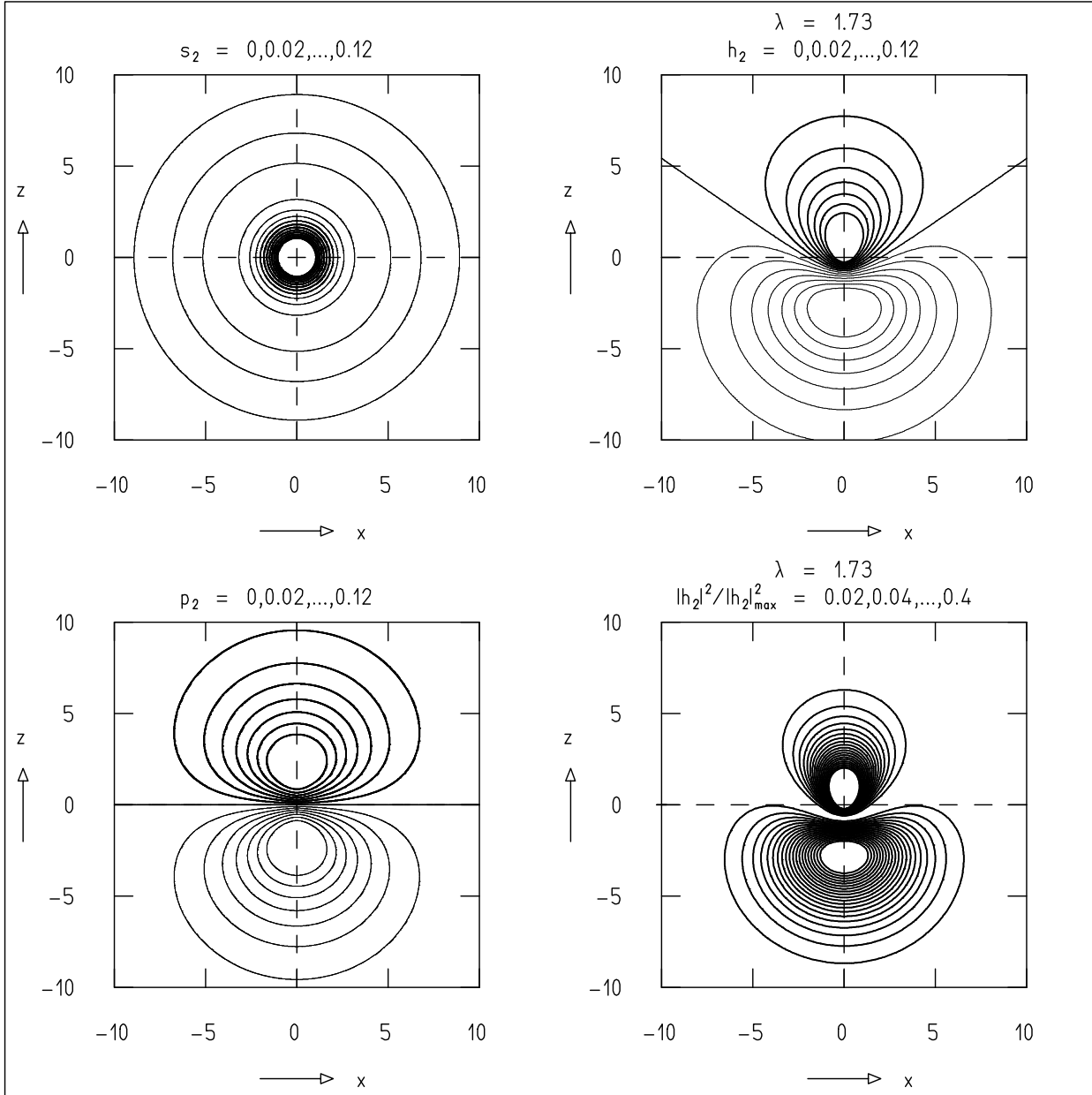
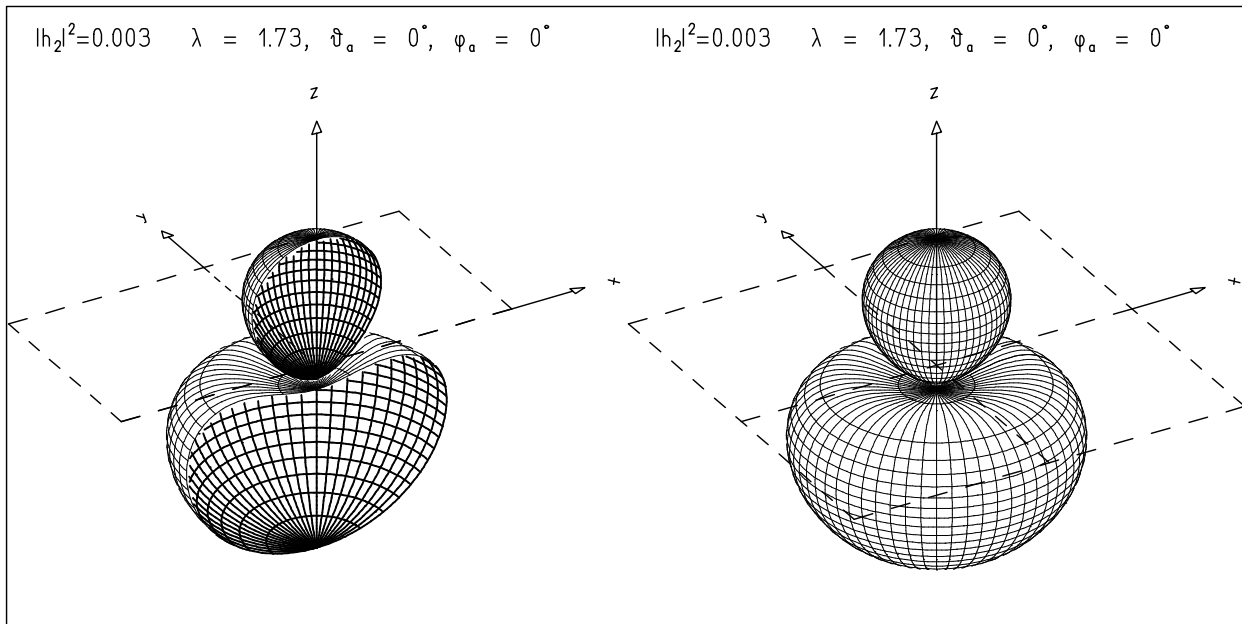


