Thermal Dipoles

(a) $$V(\underline{r}) = \frac{\mu_0}{4\pi r^3}\left(\underline{d}_1\cdot\underline{d}_2 - 3(\underline{d}_1\cdot\hat{\underline{r}})(\underline{d}_2\cdot\hat{\underline{r}})\right)$$

$$\underline{r} = \begin{pmatrix} 0 \\ 0 \\ r \end{pmatrix} \quad (\text{in } z \text{ direction}) \quad \text{so} \quad \hat{\underline{r}} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\underline{d}_1 = \begin{pmatrix} d_1 \sin\theta_1 \cos\phi_1 \\ d_1 \sin\theta_1 \sin\phi_1 \\ d_1 \cos\theta_1 \end{pmatrix} \qquad \underline{d}_2 = \begin{pmatrix} d_2 \sin\theta_2 \cos\phi_2 \\ d_2 \sin\theta_2 \sin\phi_2 \\ d_2 \cos\theta_2 \end{pmatrix}$$

$$\underline{d}_1\cdot\underline{d}_2 = d_1 d_2\left(\sin\theta_1\sin\theta_2\underbrace{\left(\cos\phi_1\cos\phi_2 + \sin\phi_1\sin\phi_2\right)}_{=\cos(\phi_1-\phi_2)} + \cos\theta_1\cos\theta_2\right)$$

$$(\hat{d}_1\cdot r)(\hat{d}_2\cdot r) = d_1 d_2 \cos\theta_1\cos\theta_2$$

$$\Rightarrow V(r) = \frac{d_1 d_2 \mu_0}{4\pi r^3}\left[\underbrace{\sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2) - 2\cos\theta_1\cos\theta_2}_{=V}\right]$$

This is rather trivial, but I thought doing this step was a good way for everybody to get into the question and understand the notation.

(b) Key knowledge: 1. Partition function $Z = \int_{\text{configurations}} e^{-E/kT}$

2. Internal energy $U = -\dfrac{\partial \ln Z}{\partial \beta}$

3. Force $\underline{F} = -\dfrac{\partial U}{\partial \underline{r}}$

1. Configurations are <u>orientations</u> of dipoles:

$\Rightarrow$ Integral is $\displaystyle\int_0^{\pi} \sin\theta_1 d\theta_1 \int_0^{2\pi} d\phi_1 \int_0^{\pi} \sin\theta_2 d\theta_2 \int_0^{2\pi} d\phi_2$

Let $\lambda = \dfrac{\mu_0 d_1 d_2}{4\pi r^3 k_B T} \ll 1$

Then $e^{-V(r)/k_BT} = e^{-\lambda v}$ (v defined above)

$$= \underbrace{1}_{0^{th}} - \underbrace{\lambda v}_{1st} + \underbrace{\lambda v^2/2}_{2nd} + \dots$$ (Taylor expand because $\lambda \ll 1$)

Order:

0th order term: Integral gives $(4\pi)^2$

1st order term:

$$\lambda \int_{-1}^{1} d\cos\theta_1 \int_{-1}^{1} d\cos\theta_2 \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \left(\sin\theta_1 \sin\theta_2 \cos(\phi_1-\phi_2) - 2\cos\theta_1\cos\theta_2\right)$$

$$= 0$$

2nd order term:

$$\frac{\lambda^2}{2} \int_{-1}^{1} d\cos\theta_1 \int_{-1}^{1} d\cos\theta_2 \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \left(\sin\theta_1 \sin\theta_2 \cos(\phi_1-\phi_2) - 2\cos\theta_1\cos\theta_2\right)^2$$

Square integrand: $\sin^2\theta_1 \sin^2\theta_2 \cos^2(\phi_1-\phi_2)$ — (A)

$-4\sin\theta_1\cos\theta_1\sin\theta_2\cos\theta_2\cos(\phi_1-\phi_2)$ — (B)

