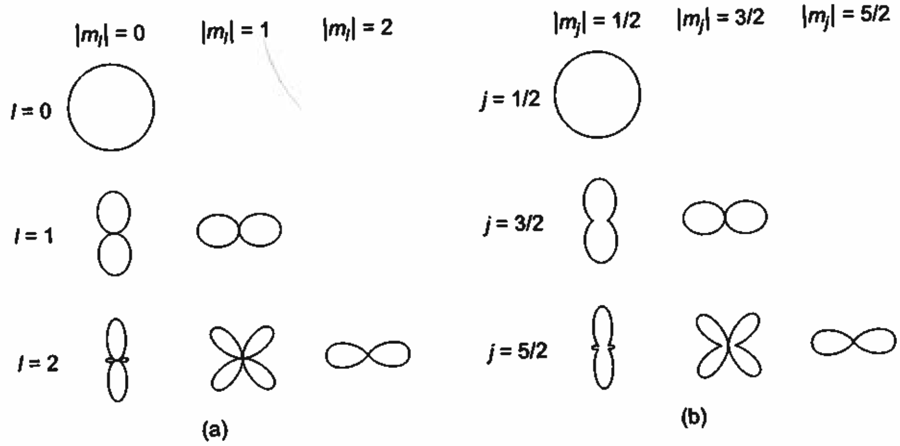

Figure 7.1 Polar density plots of (a) nonrelativistic orbitals and (b) relativistic 2-spinors

depend on j and not on ℓ. Thus $s_{1/2}$ and $p_{1/2}$ 2-spinors are *both* spherical. A relativistic filled shell also has a spherical density; for example, the ground state of the Pb atom has the configuration $6p^2$, which in a nonrelativistic scheme would have ^3P symmetry and components whose density looks like that of a p function, but in a relativistic scheme the configuration is $6p_{1/2}^2$, which has $J = 0$ and a spherical density.

Another feature that emerges from these plots is the loss of nodal structure. Because the spin-up and spin-down components of each spinor have nodes in different places, the directional properties of the angular functions are smeared out compared with the properties of the nonrelativistic angular functions. Only for the highest m value does the spinor retain the nodal structure of the nonrelativistic angular function, and that is because it is a simple product of a spin function and a spherical harmonic. The admixture of m_ℓ and $m_\ell + 1$ character approaches equality as ℓ increases and as m_ℓ approaches zero, resulting in a loss of spatial directionality. The implications of this loss of directionality for molecular structure could be significant, particularly where the structure is not determined simply from the molecular symmetry or from electrostatics.

7.3 Solutions of the Radial Dirac Equation

We now turn to the radial functions and the radial Dirac equation. Using (7.22) in (7.14) and (7.15) we arrive at the pair of coupled radial equations[2]

$$(V - E)P + c\left[\frac{\mathrm{d}Q}{\mathrm{d}r} - \frac{\kappa Q}{r}\right] = 0 \tag{7.27a}$$

$$-c\left[\frac{\mathrm{d}P}{\mathrm{d}r} + \frac{\kappa P}{r}\right] + (V - E - 2c^2)\, Q = 0. \tag{7.27b}$$

2. We omit the mass in this section, and work strictly in Hartree atomic units.