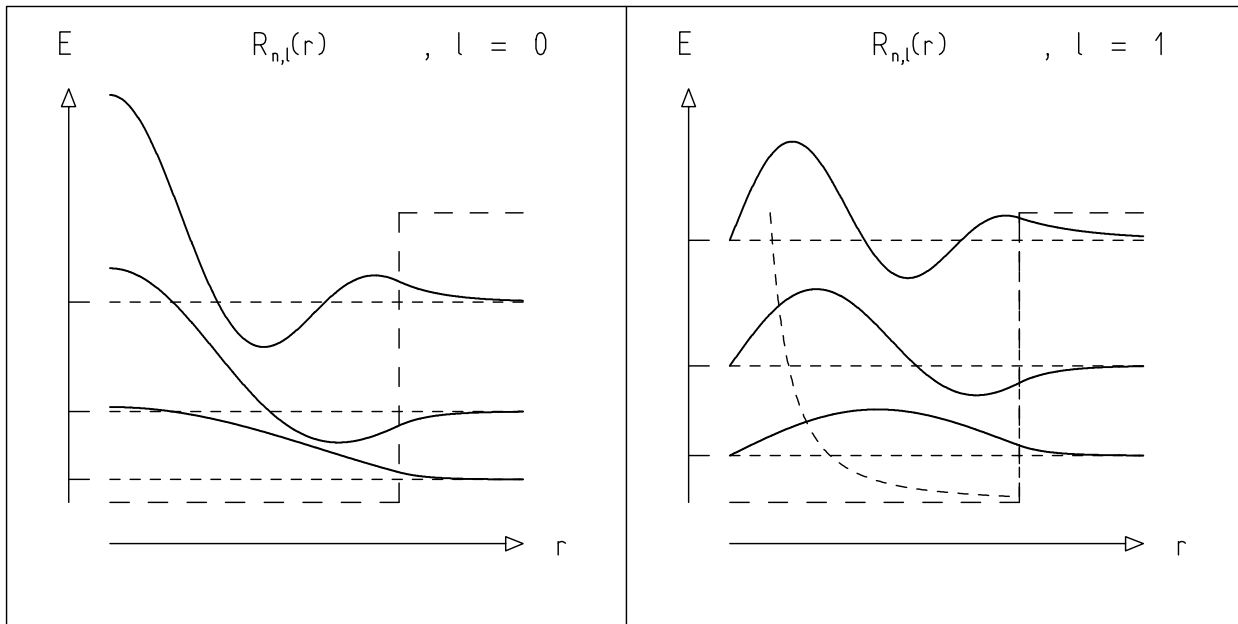
**Fig. 14.1.** The wave function  $\varphi = s_2$  is symmetric with respect to the  $xy$  plane, i.e., the plane perpendicular to the  $z$  axis. The wave function  $\varphi = p_2$  is antisymmetric. A superposition of both, the hybrid  $\varphi = h_2$ , displays neither symmetry nor antisymmetry: it is unsymmetric. Its absolute square, the probability density  $|\varphi|^2 = |h_2|^2$ , is markedly more extended along the negative  $z$  direction compared to the positive  $z$  direction.



