CHEM442-001
College of Charleston
Spring 1999
Exam II

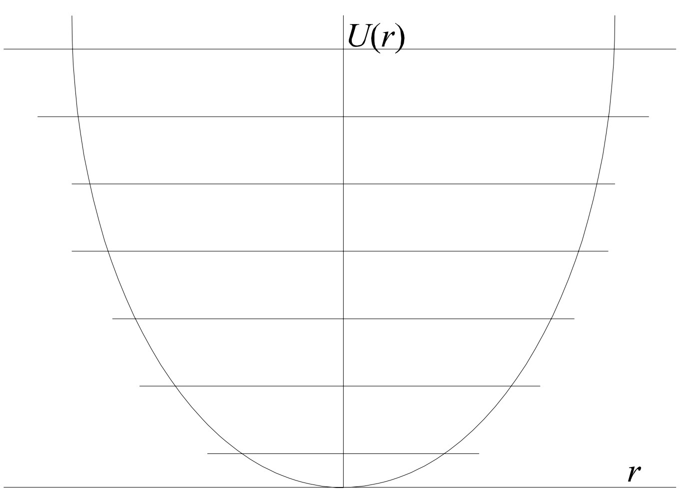
1(10). Name/identify each of the mathematical representations. The first one is an example.

$g_J = (2J + 1)$	degeneracy of rotational energy level
$\phi = \mu_1\mu_2\cdots$ where μ_i are 1-electron wave functions	_______________ trial wave function
$\dfrac{Z_a Z_b e^2}{(4\pi\epsilon_o)r_{ab}} \approx$ *constant* where a and b are nuclei	_______________ approximation
$E_\phi \geq E_\psi = E_{\text{experimental}}$	_______________ method
$\begin{vmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} & H_{13} - ES_{13} \\ H_{21} - ES_{21} & H_{22} - ES_{22} & H_{23} - ES_{23} \\ H_{31} - ES_{31} & H_{32} - ES_{32} & H_{33} - ES_{33} \end{vmatrix} = 0$	_______________ determinant
$\psi_{\text{total}} = \psi_{\text{center of mass}}\,\psi_{\text{internal}}$ and $E_{\text{total}} = E_{\text{center of mass}} + E_{\text{internal}}$	______________________________

2(15). Derive the normalized eigenfunction for a rigid rotator with $J = 1$ and $m = \pm 1$. Show all work in determining the normalization constant and the associated Legendre function.

3(25). Gaseous NaCl exists as a diatomic molecule held together by a rather weak polar covalent bond. Given the vibrational "frequency" $\bar{\nu}_o = 276\ \text{cm}^{-1}$, calculate N_1/N_0 at 1000 K.

Sketch $\psi^*\psi$ for $v = 4$ on the diagram.



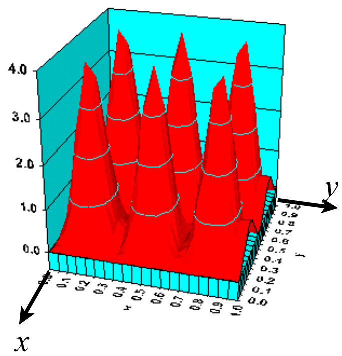
4(50). A particle is confined to a two-dimensional box in the xy plane. The mass of the particle is m and the lengths of the sides of the box are $0 \leq x \leq a$ and $0 \leq y \leq b$.

A) Write the hamiltonian operator for this system. There is no potential energy to consider. Write out the expression for the del-squared operator.

B) Based on our study of particles in one- and three-dimensional boxes, write the wave function that is used to describe this system.

C) Identify the quantum numbers corresponding to the sketch of probability given by the P-Chem cd program.

$n_x =$ $n_y =$



D) Based on our study of particles in one- and three-dimensional boxes, write the general energy expression.

Rewrite this expression in terms of $E/(h^2/8ma^2)$ for a square in which $a = b$.

Rewrite this expression in terms of $E/(h^2/8ma^2)$ for a rectangle in which $a = 2b$.

Calculate the following nine energy states, in terms of $E/(h^2/8ma^2)$, for both the square and rectangle and put your answers in the table below. Plot these energies on the graph paper provided to generate a "correlation diagram".

$n_x =$	$n_y =$	$E/(h^2/8ma^2)$ for square	$E/(h^2/8ma^2)$ for rectangle
1	1		
1	2		
1	3		
2	1		
2	2		
2	3		
3	1		
3	2		
3	3		