MATH 272, Homework 5, *Solutions*
Due March $9^{th}$

**Problem 1.** A rough model of a molecular crystal can be described in the following way. Take the scalar function

$$u(x, y) = \cos^2(x) + \cos^2(y).$$

This function $u(x, y)$ describes the *potential energy* for electrons in the crystal. Electrons are attracted to the areas with the smallest potential energy and move away from areas of high potential energy.

(a) Plot this function and include a printout. Notice what this looks like. You can imagine that each of the low points (well) is where a nucleus is located in the crystal.

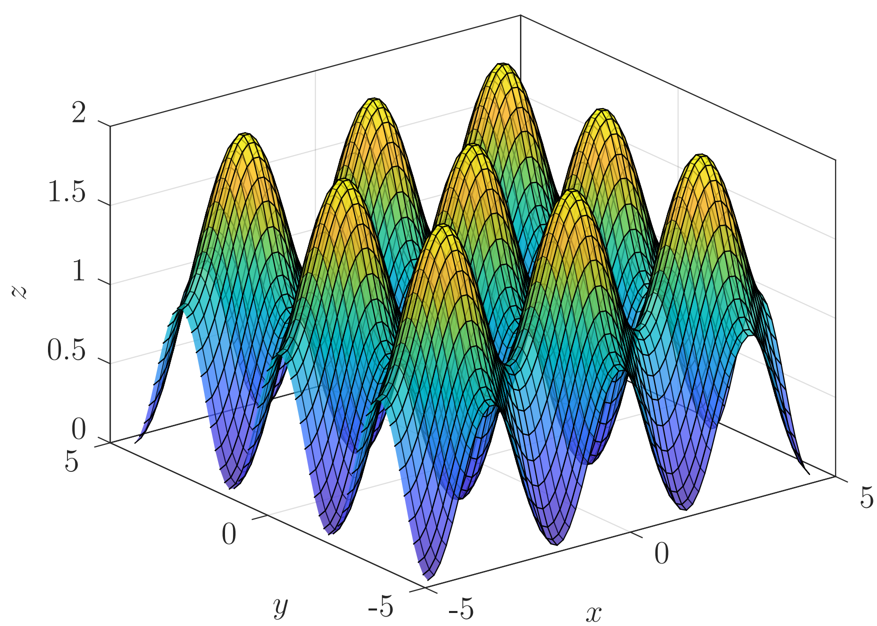
(b) Plot the level curves where $u(x, y) = 0$, $u(x, y) = \frac{1}{4}$, $u(x, y) = \frac{1}{2}$, and $u(x, y) = 1$ for the range of values $-\frac{3\pi}{2} \leq x \leq \frac{3\pi}{2}$ and $-\frac{3\pi}{2} \leq y \leq \frac{3\pi}{2}$. Picking the constant for the level curve tells you the *kinetic energy* of the electron you are looking at. It turns out that electrons (roughly) will orbit along these level curves. Notice, some level curves bleed into the different troughs of neighboring molecules which means that electrons of sufficient energy happily flow through the crystal. For what energy values do the electrons move throughout the whole crystal?

(c) Find the gradient of this function $\vec{\nabla} u(x, y)$.

(d) At what point(s) is the gradient zero? *Hint: Use your graph of the level curves to help.*

**Solution 1.**

(a) Here is the plot



(b) Here is the plot of the level curves.

