

## The hemispherical box: an example of virtual symmetry

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is satisfied with the discontinuities of  $E$  given in equation (4). Further work is in progress to derive useful boundary conditions for use in the  $\eta = 0$  limit.

I wish to thank Dr. R. J. Hosking for a helpful discussion.

School of Physical Sciences,  
The Flinders University of South Australia,  
Bedford Park,  
South Australia.

B. DAVIES  
12th May 1969

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## The hemispherical box: an example of virtual symmetry

**Abstract.** An example of accidental degeneracy in quantum mechanics arising from virtual symmetry is exhibited and discussed.

McIntosh (1964) has emphasized that a quantum-mechanical system may inherit a degeneracy through the symmetry of a larger system in which it can be embedded. We wish to report a pleasing example of this afforded by the motion of a single particle in a hemispherical box with impenetrable walls. The method of embedding used was originated by Heisenberg (private communication to Professor C. A. Coulson), though it has apparently not been published by him. Previous applications have dealt mainly with Hückel molecular orbital calculations and the study of lattice vibrations, references to which may be found in the paper by McIntosh. The eigenvalue problem pertaining to the present system, though it is rather simple and could otherwise be solved by straightforward methods, is of interest because of the manner in which it exhibits accidental degeneracy as we shall now describe.

The manifest symmetry group of the hemispherical box is  $C_{\infty v}$ , which would imply at most a twofold degeneracy in the energy levels. The actual degeneracy is much higher. To show this we follow Heisenberg's procedure as described by McIntosh and attempt to embed in a larger more symmetrical system, in this case the spherical box, so that out of a subset of the eigenfunctions of the latter we may construct the eigenfunctions of the original system. Now, although the extra symmetry of the larger system may imply additional degeneracy, the question still remains as to whether in the subset of eigenfunctions of the smaller system the residual degeneracy is greater than would otherwise have been anticipated. In the present case this does occur. Indeed, since the symmetry group of the spherical box is  $SO(3, R)$ , we first of all observe that each of its energy levels may be indexed with the angular quantum number  $l$  with a  $(2l+1)$ -fold degeneracy. Then if we select those eigenfunctions which have a node on (say) the  $xy$  plane and apply to them the projection operator  $P$  defined by

$$(Pf)(z) = \begin{cases} f(z) & z > 0 \\ 0 & z \leq 0 \end{cases}$$

we obtain the correct eigenfunctions for the hemispherical box. (Since the walls are infinite we require only that the wave function and not its derivative be continuous on the boundary.) The eigenfunctions with such a node are just those which are odd under reflection in the  $xy$  plane. This condition is met if, and only if,  $l+m$  is odd. We can see this by noting that when the magnetic quantum number  $m$  is zero, the resulting solutions (Legendre polynomials) are even in  $z$  for  $l$  even and odd otherwise. The result then follows from the fact that the operators  $L_x \pm iL_y$ , which step  $m$  by one unit, are odd in  $z$ . The energy levels of the hemispherical box may thus be indexed by the angular quantum number  $l$  and exhibit an  $l$ -fold degeneracy. This is higher than that predicted by the  $C_{\infty v}$  symmetry alone.

The 'hidden' symmetry group of the hemispherical box may be regarded as  $SU(2, C)$ , the Lie algebra being generated by  $L_z$  and two further elements which behave like  $(L_x + iL_y)^2$  and  $(L_x - iL_y)^2$ . These last two operators step the eigenvalues of  $L_z$  by two units, so that, without the need to invoke spin, all the unitary representations are physically meaningful.

Finally we remark that one may anticipate a symmetry breaking when the potential walls of the hemispherical box are of only finite height. This is because the eigenvalue problem is then no longer exactly separable in polar coordinates, nor may we assume the wave function to vanish identically on the boundary with discontinuous derivative there. For these reasons the above argument is no longer applicable and hence we should not expect the additional degeneracy which it implies. The corresponding effect in the lattice vibration and Hückel problems occurs when there are more than just nearest-neighbour interactions. The extra symmetry realized through boundary reflections is then broken on account of interactions across the boundary arising from second nearest-neighbour terms.

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Mathematical Institute and Corpus Christi College,  
Oxford.

A. JOSEPH  
23rd June 1969

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