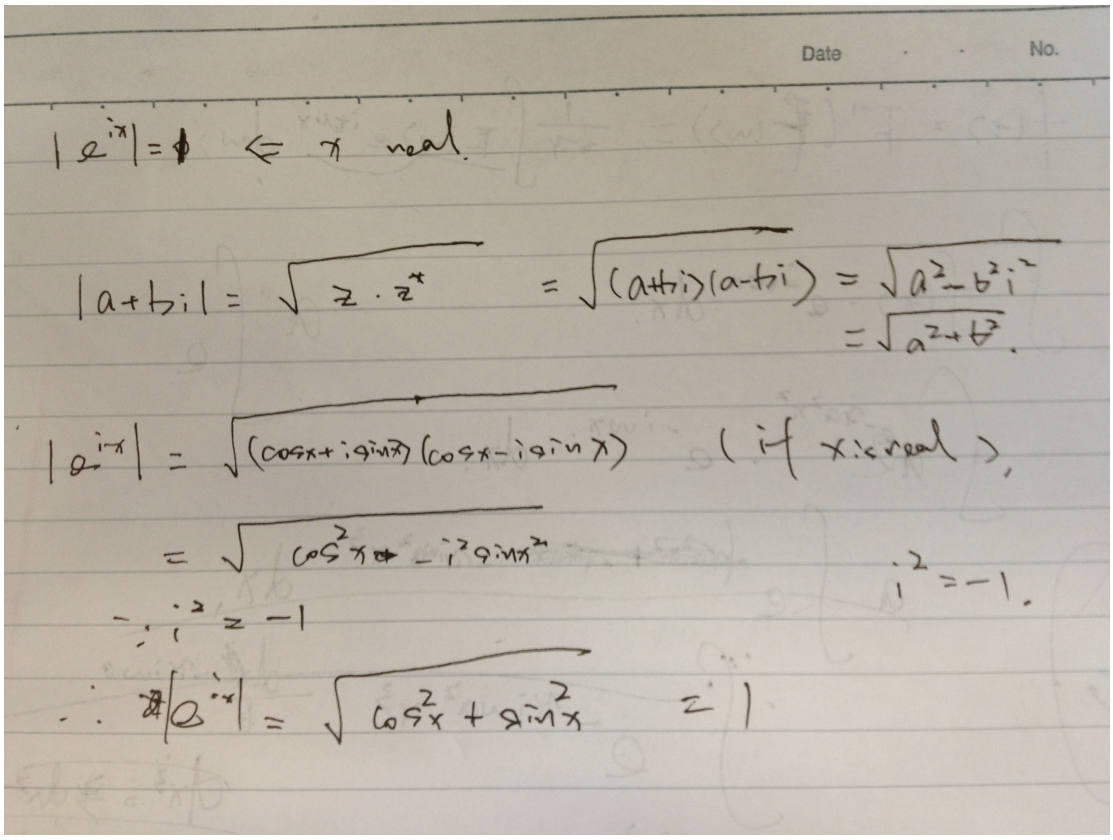
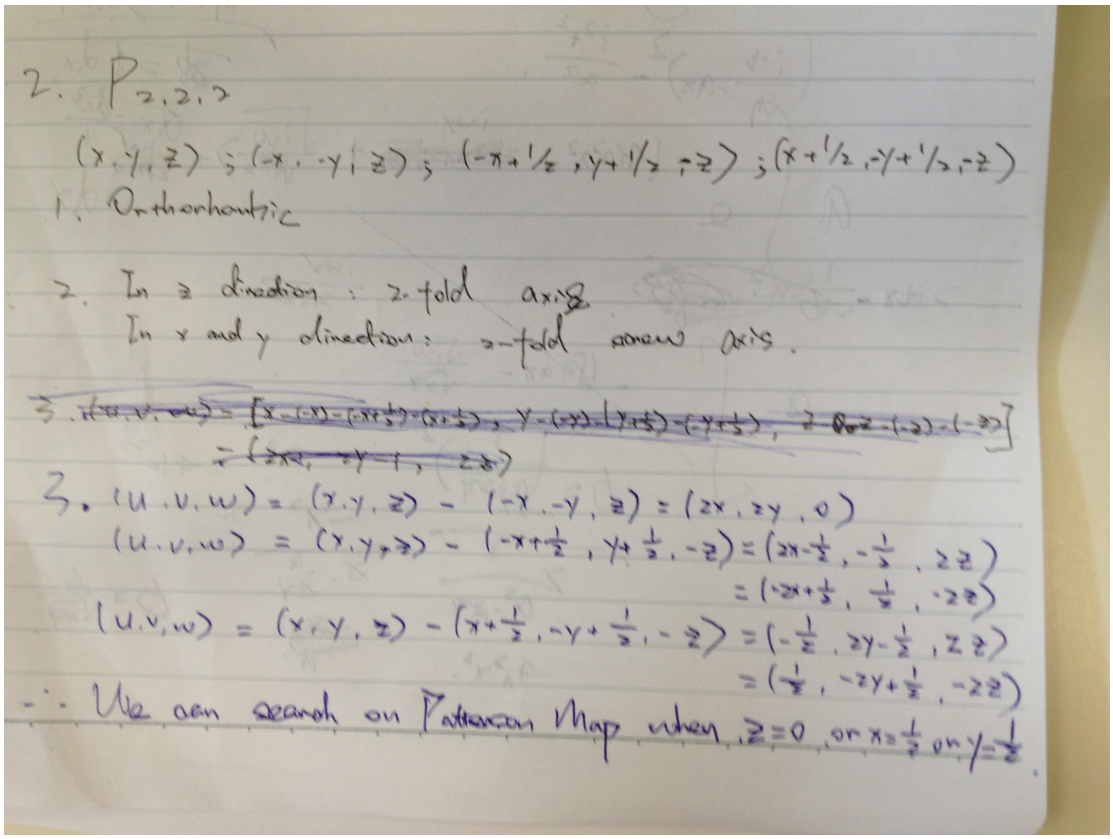
1.