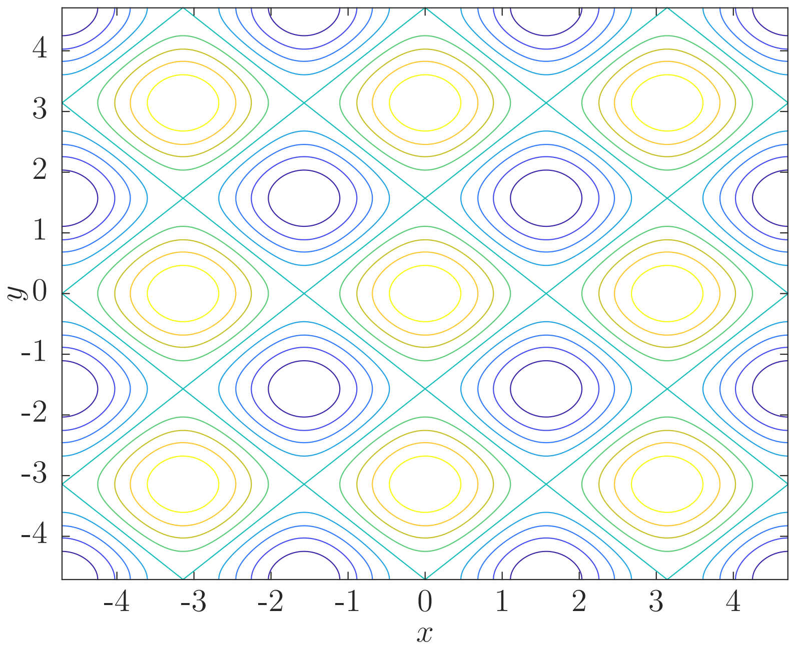



Figure 1: Contour plot labeled with relevant values. Colors match the colors in the previous figure.

(c) The gradient is

$$\vec{\boldsymbol{\nabla}} u(x,y) = \begin{pmatrix} -2\cos(x)\sin(x) \\ -2\cos(y)\sin(y) \end{pmatrix}.$$

(d) We want to find where

$$\vec{\boldsymbol{\nabla}} u(x,y) = \vec{\mathbf{0}}.$$

This gives us two equations to work with:

$$-2\cos(x)\sin(x) = 0, \tag{1}$$
$$-2\cos(y)\sin(y) = 0. \tag{2}$$

Note that (1) is zero whenever $\cos(x)$ or $\sin(x)$ is zero, which happens at $x = \frac{n\pi}{2}$ for all integers $n$. Similarly, we have that (2) is zero when $y = \frac{m\pi}{2}$ for all integers $m$. This gives us many different solutions in our given range of values.

If we think graphically, these values where the gradient is zero occur at the tops and bottoms of the peaks and valleys respectively. These are the maxima and minima of the function $u(x,y)$.

However, not all of these solutions are solutions where the electrons will want to stay put. We will have to work harder to find out which ones are minimizers of the energy!

**Problem 2.** Consider the function

$$f(x, y) = \sin\left(\frac{2\pi x}{5}\right)\sin\left(\frac{2\pi y}{5}\right).$$

comes up when you want to find out how a square shaped drum head will vibrate when hit.

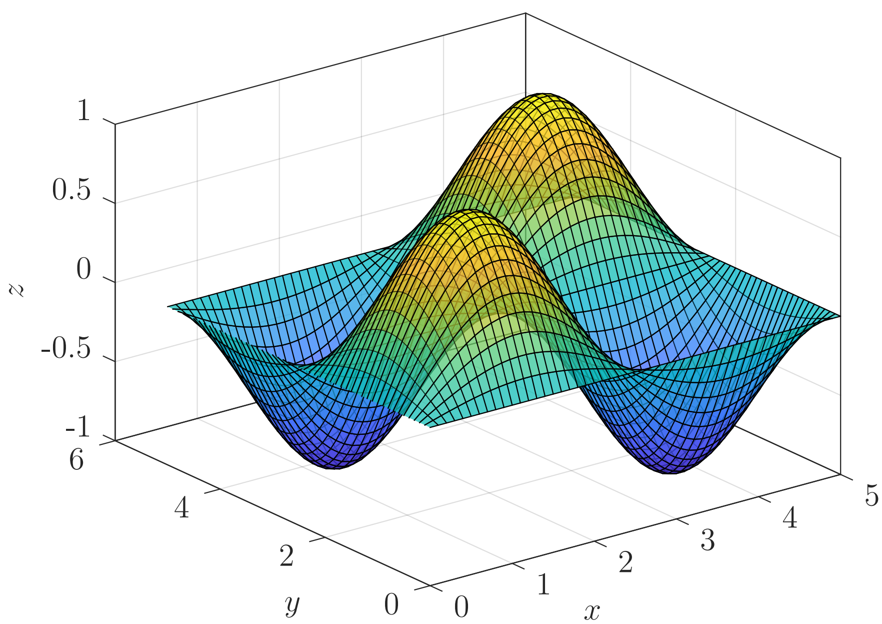
(a) Plot this function on the region $\Omega$ given by $0 \le x \le 5$ and $0 \le y \le 5$.

