Prelims Solutions

Problem J14T1

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Substituting:

$$E_{pot} = E_o + \frac{1}{2L^2}\int dxdy(\sum_{k_x,k_{x'}}\sum_{k_y,k_y'}(\sigma(ik_xik_x^{'} + ik_yik_y^{'}) + \rho g)A(\vec{k})A(\vec{k'})e^{i(\vec{k}+\vec{k'})\cdot\vec{r}})$$

The integral over x and y only affects the exponentials so we can use the identity: $\int dxdye^{i(\vec{k}+\vec{k'})\cdot\vec{r}}) = L^2\delta(k_x + k_x^{'})\delta(k_y + k_y^{'})$. Plugging into E_{pot} and using $A(-\vec{k}) = A^*(\vec{k})$ gives:

$$E_{pot} = E_o + \frac{1}{2}\sum_{k_x}\sum_{k_y}(\sigma(k_x^2 + k_y^2) + \rho g)|A(\vec{k})|^2 = E_o + \frac{1}{2}\sum_{\vec{k}}(\sigma\vec{k}^2 + \rho g)|A(\vec{k})|^2$$

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By definition the expectation $< |A(\vec{k})|^2 >$ is taken over the configuration space of $A(\vec{k})$, $\int D[A(\vec{k})]$. If this was in terms of $z(x, y)$ then the integral would be over all possible functions $z(x, y)$, i.e. for each (x, y), $z(x, y)$ ranges from $-\infty$ to $+\infty$. So here for each $\vec{k}$, $A(\vec{k})$ ranges from $-\infty$ to $+\infty$: $\int D[A(\vec{k})] = \prod_{\vec{k}}\int_{-\infty}^{\infty} dA(\vec{k})$.

$$< |A(\vec{k})|^2 >= \frac{\int D[A(\vec{k})]|A(\vec{k})|^2 e^{-\beta E_{pot}(\vec{k})}}{\int D[A(\vec{k})]e^{-\beta E_{pot}(\vec{k})}}$$

$$< |A(\vec{k})|^2 >= \frac{\int D[A(\vec{k'})]|A(\vec{k})|^2 e^{-\beta E_o - \frac{\beta}{2}\sum_{k''}(\sigma\vec{k''}^2+\rho g)|A(\vec{k''})|^2}}{\int D[A(\vec{k'})]e^{-\beta E_o - \frac{\beta}{2}\sum_{k''}(\sigma\vec{k''}^2+\rho g)|A(\vec{k''})|^2}} = \frac{\int dA(\vec{k})dA^*(\vec{k}) * |A(\vec{k})|^2 e^{-\frac{\beta}{2}(\sigma\vec{k}^2+\rho g)|A(\vec{k})|^2}}{\int dA(\vec{k})dA^*(\vec{k}) * e^{-\frac{\beta}{2}(\sigma\vec{k}^2+\rho g)|A(\vec{k})|^2}}$$

$$= \frac{1}{\beta\sigma\vec{k}^2 + \beta\rho g}$$

Hence, $a = \frac{\sigma}{k_B T}$ and $b = \frac{\rho g}{k_B T}$.

Above I have used separability of the integrals in $\int D[A(\vec{k})]$ and $dA(-\vec{k}) = dA^*(\vec{k})$. For evaluating the integrals you can change variables to real and imaginary parts of $|A(\vec{k})|^2$ and get a simple sum of gaussian integrals for example. Helpful identities: $\int_{-\infty}^{\infty} e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}}$ and $\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2}dx = \frac{1}{2} * \frac{\sqrt{\pi}}{\alpha^{\frac{3}{2}}}$.

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$$< z(\vec{r})^2 >=< \frac{1}{L^2}\sum_{\vec{k}}\sum_{\vec{k'}} A(\vec{k})A(\vec{k'})e^{i(\vec{k}+\vec{k'})\cdot\vec{r}}) >= \frac{1}{L^2}\sum_{\vec{k}}\sum_{\vec{k'}} < A(\vec{k})A(\vec{k'}) > e^{i(\vec{k}+\vec{k'})\cdot\vec{r}}) = \frac{1}{L^2}\sum_{\vec{k}} < |A(\vec{k})|^2 >$$

We can approximate this sum as an integral in $\vec{k}$ plane with maximum radius $\vec{k}_{max}$. We take the full area of the circle because $\vec{k}$ can be negative and positive (i.e. negative integer modes exist). Hence,

$$< z(\vec{r})^2 >\approx \frac{1}{L^2}\int_0^{|\vec{k}_{max}|}\frac{2\pi k dk}{(\frac{2\pi}{L})^2}\frac{1}{\beta\sigma k^2+\beta\rho g} = \frac{k_B T}{4\pi\sigma}ln(\frac{\beta\sigma k_{max}^2+\beta\rho g}{\beta\rho g})$$

And so,

$$\sqrt{< z(\vec{r})^2 >} \approx \sqrt{\frac{k_B T}{4\pi\sigma}ln(\frac{\sigma}{\rho g}k_{max}^2+1)}$$

Now using the assumption $k_{max}a/b >> 1$, I finally get:

$$\sqrt{< z(\vec{r})^2 >} \approx \sqrt{\frac{k_B T}{4\pi\sigma}ln(\frac{\sigma}{\rho g}k_{max}^2)}$$

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The shortest wavelength mode that can exist on the surface of the water is a wavelength on the order of the intermolecular distance λ_{min} between water molecules $\rightarrow k_{max} \approx \frac{2\pi}{\lambda_{min}}$.