

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.

$E_{\min} =$

$\theta_{\min} =$

$\phi_{\min} =$

- (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).

$E(\theta, \phi) \approx$

- (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?

$E_{\min} =$

$x_{\min} =$

$y_{\min} =$

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?