PROBLEM SET SOLUTIONS

CHAPTER 1, Levine, *Quantum Chemistry,* 5^{th} Ed.

1.12 Which of the following functions meet ALL the requirements of a probability density function (a & b are positive constants)?

The requirements for a probability density function (i.e. $|\psi|^2$) are that it is normalized (i.e. $\int_{-\infty}^{\infty}|\psi|^2\, dx = 1$), real (i.e. , $|\psi|^2$ is real) & non-negative (i.e. $|\psi|^2$ is non-negative). Do these functions meet the above conditions?

(a) No - e^{iax} is not real

(b) No - x $\exp(-bx^2)$ can be negative

(c) No - exp $(-bx^2)$ is not normalized:

$$\int_{\infty}^{\infty} \exp(-bx^2)\, dx = 2 \int_0^{\infty} \exp(-bx^2)\, dx = 2\ (1/2)\ \mathrm{SQRT}\ ((\pi/b)) = \mathrm{SQRT}\ ((\pi/b))$$

1.22 Find the absolute value & phase of the following functions.

Use r = absolute value = $|z|$ = SQRT ($x^2 + y^2)^2$, $z = x + i y$, θ = phase, $\tan \theta = y/x$, $x = r \cos \theta$, $y = r \sin \theta$.

(a) $z = x + i y = i \Rightarrow x = 0, y = 1$. So $r = (0^2 + 1^2)^{(1/2)}$ = SQRT (1) = 1. $\tan \theta = y/x = 1/0 = \infty \Rightarrow \theta = 90^o = \pi/2$

(b) $z = x + i y = 2 \exp(i\pi/3) = 2 [\cos \pi/3 + i \sin \pi/3] = 2 (1/2 + i$ SQRT(3)/2) $\Rightarrow x = 1, y =$ SQRT(3). So $r = (1 + 3)^{(1/2)} = (4)^{(1/2)} = |2|$. $\tan \theta =$ SQRT(3)/(1) = SQRT(3) $\Rightarrow \theta = \pi/3$

(c) (c) $z = x + i y = -2 \exp(i\pi/3) = -2 [\cos \pi/3 + i \sin \pi/3] = -2 (1/2 + i$ SQRT(3)/2) $\Rightarrow x = -1, y =$ -SQRT(3). So $r = (1 + 3)^{(1/2)} = (4)^{(1/2)} = |2|$. $\tan \theta =$ SQRT(3)/(1) = SQRT(3) $\Rightarrow \theta = \pi/3$

(d) $z = x + i y = 1 - 2i \Rightarrow x = 1, y = -2$. $r = (1^2 + (-2)^2)^{(1/2)}$ = SQRT (5), $\tan \theta = y/x = -2/1 = -2$, $\theta = \tan^{-1}(-2) = 296^o 27'$