**Fig. 14.2.** The functions displayed in Fig. 14.1 are shown here in the form of contour plots in the  $xz$  plane. Function values are positive on blue lines, negative on magenta lines, and vanish on red lines. The unit length used for the scales in  $x$  and  $z$  is the Bohr radius.



**Fig. 14.3.** The probability density shown in the bottom right of Figs. 14.1 and 14.2 is displayed here as a contour-surface plot. On the left it is shown for the half-space  $y > 0$  only and thus appears as cut open. On the right the surface is closed since it is shown in full space.



**Fig. 14.4.** Radial wave functions and their eigenvalues in a 3D square-well potential. The eigenvalues are systematically higher for states with  $\ell = 1$  (right) compared to the corresponding states with  $\ell = 0$  (left).

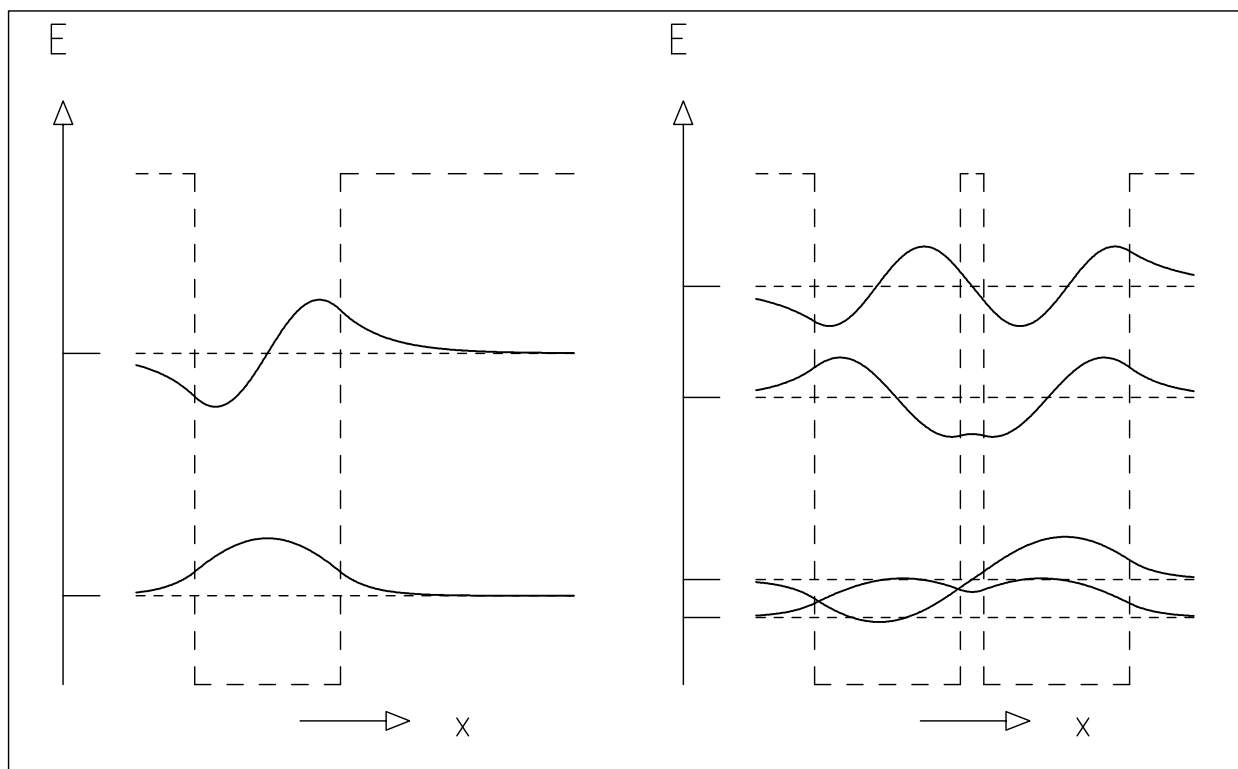
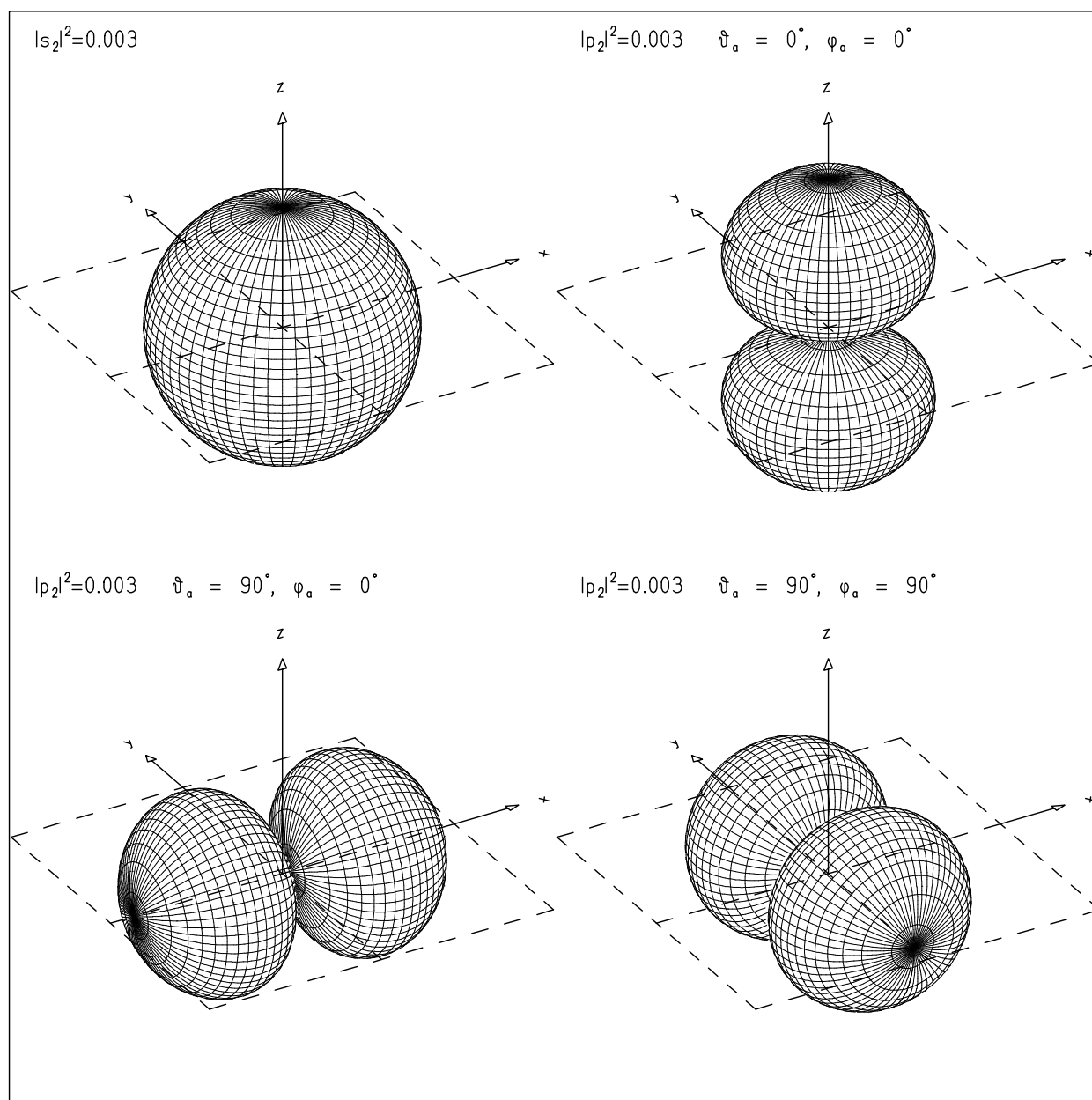
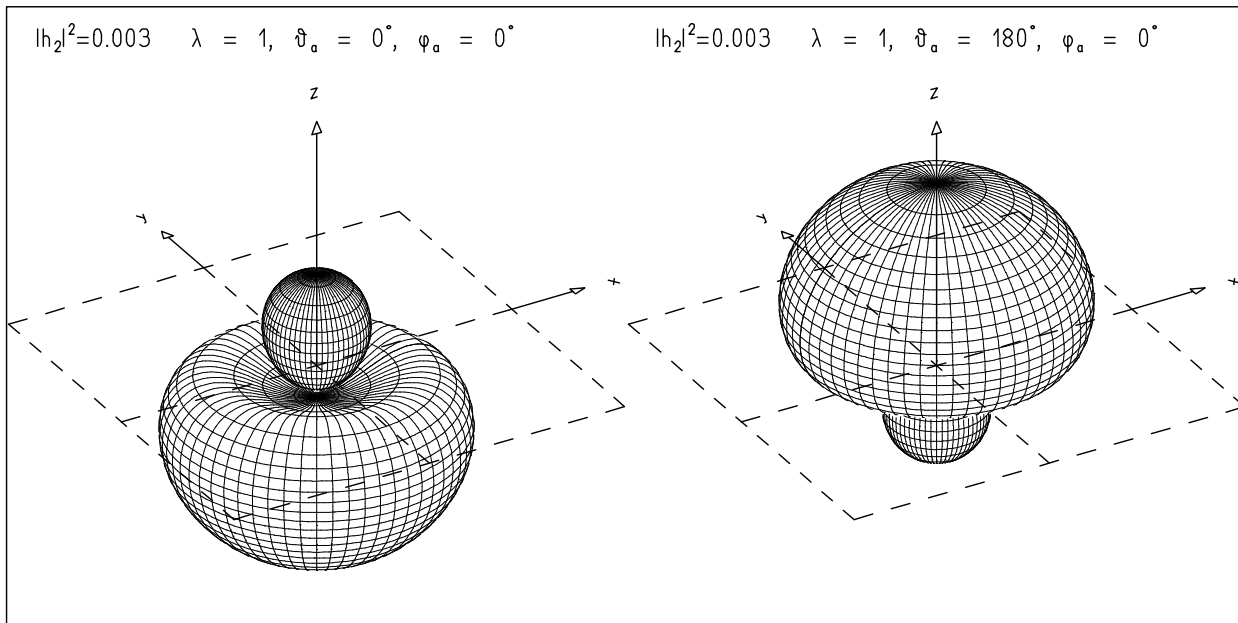