(b) What is the value the function $f(x, y)$ on the boundary of the given region $\Omega$ (i.e, when $x = 0$, $x = 5$, $y = 0$, and $y = 5$)?

(c) Show that $f(x, y)$ is an eigenfunction of the Laplacian $\Delta$. That is, $\Delta f = \lambda f$ for some eigenvalue $\lambda$. What is the eigenvalue?

**Solution 2.**

(a) Here is the plot of the vibrating square drum head:




(b) When $x = 0$ we have

$$f(0, y) = \sin\left(\frac{2\pi 0}{5}\right)\sin\left(\frac{2\pi y}{5}\right) = 0.$$

Similarly, when $x = 5$ $f(5, y) = 0$, when $y = 0$ $f(x, 0) = 0$, and when $y = 5$ $f(x, 5) = 0$.

These are the boundary of the drum head. That is, where the head of the drum is clamped down.

(c) We have

$$
\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{2\pi}{5}\cos\left(\frac{2\pi x}{5}\right)\sin\left(\frac{2\pi y}{5}\right), \\
\frac{\partial^2 f}{\partial x^2} &= \frac{-4\pi^2}{25}\sin\left(\frac{2\pi x}{5}\right)\sin\left(\frac{2\pi y}{5}\right), \\
\frac{\partial f}{\partial y} &= \frac{2\pi}{5}\sin\left(\frac{2\pi x}{5}\right)\cos\left(\frac{2\pi y}{5}\right), \\
\frac{\partial^2 f}{\partial y^2} &= \frac{-4\pi}{25}\sin\left(\frac{2\pi x}{5}\right)\sin\left(\frac{2\pi y}{5}\right).
\end{aligned}
$$

Then we have

$$
\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = -\frac{8\pi^2}{25}\sin\left(\frac{2\pi x}{5}\right)\sin\left(\frac{2\pi y}{5}\right) = -\frac{8\pi^2}{25} f(x,y).
$$

So, the way a drum head vibrates is an eigen-problem.

**Problem 3.** Consider the following vector field

$$\vec{\boldsymbol{E}}(x,y,z) = \begin{pmatrix} \frac{x}{(x^2+y^2+z^2)^{3/2}} \\ \frac{y}{(x^2+y^2+z^2)^{3/2}} \\ \frac{z}{(x^2+y^2+z^2)^{3/2}} \end{pmatrix},$$

which models the electric field of an proton (in units of of charge $q=1$) placed at the origin.

(a) Show that $\vec{\boldsymbol{E}}(x,y,z) = -\vec{\boldsymbol{\nabla}}V(x,y,z)$ where $V(x,y,z) = \frac{1}{\sqrt{x^2+y^2+z^2}}$. We refer to $V(x,y,z)$ as the electrostatic potential or voltage.

(b) Let $\Omega$ be a box with side lengths two centered at the origin. Compute the total flux of $\vec{\boldsymbol{E}}$ through the surface of the box $\Sigma$. That is,

$$\int_\Gamma \vec{\boldsymbol{E}}(x,y,z)\cdot\hat{\boldsymbol{n}}d\Sigma.$$

(c) Does the total flux depend on the size or shape of the box?

(d) Using the provided argument, one can compute

$$\int_\Omega \vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{E}}(x,y,z)d\Omega.$$

- Compute $\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{E}}$ and note that this is zero everywhere except at $(x,y,z)=(0,0,0)$.
- Note that the two integrals in this problem are equal. This is known as the *divergence theorem* and it is a special case of a more general theorem called *Stokes' theorem* which generalizes the fundamental theorem of calculus. Hence, you can now argue why

$$\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{E}} = 4\pi\delta(x,y,z),$$

