Chemistry 20262 Spring 2018
Professor J. Daniel Gezelter Due Fri. 2/2/2018

Problem Set 2

1. Derive the following trigonometric identity:

$$\cos(nx) = 2\cos x\cos((n-1)x) - \cos((n-2)x)$$

(Hint: you will want to turn the cosines into complex exponentials and then turn them back to cosines again.)

2. Define the following function:

$$\Psi(x,t) = e^{i\omega t}\sin x + e^{4i\omega t}\sin 2x$$

Show that

$$|\Psi(x,t)|^2 = f(x) + g(x)\cos 3\omega t$$

and expand $f(x)$ and $g(x)$ in terms of $\sin x$ and $\sin 2x$.

3. Use Mathematica to plot the following functions from problem 2 versus x, for $0 \leq x \leq 2\pi$:

a) $\sin x$

b) $\sin 2x$

c) $|\Psi(x,t)|^2$ when $t = 0$

d) $|\Psi(x,t)|^2$ when $3\omega t = \pi/2$

e) $|\Psi(x,t)|^2$ when $3\omega t = \pi$

4. Evaluate the following limits, if they exist:

a) $\lim_{(x,y)\to(2,\pi)} x^2 \sin\frac{y}{x}$

b) $\lim_{(x,y)\to(a,b)} \frac{x^2+y^2}{xy}$

5. Determine all the partial derivatives up to second order of $f(x,y) =$

a) $xe^y + y$

b) $y\sin x + x^2$

6. Show that $f_{xy} = f_{yx}$ for $f(x,y) = x^2 e^{-y^2}$

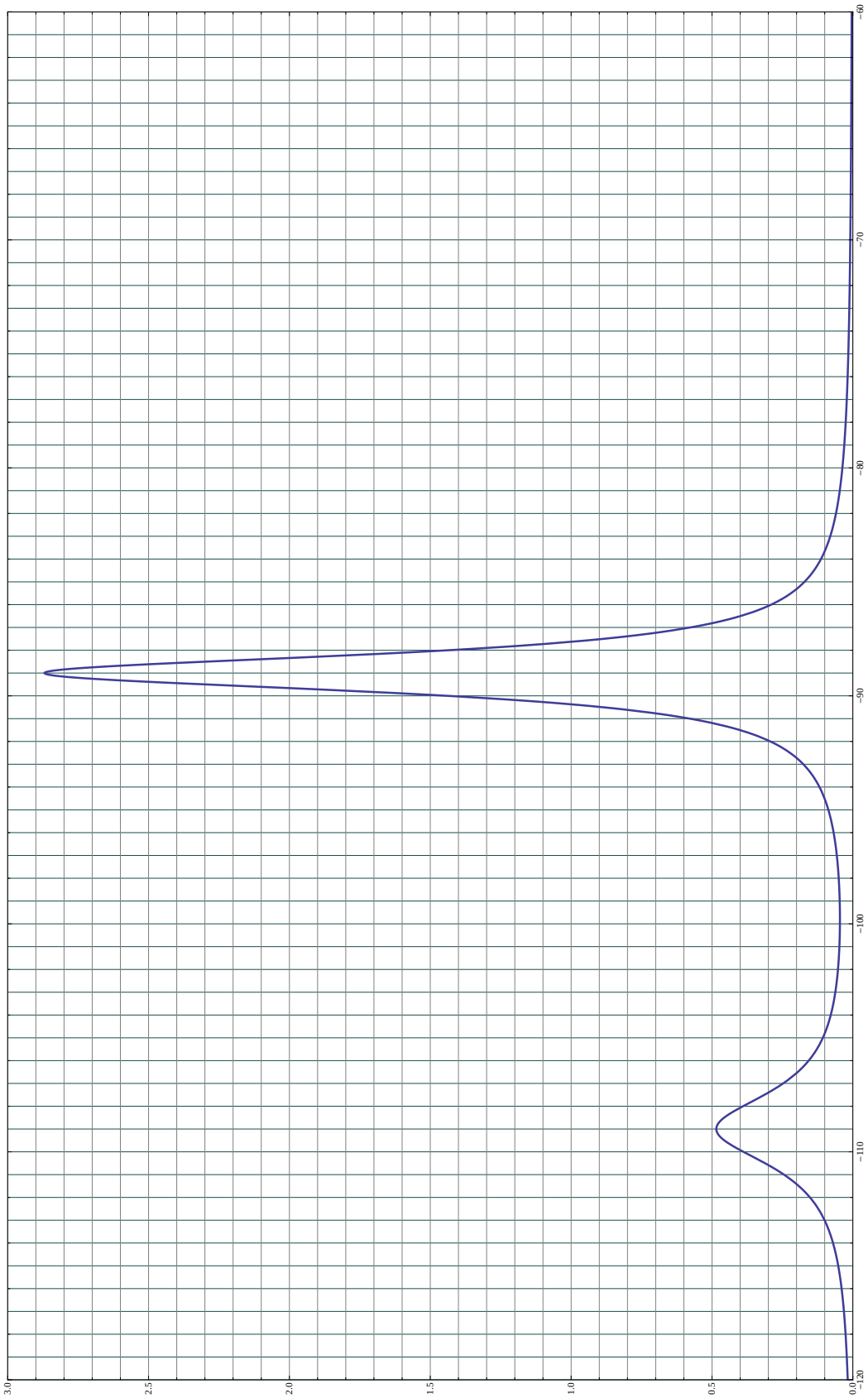
7. Show that $f_{xy} = f_{yx}$ for $f(x,y) = e^{-y}\cos xy$