Date
No.
$|e^{ix}| = 1 \Leftarrow x$ real.
$|a+bi| = \sqrt{z \cdot z^*} = \sqrt{(a+bi)(a-bi)} = \sqrt{a^2 - b^2 i^2}$
$= \sqrt{a^2+b^2}$.
$|e^{ix}| = \sqrt{(\cos x + i \sin x)(\cos x - i \sin x)}$ (if x: real),
$= \sqrt{\cos^2 x - i^2 \sin^2 x}$
$i^2 = -1$.
$\therefore i^2 = -1$
$\therefore |e^{ix}| = \sqrt{\cos^2 x + \sin^2 x} = 1$

2.


2. $P_{2,2,2}$
(x,y,z); $(-x,-y,z)$; $(-x+1/2, y+1/2, z)$; $(x+1/2, -y+1/2, -z)$
1. Orthorhombic
2. In z direction: 2-fold axis
In x and y direction: 2-screw axis.
3. $(u,v,w) = (x,y,z) - (-x,-y,z) = (2x, 2y, 0)$
$(u,v,w) = (x,y,z) - (-x+\frac{1}{2}, y+\frac{1}{2}, -z) = (2x-\frac{1}{2}, -\frac{1}{2}, 2z)$
$= (-2x+\frac{1}{2}, \frac{1}{2}, -2z)$
$(u,v,w) = (x,y,z) - (x+\frac{1}{2}, -y+\frac{1}{2}, -z) = (-\frac{1}{2}, 2y-\frac{1}{2}, 2z)$
$= (\frac{1}{2}, -2y+\frac{1}{2}, -2z)$
$\therefore$ We can search on Patterson Map when $z=0$ or $x=\frac{1}{2}$ or $y=\frac{1}{2}$.

3.

The protein chosen: **Cytochrome P450cam (EC: 1.14.15.1)**

2LQD: NMR

2ZWT: X-ray Crystallography

Summary:

Cytochrome P450 is a family of enzymes for detoxification by adding oxygen to them, and destroying the unusual chemicals, like drugs. It exists in almost all organisms. Here, I choose the best-studied cytochrome p450 enzyme, cytochrome p450cam, which adds oxygen to camphor to detoxify it. 2LQD and 2ZWT are two recently studied structures by respectively NMR an X-ray crystallography. Similarities and differences are shown as following.