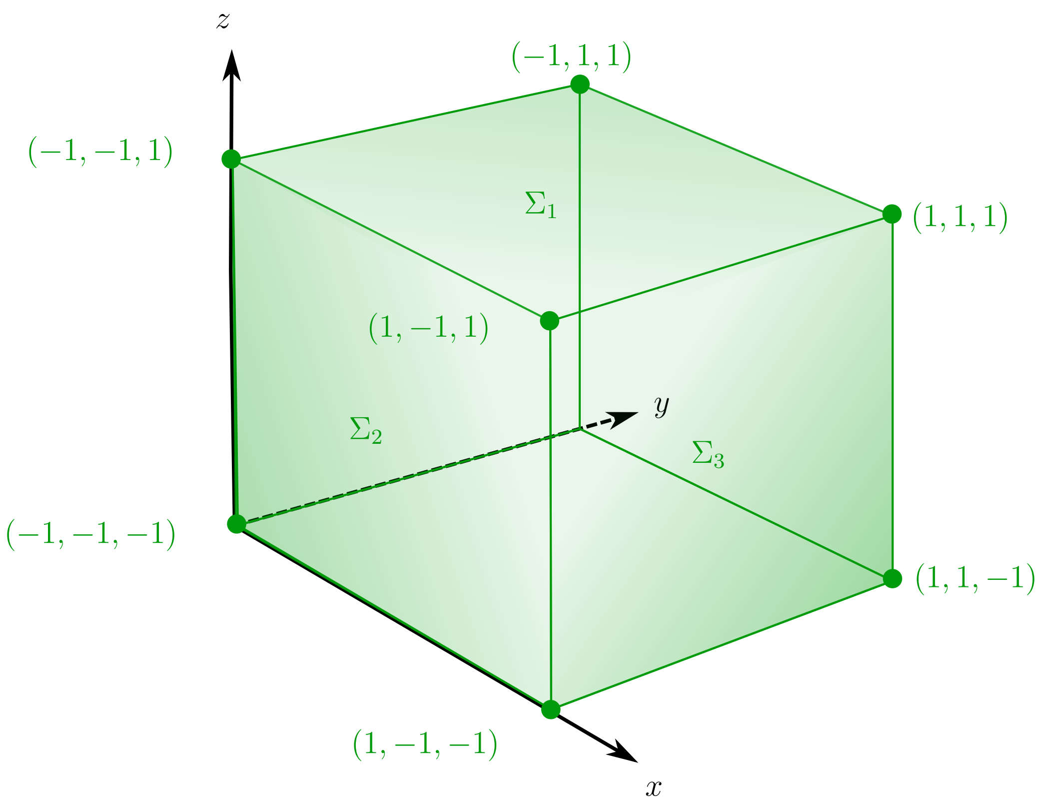
where $\delta(x,y,z)$ is the 3-dimensional Dirac delta.

**Solution 3.** (a) We compute $-\vec{\boldsymbol{\nabla}}V$,

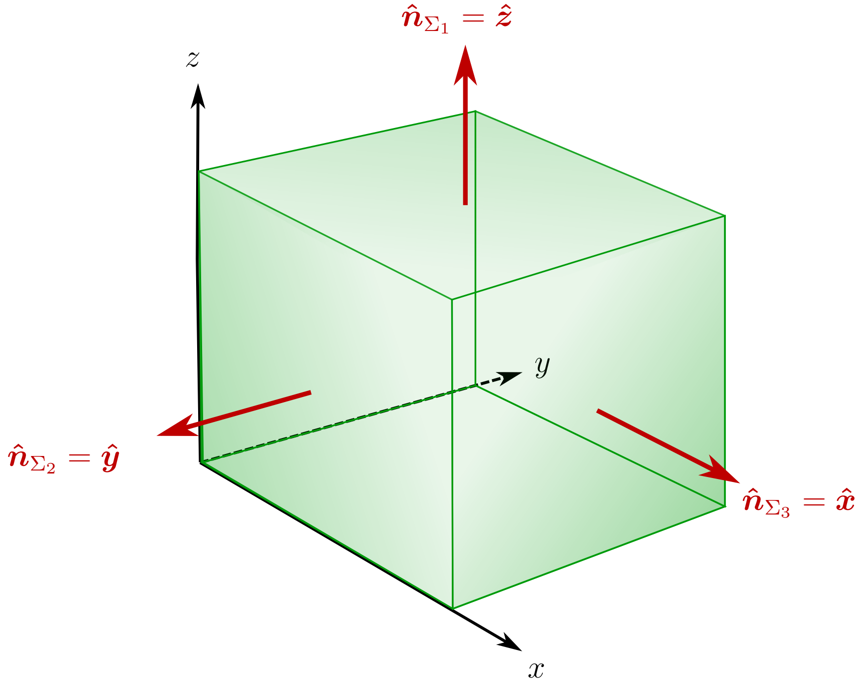
$$\begin{aligned} -\vec{\boldsymbol{\nabla}}V &= \begin{pmatrix} -\frac{\partial V}{\partial x} \\ -\frac{\partial V}{\partial y} \\ -\frac{\partial V}{\partial z} \end{pmatrix} \\ &= \begin{pmatrix} \frac{x}{(x^2+y^2+z^2)^{3/2}} \\ \frac{y}{(x^2+y^2+z^2)^{3/2}} \\ \frac{z}{(x^2+y^2+z^2)^{3/2}} \end{pmatrix}. \end{aligned}$$