$+4\cos^2\theta_1\cos^2\theta_2$ — (C)

Three integrals to do:

A) $$\underbrace{\int_{-1}^{1} dx_1 (1-x_1^2)}_{=\left[x-\frac{x^3}{3}\right]_{-1}^{1}=\frac{4}{3}} \underbrace{\int_{-1}^{1} dx_2 (1-x_2^2)}_{=4/3} \underbrace{\int_0^{2\pi} d\phi_1}_{2\pi} \underbrace{\int_0^{2\pi} d\phi_2 \cos^2(\phi_1-\phi_2)}_{\pi} = \frac{32\pi^2}{9}$$

B) $$\int d\phi_1 \cos(\phi_1-\phi_2) = 0$$

C) $$4\underbrace{\int_{-1}^{1} dx_1\, x_1^2}_{2/3} \underbrace{\int_{-1}^{1} dx_2\, x_2^2}_{2/3} \underbrace{\int_0^{2\pi} d\phi_1}_{2\pi} \underbrace{\int_0^{2\pi} d\phi_2}_{2\pi} = \frac{64\pi^2}{9}$$

Hence 2nd order term is $$\frac{\lambda^2}{2}\left(\frac{32\pi^2}{9}+\frac{64\pi^2}{9}\right) = \frac{16\pi^2}{3}\lambda^2$$

$$\Rightarrow \quad Z = (4\pi)^2\left(1+\lambda^2/3\right) + \text{higher order in } \lambda.$$

2. $$\frac{\partial Z}{\partial \beta} = \frac{\partial Z}{\partial \lambda}\frac{\partial \lambda}{\partial \beta} = (4\pi)^2 \cdot \frac{2\lambda}{3} \cdot \frac{\mu_0 d_1 d_2}{4\pi r^3}$$

$$\left(\lambda = \frac{\mu_0 d_1 d_2}{4\pi r^3}\beta\right)$$

$$\boxed{U = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial Z/\partial \beta}{Z} = \frac{-\mu_0 d_1 d_2}{4\pi r^3} \cdot \frac{2\lambda}{3+\lambda^2}}$$

To leading order in λ, forget λ^2 in denominator:

$$U \simeq -\frac{2}{3} \cdot \frac{\mu_0 d_1 d_2}{4\pi r^3} \lambda = -\left(\frac{\mu_0 d_1 d_2}{4\pi}\right)^2 \cdot \frac{1}{k_B T} \cdot \frac{2}{3} \cdot \frac{1}{r^6}$$

<u>Step 3</u>

Force $$\boxed{F = -\frac{\partial U}{\partial r} = \left(\frac{\mu_0 d_1 d_2}{4\pi}\right)^2 \frac{1}{k_B T} \frac{4}{r^7}}$$

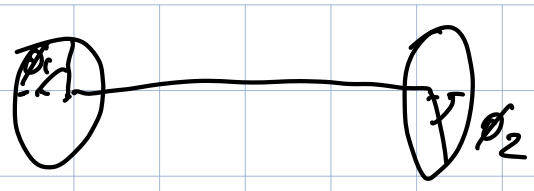
Also nicely expressed as $F = \lambda^2 \cdot \frac{4 k_B T}{r}$

This is pointing in the $\hat{\underline{r}}$ direction so is a <u>repulsive</u> force.

Suggested marking Scheme:

- 2 points for understanding steps necessary to get to result
- 1 for realising one needs second order expansion of exponential in partition function
- 3 for technical details/execution of integrals
- 1 for answer/understanding direction of force

(c) This is a SYMMETRY argument, but for the marks they should expand at least a little beyond just saying "symmetry".



For example, you could focus on the ϕ variable ... the potential involves only $\phi_1 - \phi_2$ but is completely symmetric under rotation.

- This means any transverse force would be in an arbitrarily chosen direction (as $\phi_1 = 0$ has no meaning) therefore must be zero.