Quiz 7

Answer the questions in the spaces provided. If you run out of room for an answer, continue on the back of the page.

Question:	1	2	Total
Points:	25	0	25
Score:			

Name: ____________________

1. Suppose we have a molecule with two angles θ and ϕ. The energy with respect to θ is $\epsilon_\theta(\theta) = 1 - \cos(\theta - \alpha)$, and the energy with respect to ϕ is $\epsilon_\phi(\phi) = 1 - \cos(2\phi - \beta)$ where α and β are real constants.

   (a) (10 points) What is an absolute minimum of the total energy $E(\theta, \phi) = \epsilon_\theta(\theta) + \epsilon_\phi(\phi)$ and at what angles does this minimum occur? Note, because this is a periodic function, it has an infinite number of minima, but just find one.

   Solution: Both energy components will be 0 when the argument to the cos is zero.

$$
\begin{aligned}
0 &= \theta_{\text{min}} - \alpha \\
\boxed{\theta_{\text{min}} = \alpha} \\
0 &= 2\phi - \beta \\
\boxed{\phi_{\text{min}} = \frac{\beta}{2}} \\
\boxed{E_{\text{min}} = 0}
\end{aligned}
$$

   (b) (5 points) Now Taylor expand this energy function around some point $(\theta = \alpha, \phi = \beta/2)$ to the first non-vanishing order (the lowest order that does not make the function zero everywhere).

   Solution:

$$
\begin{aligned}
E^{(0)}(\theta, \phi) &= 1 - \cos 0 + 1 - \cos 0 = 0 \\
E^{(1)}(\theta, \phi) &= 0
\end{aligned}
$$

   because this point is a extremum of the function (a minimum to be exact, as found above).

$$
\begin{aligned}
E^{(2)}(\theta, \phi) = \frac{1}{2}\Bigg(&\left.\frac{\partial^2 E}{\partial \theta^2}\right|_{\alpha, \beta/2} (\theta - \alpha)^2 \\
&+ \left.\frac{\partial^2 E}{\partial \phi^2}\right|_{\alpha, \beta/2} (\phi - \beta/2)^2 \\
&+ 2\left.\frac{\partial^2 E}{\partial \theta \partial \phi}\right|_{\alpha, \beta/2} (\theta - \alpha)(\phi - \beta/2)\Bigg) \\
E(\theta, \phi) \approx \frac{1}{2}&(\theta - \alpha)^2 + 2\left(\phi - \frac{\beta}{2}\right)^2
\end{aligned}
$$

   (c) (10 points) Someone else has found a Taylor series for a different energy function:

$$
E(x, y) \approx (x + a)^2 + (y + b)^2.
$$

If the angles x and y are constrained such that $x + y = m$, what is the minimum energy and the angles at which it occurs for this constrained system?

Solution:

$$\mathcal{L}(x, y, \lambda) = (x+a)^2 + (y+b)^2 - \lambda(x+y-m)$$
$$0 = \frac{\partial \mathcal{L}}{\partial x} = 2(x+a) - \lambda$$
$$0 = \frac{\partial \mathcal{L}}{\partial y} = 2(y+b) - \lambda$$
$$0 = \frac{\partial \mathcal{L}}{\partial \lambda} = x + y - m$$
$$0 = \frac{\lambda}{2} - a + \frac{\lambda}{2} - b - m$$
$$\lambda = a + b + m$$
$$\boxed{x = \frac{1}{2}(-a+b+m) \qquad y = \frac{1}{2}(a-b+m)}$$
$$\boxed{E_{\text{min}} = \frac{1}{2}(a+b+m)^2}$$

2. For fun if you finish early: Let's impose essentially the same constraint on our initial energy function from (a) and (b):
$$\theta + \phi = m.$$
What is the energy minimum of the Taylor series approximation? Can you find the constrained energy minimum without doing a Taylor series expansion?

Solution:

$$E_{\text{min}} = \frac{1}{10}(2\alpha + \beta - 2m)^2$$
$$\theta = \frac{1}{5}(\alpha - 2\beta + 4m)$$
$$\phi = \frac{1}{5}(-\alpha + 2\beta + m)$$

It would be very difficult to solve this without doing a Taylor series expansion.