(b) This portion requires computing six different (however, symmetric) integrals. One can reduce the argument down to a single integral via a bit of physical/mathematical reasoning. Note that the field $\vec{\boldsymbol{E}}$ is radially symmetric in that the field points radially outward from the origin and the strength falls off as we move away from the origin. Fundamentally, this means that each face of the cube receives the same amount of flux through it.

Picture the situation as follows. We have the cube surface broken up into 6 faces. We will label these faces as $\Sigma_1$, $\Sigma_2, \ldots, \Sigma_6$.




One can take $\Sigma_4$, $\Sigma_5$, and $\Sigma_6$ to be the faces opposite to $\Sigma_1$, $\Sigma_2$ and $\Sigma_3$ respectively. Each face then has a unique outward normal vector which we can denote by $\hat{\boldsymbol{n}}_{\Sigma_j}$ for the face $\Sigma_j$.




Thus, our integral over the cubic surface $\Sigma$ is given by

$$\iint_{\Sigma} \vec{\boldsymbol{E}} \cdot d\Sigma = \sum_{j=1}^{6} \iint_{\Sigma_j} \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}}_{\Sigma_j} d\Sigma_j.$$

By the symmetry argument before, we can simplify this further as

$$\iint_{\Sigma} \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}} d\Sigma = 6 \iint_{\Sigma_1} \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}}_{\Sigma_1} d\Sigma_1.$$

Now, we can evaluate this integral

$$\begin{aligned}
6 \iint_{\Sigma_1} \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}}_{\Sigma_1} d\Sigma_1 &= \int_{-1}^{1} \int_{-1}^{1} \vec{\boldsymbol{E}}(x, y, 1) \cdot \hat{\boldsymbol{z}} dx dy \\
&= 6 \int_{-1}^{1} \int_{-1}^{1} \frac{1}{(x^2 + y^2 + 1)^{3/2}} dx dy \\
&= 6 \int_{-1}^{1} \frac{2}{(y^2 + 1)\sqrt{y^2 + 2}} dy \\
&= 6 \frac{2\pi}{3} \\
&= 4\pi.
\end{aligned}$$

Note that the divergence of $\vec{\boldsymbol{E}}$ is zero everywhere aside from the origin. Hence, the only possible source of flux comes from the origin and our previous argument discussed the symmetry of this field. So long as we integrate in a surface that encloses the origin, we will have the same answer. This leads us to (d).

We have already computed $\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}}$ and noted this in an earlier problem. It's now very physically reasonable to suspect that we have the following identity

$$\int_{\Omega} \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}} d\Omega = \int_{\Sigma} \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}} d\Sigma,$$

since the amount of "source behavior" in the region $\Omega$ should directly correspond to the flux that will pass through the boundary. To picture this literally, if we pump in water at $(0,0,0)$, we know how much water we pumped in by seeing how much flows through any surface surrounding the origin.

Thus, our argument is that

$$\int_{\Omega} \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}} d\Omega = 4\pi.$$

Now, $\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}}$ is zero aside from at $(x,y,z) = (0,0,0)$, and thus $\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}}$ must mimic the Dirac delta by being infinite at the origin (which we observed previously). Hence, we conclude that

$$\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}} = 4\pi\delta(x,y,z).$$

Furthermore, if we relate this to the Maxwell equation for the electric field $\vec{\boldsymbol{E}}$ due to a charge distribution $\rho(x,y,z)$, i.e.,

$$\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}} = \rho/\epsilon_0,$$

we see that a point charge corresponds to a distribution $\delta(x,y,z)$ times some constant.