Dipole Tilt

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The dipole-dipole energy is,

$$E_{dd} = \frac{1}{2}\int \mathrm{d}\mathbf{x}|\Psi(\mathbf{x})|^2 \int \mathrm{d}\mathbf{x}' U(\mathbf{x}-\mathbf{x}')|\Psi(\mathbf{x}')|^2 = \frac{1}{2}\int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{x}' n(\mathbf{x}) U(\mathbf{x}-\mathbf{x}') n(\mathbf{x}') \tag{1}$$

where we'll use the dipole-dipole potential,

$$U(\mathbf{x}) = \frac{C_{dd}}{4\pi}\frac{1-3\cos^2\vartheta}{|\mathbf{x}|^3} \tag{2}$$

Now, let's say, using the convolution theorem,

$$\Phi(\mathbf{x}) \equiv \int \mathrm{d}\mathbf{x}' U(\mathbf{x}-\mathbf{x}') n(\mathbf{x}') = \mathcal{F}^{-1}\left[\tilde{U}(\mathbf{k})\tilde{n}(\mathbf{k})\right] \tag{3}$$

so, $\tilde{\Phi}(\mathbf{k}) = \tilde{U}(\mathbf{k})\tilde{n}(\mathbf{k})$

$$\frac{1}{2}\int \mathrm{d}\mathbf{x}\, n(\mathbf{x})\Phi(\mathbf{x}) = \frac{1}{2(2\pi)^3}\int \mathrm{d}\mathbf{k}\, \tilde{n}(-\mathbf{k})\tilde{\Phi}(\mathbf{k}) \tag{4}$$

(using Plancherel's theorem). Since the density is real, therefore,

$$E_{dd} = \frac{1}{2(2\pi)^3}\int \mathrm{d}\mathbf{k}\, \tilde{n}^2(\mathbf{k})\tilde{U}(\mathbf{k}) \tag{5}$$

Now, let's take an ansatz for the wavefunction,

$$\Psi(\mathbf{x}) = \left(\frac{2}{\pi}\right)^{\frac{3}{4}} \frac{1}{\sqrt{\alpha\beta\gamma}} \mathrm{e}^{-\frac{x^2}{\alpha^2}-\frac{y^2}{\beta^2}-\frac{z^2}{\gamma^2}} \tag{6}$$

which gives the Fourier-transformed density,

$$\tilde{n}(\mathbf{k}) = \mathrm{e}^{-\frac{1}{8}(k_x^2\alpha^2+k_y^2\beta^2+k_z^2\gamma^2)} = \mathrm{e}^{-\frac{1}{8}\mathbf{k}^{\mathrm{T}}M\mathbf{k}} \tag{7}$$

with,

$$M = \begin{pmatrix} \alpha^2 & 0 & 0 \\ 0 & \beta^2 & 0 \\ 0 & 0 & \gamma^2 \end{pmatrix} \tag{8}$$

Meanwhile, the Fourier-space dipole-dipole potential is,

$$\tilde{U}(\mathbf{k}) = \int \mathrm{d}\mathbf{x}\, \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\mathbf{k}} U(\mathbf{x}) = \frac{C_{dd}}{3}\left(3\cos^2\varphi - 1\right) \tag{9}$$

where

$$\cos\varphi = \frac{\mathbf{k}\cdot\hat{\mathbf{d}}}{|\mathbf{k}|} = \frac{1}{|\mathbf{k}|}\left(k_x\sin\theta\cos\phi + k_y\sin\theta\sin\phi + k_z\cos\theta\right) \tag{10}$$

and where θ, ϕ are polarization angles of the dipoles with respect to the z axis.

We are then left to calculate the integral,

$$E_{dd} = A\int \mathrm{d}\mathbf{k}\, \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}}M\mathbf{k}}\left(3\cos^2\varphi - 1\right) \tag{11}$$

where $A = \frac{C_{dd}}{6(2\pi)^3}$. The term with no cosine is trivial,

$$E_{dd} = 3A\int \mathrm{d}\mathbf{k}\, \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}}M\mathbf{k}}\cos^2\varphi - A\frac{8\pi^{3/2}}{\alpha\beta\gamma} \tag{12}$$

And so we need to calculate integrals of the form,

$$\int \mathrm{d}\mathbf{k}\, \frac{k_i k_j}{|\mathbf{k}|^2} \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}} M \mathbf{k}} \tag{13}$$

First, we use the fact that (Schwinger parameter identity),

$$\frac{1}{k^2} = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-tk^2} \tag{14}$$

so,

$$\int \mathrm{d}\mathbf{k}\, \frac{k_i k_j}{|\mathbf{k}|^2} \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}} M \mathbf{k}} = \int_0^\infty \mathrm{d}t \int \mathrm{d}\mathbf{k}\; k_i k_j \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}} (M + \mathbb{1}4t) \mathbf{k}} \tag{15}$$

which can be evaluated,

$$\int_0^\infty \mathrm{d}t \int \mathrm{d}\mathbf{k}\; k_z^2 \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}} (M + \mathbb{1}t) \mathbf{k}} = \int_0^\infty \mathrm{d}t \frac{16\pi^{3/2}}{(\gamma^2 + 4t)^{3/2} \sqrt{(\alpha^2 + 4t)(\beta^2 + 4t)}} = \frac{8\pi^{3/2}}{\alpha\beta^2\gamma - \alpha\gamma^3} \left(\beta - \frac{\alpha\gamma \mathrm{E}\left(\csc^{-1}\left(\frac{\alpha}{\sqrt{\alpha^2 - \gamma^2}} \right) | \frac{\alpha^2 - \beta^2}{\alpha^2 - \gamma^2} \right)}{\sqrt{\alpha^2 - \gamma^2}} \right) \tag{16}$$

and similarly for k_x^2 and k_y^2 (with appropriate change of $\alpha \leftrightarrow \beta \leftrightarrow \gamma$), meanwhile it is zero otherwise (i.e. all integrals containing cross terms like $k_x k_y$ moments vanish). The function $\mathrm{E}(q|m)$ is the elliptic integral of the second kind,

$$\mathrm{E}(q|m) = \int_0^q \mathrm{d}p\, \sqrt{1 - m \sin^2 p} \tag{17}$$

Now let's simplify a bit. We're only considering tilt angles along the xz plane, so $\phi = 0$, and thus the k_y^2 integral will not appear.

$$\begin{aligned} E_{dd} = &-A\frac{8\pi^{3/2}}{\alpha\beta\gamma} + 3A \int_0^\infty \mathrm{d}t \int \mathrm{d}\mathbf{k}\; \mathrm{e}^{-\frac{1}{4}\mathbf{k}^{\mathrm{T}} M \mathbf{k}} (k_x^2 \sin^2\theta + k_z^2 \cos^2\theta) &(18)\\ = &-A\frac{8\pi^{3/2}}{\alpha\beta\gamma} + 3A \left(\sin^2\theta F[\beta, \gamma, \alpha] + \cos^2\theta F[\alpha, \beta, \gamma] \right) &(19) \end{aligned}$$

where now I've defined the function,

$$F[a, b, c] = \frac{8\pi^{3/2}}{ab^2c - ac^3} \left(b - \frac{ac}{\sqrt{a^2 - c^2}} \mathrm{E}\left[\csc^{-1}\left(\frac{a}{\sqrt{a^2 - c^2}} \right) \middle| \frac{a^2 - b^2}{a^2 - c^2} \right] \right) \tag{20}$$