8. Show that if the concentration of a solute is given by the function $c(x,t) = (4\pi Dt)^{-1/2} e^{-x^2/4Dt}$, it will satisfy the diffusion equation $\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$

9. The energy of a chemical system, $U = k_B T^2 \left(\frac{\partial \ln Q}{\partial T}\right)_{N,V}$ where Q is something called the "partition function". For an ideal gas, this function, $Q(N,V,T) = \frac{1}{N!}\left(\frac{2\pi m k_B T}{h^2}\right)^{3N/2} V^N$. If k_B, m, and h are constants, determine U for an ideal gas as a function of T. For now, this is purely an exercise in partial differentiation.

10. Extra Credit. Attached on the next two pages are two separate copies of the same (simulated) trace from a very early proton NMR experiment. The integrated area under each of the peaks tells us about the relative number of protons in the molecule that have the same chemical shifts. In the days before automated NMR spectrometers and computers, the integration had to be done by particularly clever students to figure out the structure of the molecule being studied.

    Find *two* **different** *and* **independent** *methods* for calculating the relative number of protons for each of these two peaks *without using a computer*. Compare your results. Hint: One of the methods may destroy the spectrum. Feel free to print out multiple copies of the problem set to experiment with your methods.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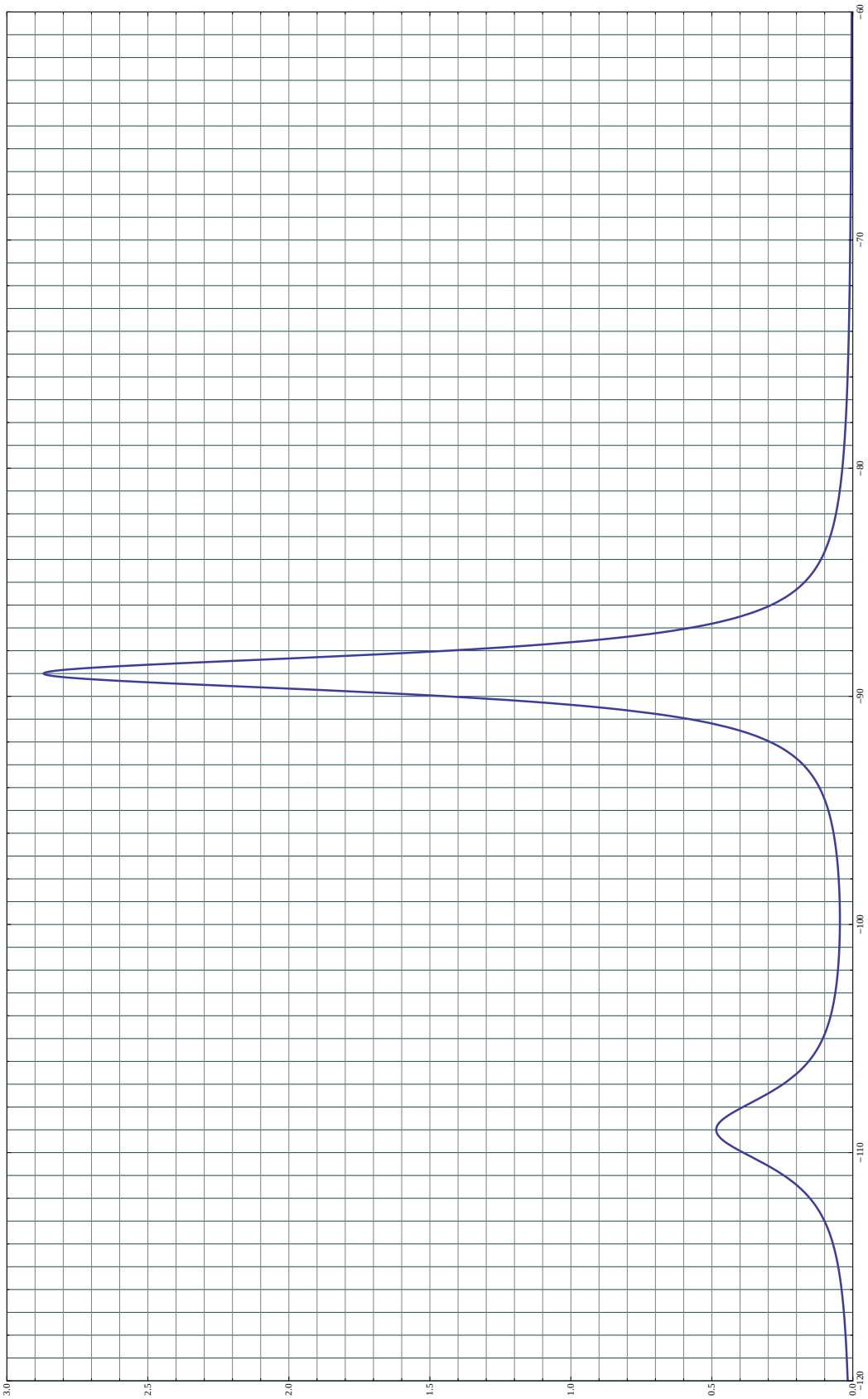
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