Name:________________________ Date:____________

Time for Completion:____________

Honours QM HW #2

1. Using Dirac notation show that the trace of operators is cyclic; i.e. $\mathrm{Tr}\,(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}\,(\hat{B}\hat{C}\hat{A})$. Again, using Dirac notation, prove what $\sum_n \psi_n^*(\boldsymbol{x}')\,\psi_n(\boldsymbol{x}) = \delta(x - x')$, where $\psi_n(\boldsymbol{x}) = \langle \boldsymbol{x}|\psi_n\rangle$ in a CON basis $|\psi_n\rangle$.

2. Prove that the determinant of a unitary operator is in general a complex number of unit modulus. NB: $\det(\hat{A}\hat{B}) = \det(\hat{A})\,\det(\hat{B})$. You may do this in a vector space in which your operator can be explicitly represented by a matrix. In that case it is useful to recall that for a matrix M $\det M^T = \det M$, where M^T is the transpose of M.

3. Prove that $\mathrm{Tr}\,(\hat{A})$ and $\det(\hat{A})$ is independent of the basis used to represent $\hat{A}$. Hint the determinant is cyclic, and these first few problems have a lot to do with unitary matrices...

4. Prove that if $\hat{A}$ is diagonalizable in some basis $|a_n\rangle$ then $\mathrm{Tr}\,(\hat{A}) = \sum_n a_n$, where a_n are the eigenvalues of $\hat{A}$. Show also that $\det(\hat{A}) = \prod_n a_n$ and

$$\det(\hat{A}) = \exp\Big(\mathrm{Tr}\,\big(\log(\hat{A})\big)\Big). \tag{1}$$

   Hint: for the last part first examine $\log\big(\det(\hat{A})\big)$.

5. Remember Problem 3 from HW Set 0? We're not done with it just yet. Suppose we have a linear combination of two stationary states at $t = 0$,

$$|\psi(\theta,\, t = 0)\rangle = c_1|n_1\rangle + c_2|n_2\rangle, \qquad n_1 \neq n_2, \tag{2}$$

   and where we have chosen to represent the orthonormal stationary states by

$$\langle\theta|n_i\rangle = \frac{1}{\sqrt{2\pi R}}e^{i\,n_i\,\theta}, \qquad n_i \in \mathbb{Z}. \tag{3}$$

   What is $|\psi(t)\rangle$? What are $P(n = n_1,\, t)$ and $P(n = n_2,\, t)$, the probabilities of measuring $n = n_1$ and $n = n_2$ as a function of time, respectively? Suppose for the moment that $c_1 = 0$; what is $\langle\hat{\theta}\rangle(t)$? Similarly for $c_2 = 0$. Compute $\langle\hat{\theta}\rangle$ for general c_i and see that a nontrivial t dependence emerges (make sure your answer for general c_i reduces to the results you found when an individual $c_i = 0$).

6. Demonstrating the acausality of the non-relativistic Schroödinger Equation. Suppose you have a free particle of mass m whose wavefunction is localized at $t = 0$ such that

$$\psi(x,\, t\, =\, 0) = \frac{1}{\sqrt{a}}\theta\left(a/2 - x\right)\theta\left(a/2 + x\right). \tag{4}$$

(Note #1 (interesting but not necessarily useful for solving the problem): notice that $\theta(x) = \int_{-\infty}^{x} dx'\delta(x')$.)

(Note #2: we could have done something more "realistic" in this problem like starting with the particle in an infinite square well for $t < 0$ and then suddenly removing the potential at $t = 0$. In the end, one finds again acausality, but the results are much more messy mathematically than what we will find below.)

(a) Show that, assuming $x \gg a$,

$$\psi(x,\, t) \simeq \sqrt{\frac{t}{\pi\, a\, m}}\frac{1-i}{x}\sin\left(\frac{m\, a\, x}{2t}\right)e^{i\, m\, x^2/2\, t}. \tag{5}$$

Find $|\psi(x\, t)|^2$ for this approximation. Clearly for any $t > 0$ there is a nonzero probability of finding the particle for in any interval $x + dx$!

Note that if you find yourself with an intermediate expression that looks like

$$\psi(x,\, t) = \frac{1}{\sqrt{a}}\int_{-\infty}^{\infty} dp\, e^{-i\frac{p^2}{2m}t}\, e^{i\, p(x-x')}\frac{\sin(a\, p/2)}{p}, \tag{6}$$

then you may be in possession of a correction expression but one that might not lead you to the answer most easily...