The overall secondary structures of these two models are similar. Both involve lots of α-helices in the middle of its structure. Also the major mechanisms of these two structures are also similar.

There are might be some differences between these two. The first one is x-ray crystallography is great to use in a position that a substrate or ligand is added because it's a fixed method. NMR structure is great to measure the structure in a solution and determine the conformational change in it because of its vibration.

http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2635880/?tool=pubmed

4.

a.

Single amino acid's side chain error might affect the original structure amplitudes, but it will not affect the final structure amplitudes after refinement is done. Commonly, A small number of structure amplitudes errors will not affect the overall structure amplitudes, because small errors can be refined by some refinement tools.

b.

There are multiple refinement data. For example, we can take 5-10% of your structure amplitudes out of the refinement list. Then we use the other 90-95% of the structure amplitudes in modifying the model to fit the observed data. We do this process repeatedly. If errors are little, it always can be excluded eventually, which proves that a small amount of error will not affect the structure.

5.

As to experimental phasing like (MIR and MAD) to determine the structure of protein N, the isomorphism is the greatest advantage. That means a single sample is used in the experiment. Unit cells will change because of radiation if we measure one sample first, and measure anther later. Thus every cell is identical and molecule is in the sample place within that unit cell, partly compensating for the low S/N, and lowering the occurrence of errors. The disadvantage might be that it is so complicated and heavy, requiring lots of lab and computational work. As to molecular replacement using protein M as a search model, the greatest advantage is saving the time and effort. There is no need to do experimental job and prepare heavy atom derivatives, which is much more simplified than experimental phasing. The disadvantage might be the

inability to correct errors in model, which is greater with molecular replacement than with experimental phasing. The errors might occur at the starting point, (i.e. The reference structure we assume homologous might have some great differences in some way, which could lead to great errors.)

6.
12 different parameters: 1.Slide, 2.Rise, 3.Shift, 4.Twist, 5.Rol, 6.Til, 7.Stagger, 8.Stretch, 9.Shear, 10.Buckle, 11.Propellen twist, 12.Opening
The first three base pair models illustrate that base pairs do not exactly cross the center of the helix as the same way, and some might move a little bit away from average. The next three base pair model illustrates that base pairs are not equally parallel with each other. The last six base pairs illustrates that base pairs may not necessarily in a planar, and H-bonds may not necessarily line up.

7. This single long-space repeat distance is 38.7nm.
It comes from troponin bridges between thick and thin filaments to transmit force.
In contracting muscle diffracting pattern, the two repeat should also be the same distance. The distance of Actin LLs should be a little longer, and the distance of Myosin LLs should be a little shorter, which means Actin LLs and Myosin LLs move toward to each other.

8.
The summary is arranged from faster time scales to longer time scales.
The first computational tool in characterizing biological structure is quantum models (Quantum Monte Carlo, Post Hartee-Fock, Kolus-Shan DFT), and the time scale is around picoseconds. This tool deserves quantum approach and simulates system with quantum mechanics.
The next one is Atomic models (explicit solvent & implicit solvent), and the time scale is around microseconds. In this model, we get structures at atomic levels, like atoms in amino acid can be discerned in this model.
Coarse-grained and mean-field models have a time scale around milliseconds. The difference between this model and atomic model is that fewer parameters were given in this model than in the atomic model.
Then we get the mechanic model whose time scale is around seconds. This model treats the whole amino acid as the manipulating factor and offers statistical data for motion.
The final model is kinetic model whose time scale is around hours. We can see fold and unfold in this time scale of model.

It’s very difficult to watch long scale structure like protein fold directly in a very quick time, if we use this computational tool to model our structure. So we need to derive the structure from faster time scale to longer time scale. First, we model a faster time scale and measure the structure of the longer time scale. Next, we calibrate the results of modeling based on the experimental data on the higher length scale.

Then, we can calibrate the next time scale model according to this approach. These steps could be repeated from nanoseconds to hours. Then we get the longer time scal model of the structure.

9.