MATH 261, Spring 2001 **Due Date:**_____ **Name(s):** _____

Honors Project 16: The Shape of Atomic Orbitals

Certain functions are known to describe the shapes of atomic orbitals, which are building blocks for describing the electron charge clouds of atoms and molecules. The different types of shapes are distinguished by letters and numbers:

$l = 0$	s-orbital
$l = 1$	p-orbital
$l = 2$	d-orbital
$l = 3$	f-orbital
$\vdots$	$\vdots$

For each type there are $2l + 1$ subtypes. These are distinguished by a number m_l and its values range from $m_l = -l, \ldots, l$. Two formulas have been found that yield functions $P_l^{m_l}$ that describe the θ-dependence of orbital shapes; they are

$$P_l^0(z) = \frac{1}{2^l l!}\frac{d^l}{dz^l}\left((z^2-1)^l\right), \quad P_l^{m_l}(z) = (1-z^2)^{m_l/2}\frac{d^m}{dz^m}P_l^0(z).$$

After one finds these in terms of z, z is replaced by $\cos\theta$ (θ is one of the usual spherical coordinates ρ, θ, ϕ, and ranges in value from 0 to π).

Problems:

1. Find $P_l^{m_l}(\cos\theta)$ for $l = 0$ to $l = 3$, including all appropriate choices of m_l.
2. Find the nodal structure. (That is, as θ varies from 0 to π, at how many places does each function take on a value of zero?)
3. Evaluate the overlap of any two of the functions. That is, find

$$\int_0^\pi P_l^{m_l}(\cos\theta)P_{l'}^{m_{l'}}(\cos\theta)\sin\theta d\theta.$$

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