(b) Now solve the problem exactly, finding that

$$\psi(x,\, t) - \frac{1}{2\sqrt{a}}\left[\operatorname{erf}\left(\frac{1-i}{4}\sqrt{\frac{t}{m}}(a-2x)\right) + \operatorname{erf}\left(\frac{1-i}{4}\sqrt{\frac{t}{m}}(a+2x)\right)\right], \tag{7}$$

where $\operatorname{erf}(x)$ is the error function, the integral of the Gaussian distribution,

$$\operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}}\int_0^x dt\, e^{-t^2}. \tag{8}$$

Remember that once you have a solution in terms of a definite integral you are free to quote the result of canned software (so long as you cite your source!).

(c) Using your favorite mathematical software, plot $|\psi(x,\, t)|^2$ from Eq. (7) for $a = m = 1$ and $t = 0.001$. Note the rapid oscillations that peak near $a/2 = 1/2$. This oscillatory peaking is a general result in expanding in a complete Fourier basis known as Gibbs' Phenomenon. Now make a new graph and plot both $|\psi(x,\, t)|^2$ from Eq. (5) and Eq. (7) keeping $a = m = 1$; make one graph for $t = 0.1$ (with x out to 5) and one for $t = 1$ (with x out to 20).

7. Suppose that we construct a system such that we have a static, constant magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ (where here the hat represents a unit vector as opposed to an operator), and at $t = 0$ we measure the electron to be polarized along the positive x-axis. What is the expectation value for the spin of the electron as a function of time for $t > 0$? I.e., what is $\langle\hat{\boldsymbol{S}}\rangle(t)$? The following might be useful:

   (a) The Hamiltonian for the coupling of spin to a magnetic field is

   $$\hat{H} = -\tilde{\omega}\hat{\boldsymbol{S}}\cdot\boldsymbol{B}, \tag{9}$$

   where $\tilde{\omega} = e/m_e$ in natural units.

   (b) The expansion of the state polarized along the positive x-axis in the basis of states polarized along the z-axis is

   $$|+,\, x\rangle = \frac{1}{\sqrt{2}}|+,\, z\rangle + \frac{1}{\sqrt{2}}|-,\, z\rangle. \tag{10}$$

   (c) In the basis of spinors aligned along the z-axis, $\{|+,\, z\rangle,\, |-,\, z\rangle\}$ $\hat{\boldsymbol{S}} = \boldsymbol{\sigma}/2$, where the σ_i are the Pauli matrices; i.e.,

   $$\langle i,\, z|\hat{S}_j|k,\, z\rangle = \frac{1}{2}\big(\sigma_j\big)_{i,k}. \tag{11}$$

   You should find that

   $$\langle\hat{\boldsymbol{S}}\rangle(t) = \left\langle\begin{pmatrix}\hat{S}_x\\ \hat{S}_y\\ \hat{S}_z\end{pmatrix}\right\rangle(t) = \begin{pmatrix}\frac{1}{2}\cos\omega t\\ \frac{1}{2}\sin\omega t\\ 0\end{pmatrix} \tag{12}$$

Bonus

1. Let's investigate the Gibbs Phenomenon for the free particle on a circle. Suppose that

   $$\psi(\theta) = \frac{1}{\sqrt{a\,R}}\theta(a/2+\theta)\theta(a/2-\theta), \tag{13}$$

   and we choose as our basis states $|n,\, j\rangle$ where

   $$\langle\theta|n,\, j\rangle = \frac{1}{\sqrt{\pi\,R}}\cos\big(n\,\theta - j\frac{\pi}{2}\big)\big[1 - \frac{1+\sqrt{2}}{2}\delta_{n,0}\big], \tag{14}$$

   $n \in \mathbb{N}$ and $j = 0$ or 1. Expand $\psi(\theta)$ in the above basis. Define $\psi_m(\theta)$ as the function given by the series expansion of $\psi(\theta)$, Eq. (13), truncated after $m+1$ terms. Plot on one graph for $\theta \in [-\pi,\, \pi]$ your results for the original $\psi(\theta)$, Eq. (13), and your $\psi_m(\theta)$ when you take $m = 0,\, 1,\, 5,\, 50$.

2. Explicitly evaluate the sum you found in the previous problem to recover the original wavefunction.