

$\coth X \approx 1 + \frac{1}{3}X^2$ FOR $X \ll 1$

$$\bar{u}(r) \approx -kT\left[1 + \frac{1}{3}\left(\frac{a}{kT}\right)^2 - 1\right]$$

$$= \frac{-a^2}{3kT} = -\left(\frac{Qp}{4\pi\varepsilon_0 r^2}\right)^2 \frac{1}{kT}$$

$\boxed{\text{GOES LIKE } \dfrac{1}{r^4}}$

So $\dfrac{\bar{u}(r)}{kT} = -\left[X \coth X - 1\right] \qquad X \equiv \dfrac{a}{kT}$

$\to -\dfrac{1}{3}X^2 \quad X \ll 1$

$\to -X \quad X \gg 1$

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In[2]:= u[x_] := -(x*Coth[x] - 1)
In[3]:= Plot[u[x], {x, .1, 4}]
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