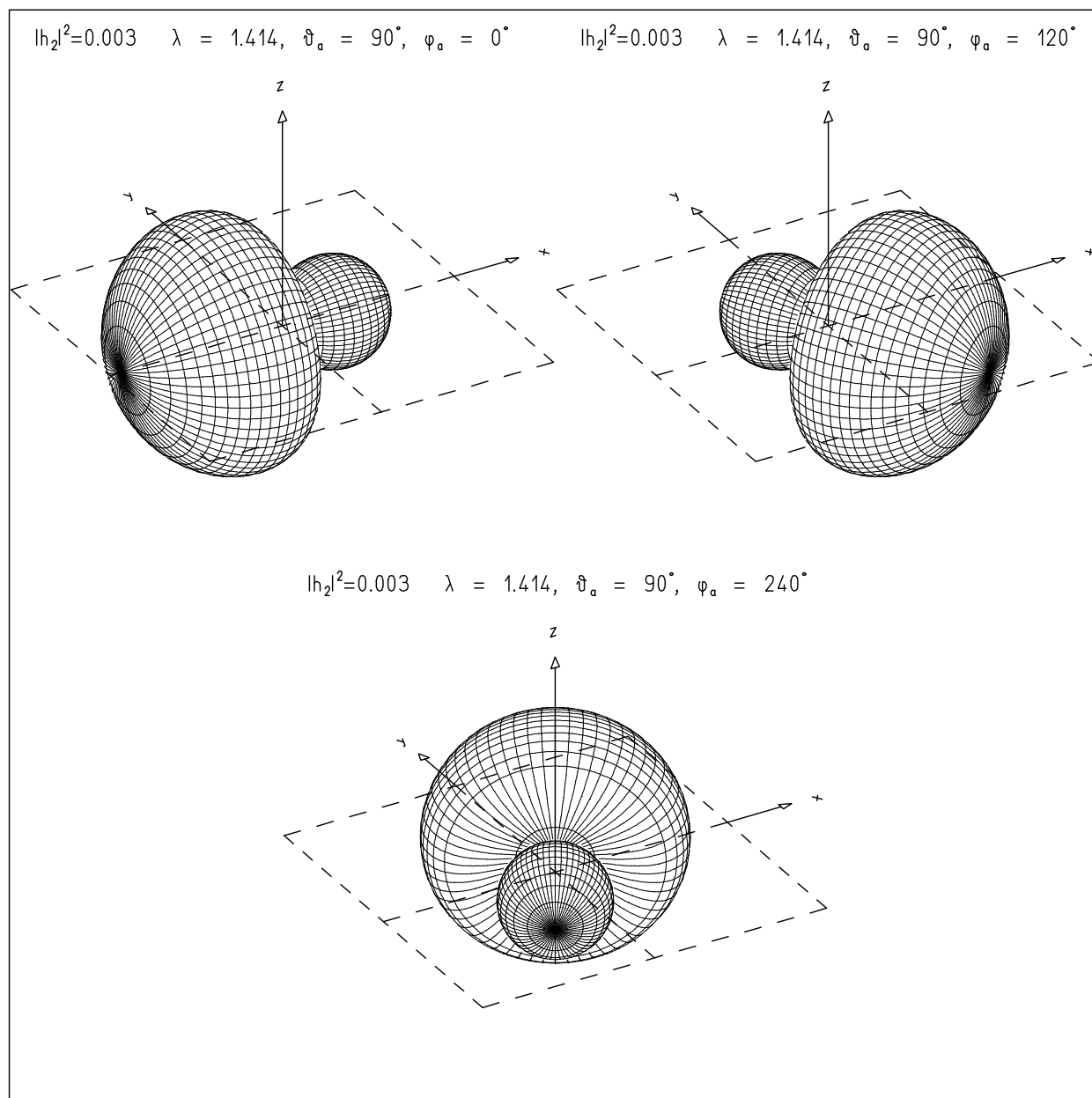
Fig. 14.5. Eigenvalues and eigenfunctions in a 1D potential. For every state in a single well (left), there are two states in the double well: one with lower, the other with higher energy than in the single well. The state of lower energy is *binding*, that of higher energy is *anti-binding*.



**Fig. 14.6.** Contour-surface plots illustrating the four orthogonal states  $s_2, p_{2z}, p_{2x}, p_{2y}$ .

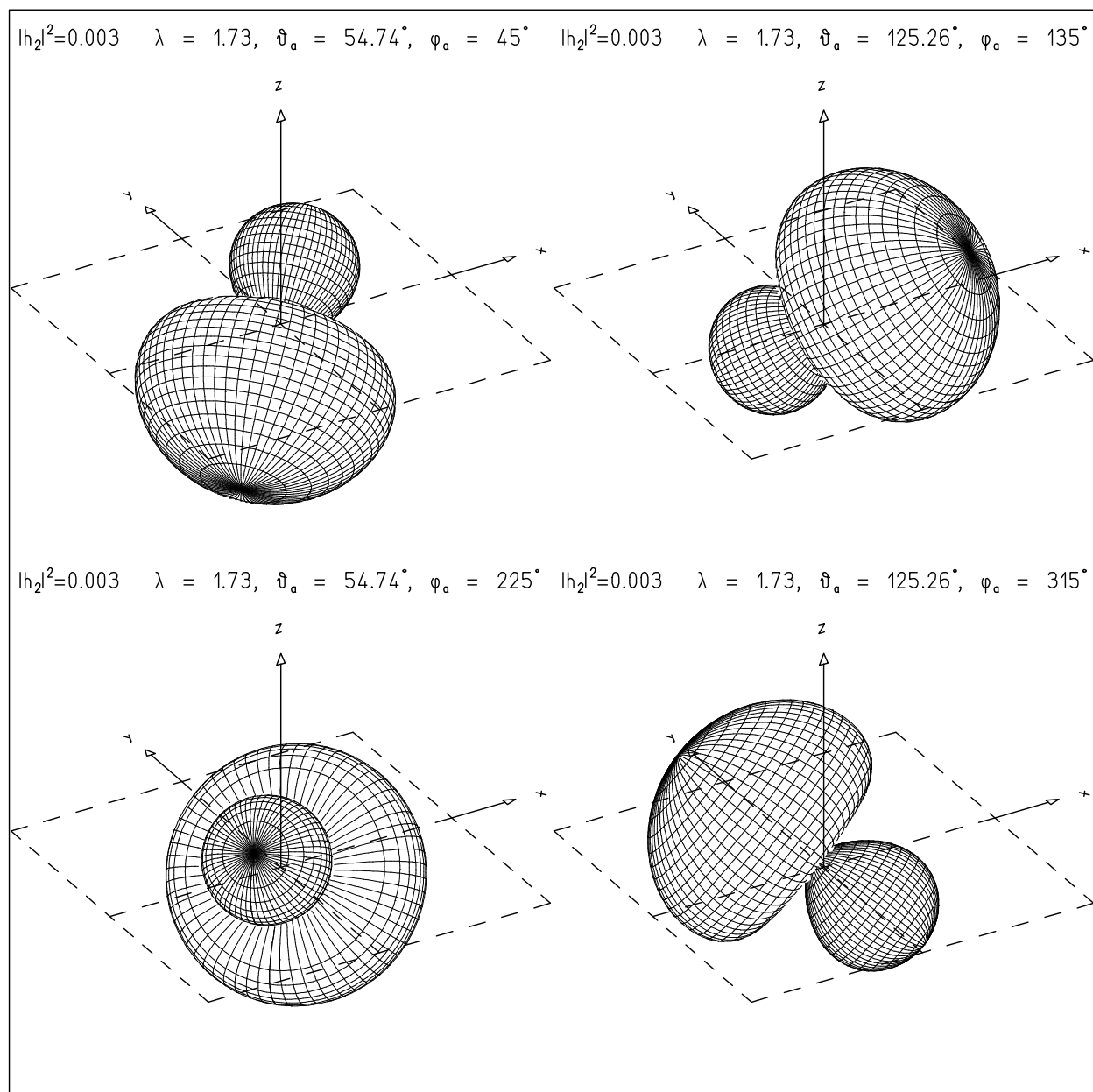


**Fig. 14.7.** *sp* hybrids for  $n = 2$ : Contour-surface plots of  $|h_{21}|^2$  and  $|h_{22}|^2$ .

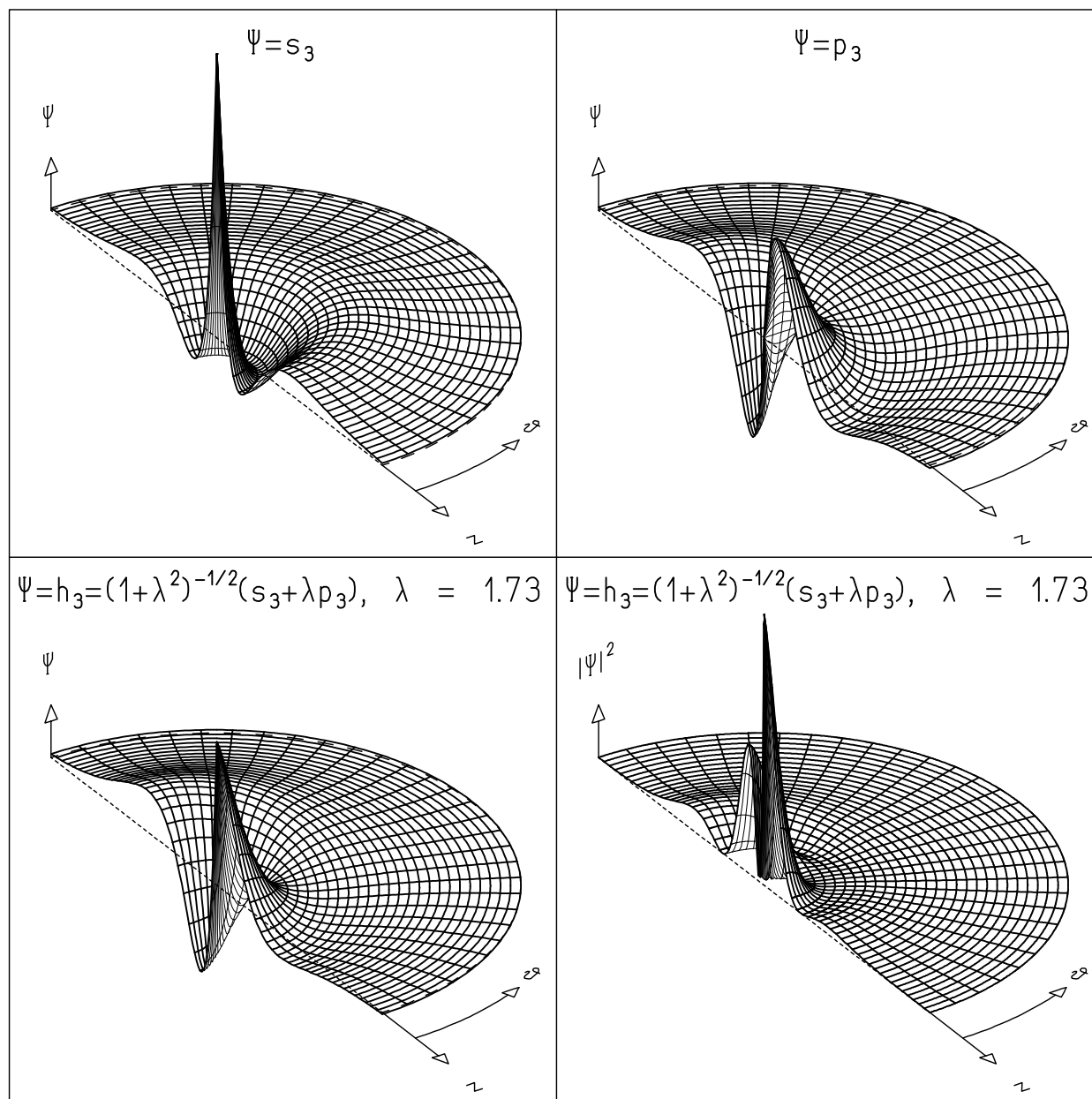


**Fig. 14.8.** Contour-surface plots of  $sp^2$  hybrids for  $n = 2$ .

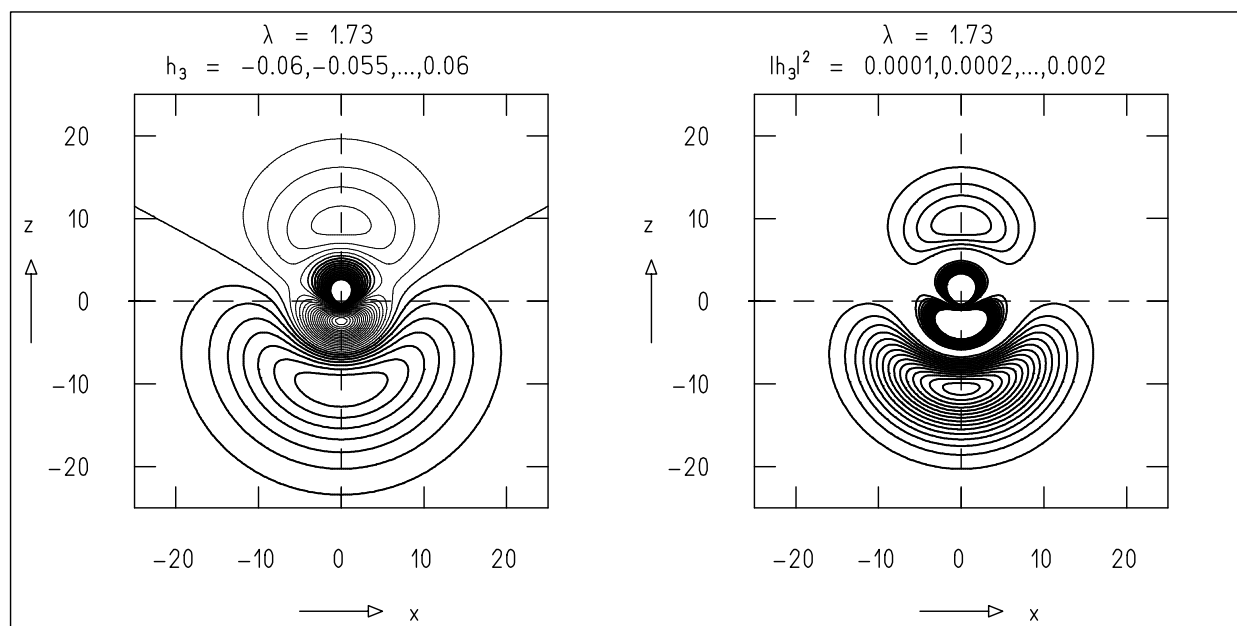




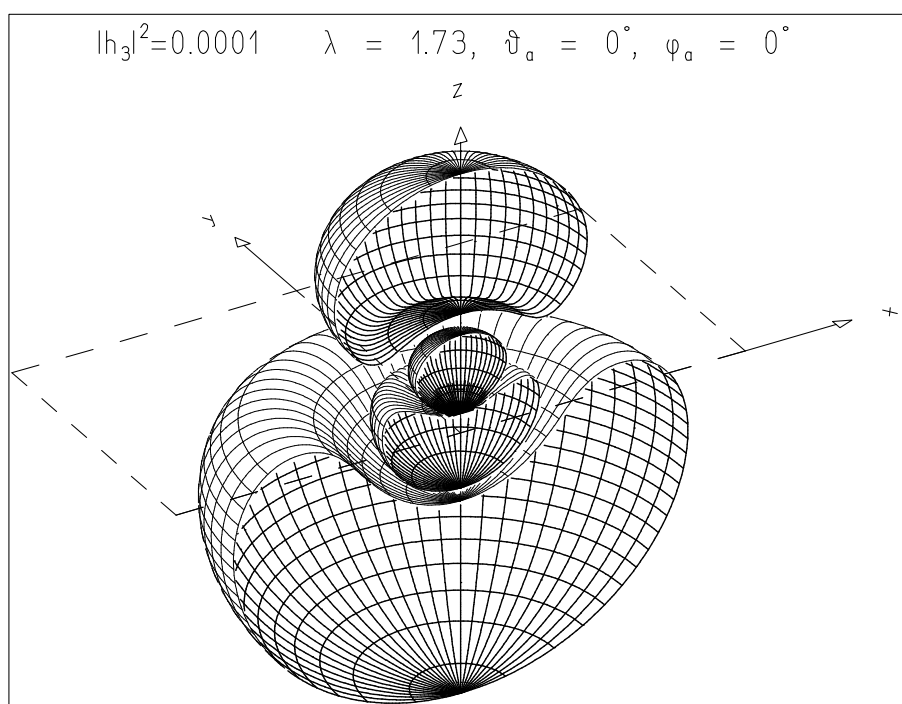
**Fig. 14.9.** Contour-surface plots of  $sp^3$  hybrids for  $n = 2$ .



**Fig. 14.10.** The wave functions  $\varphi = s_3$ ,  $\varphi = p_3$ , their superposition  $\varphi = h_3$ , and its absolute square, the probability density  $|\varphi|^2 = |h_3|^2$ . In comparison to Fig. 14.1 the scale in the  $r\vartheta$  plane is different; the functions shown here extend over a wider region.



**Fig. 14.11.** The functions  $\varphi = h_3$  and  $|\varphi|^2 = |h_3|^2$  displayed in Fig. 14.10 are shown here in the form of contour plots in the  $xz$  plane. Function values are positive on blue lines, negative on magenta lines, and vanish on red lines. The unit length used for the scales in  $x$  and  $z$  is the Bohr radius. Note the difference in scale with respect to Fig. 14.2.



**Fig. 14.12.** The probability density of the  $sp^3$  hybrid for  $n = 3$  shown as contour-surface plot in the half-space  $y > 0$ .