



Article scientifique

Article

1940

Published version

Open Access

This is the published version of the publication, made available in accordance with the publisher's policy.

On the Problem of Degeneracy in Quantum Mechanics

Jauch, Joseph-Maria; Hill, E.L.

How to cite

JAUCH, Joseph-Maria, HILL, E.L. On the Problem of Degeneracy in Quantum Mechanics. In: Physical review, 1940, vol. 57, n° 7, p. 641–645. doi: 10.1103/PhysRev.57.641

This publication URL: <https://archive-ouverte.unige.ch/unige:162207>

Publication DOI: [10.1103/PhysRev.57.641](https://doi.org/10.1103/PhysRev.57.641)

where D^2 is defined as in Eq. (19) and A_4 and B_4 are arbitrary constants.

This solution represents a state of the rotating space charge in which "spokes" of increased density maintain a fixed position relative to a coordinate system rotating with angular velocity Ω_0 . Fig. 2 is intended to represent this state of affairs. The a.c. at any point is then due only to changes in charge density and not at all to changes in electron velocity.

6. DISCUSSION

We have assumed throughout that the boundaries are perfectly conducting and that electrons travel in circles around the axis so that no current

flows from the inner to the outer conductor. Thus no d.c. power is being fed into the system, and we cannot expect to make any estimates of a.c. power output. This is also evident from the fact that currents and voltages calculated from our solutions are always $\pi/2$ out of phase. For the same reason it is impossible to estimate the resistance which a tube will present to an a.c. signal. This situation could be remedied by introducing a small d.c. radial velocity, but this increases the complexity of the a.c. equations so that they are quite unmanageable by our present technique.

It is a pleasure to acknowledge our indebtedness to Mr. W. C. Hahn for many stimulating discussions and suggestions.

APRIL 1, 1940

PHYSICAL REVIEW

VOLUME 57

On the Problem of Degeneracy in Quantum Mechanics

J. M. JAUCH AND E. L. HILL

Department of Physics, University of Minnesota, Minneapolis, Minnesota

(Received January 25, 1940)

The problem of degeneracy in quantum mechanics is related to the existence of groups of contact transformations under which the Hamiltonian is invariant. The correspondence between transformations in classical and quantum theories is developed. The Fock-Bargmann treatment of the symmetry group of the hydrogenic atom comes under this theory. The symmetry group of the

2-dimensional Kepler problem is found to be the 3-dimensional rotation group; that of the n -dimensional isotropic oscillator is isomorphic to the unimodular unitary group in n dimensions. The 2-dimensional anisotropic oscillator has the same symmetry as the isotropic oscillator in classical mechanics, but the quantum-mechanical problem presents complications which leave its symmetry group in doubt.

INTRODUCTION

IN the study of quantum-mechanical problems the question of the degeneracy of the energy levels plays an important role. It is often the case that this degeneracy is associated with simple symmetry properties of the Schrödinger equation, and considerable attention has been paid to the symmetry conditions associated with the rotation-reflection group and the group of permutations of identical particles.¹

On the other hand, certain problems possess symmetry properties of more subtle types. It was shown by Fock² some years ago that the

Schrödinger equation for the hydrogen atom actually has the symmetry of the 4-dimensional rotation group for the bound states, and the symmetry of the Lorentz group for the positive energy states. The degeneracy of the system with respect to the quantum number l is due to the invariance under these wider groups, of which the 3-dimensional rotations form a sub-group. This interpretation was verified and extended by Bargmann,³ who showed the formal relationship of the Lenz-Pauli integrals with these groups. In spite of the satisfactory way in which these considerations clarified the hydrogen atom problem, they seem peculiar to this case, and it is not clear at once whether they can be extended to other examples.

¹E. g., E. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren* (Vieweg & Sohn, 1931).

²V. Fock, *Zeits. f. Physik* **98**, 145 (1935).

³V. Bargmann, *Zeits. f. Physik* **99**, 578 (1936).

In this paper we wish to develop further the relation between general contact-transformation theory and the problem of degeneracy. We shall show that in certain cases at least, including the hydrogen atom, the degeneracy arises from the invariance of the Hamiltonian under a group of contact-transformations. These more general *dynamical* groups, involving simultaneous transformations on the coordinates and momenta, contain as sub-groups the usual *geometrical* groups based on point transformations of the coordinates. It remains unclear whether all cases of degeneracy can be explained in this way, and we shall discuss one case (2-dimensional anisotropic oscillator) which presents complications, and is unsolved as yet from this point of view.

It should be remarked that degeneracies can arise from finite groups of discrete transformations as well as from continuous groups. Such is the case, for example, with the permutations on identical particles, the Kramers spin-doubling,⁴ the doubling of the energy levels in the Dirac theory of the hydrogen atom, etc. These are characterized by the constant number of degenerate components for the various levels. We shall restrict ourselves here to continuous groups possessing infinitesimal elements.

CONTINUOUS GROUPS OF CONTACT-TRANSFORMATIONS IN CLASSICAL MECHANICS

We shall base our discussion of the quantum-mechanical theory on the corresponding classical problem. As a preliminary we give a brief statement of the classical theory.⁵

In the transformation theory of classical dynamics attention is focused on the existence of integrals of the equations of motion of the form

$$F(q_1, \dots, q_n; \quad p_1, \dots, p_n) = \text{const.}, \quad (1)$$

where the q 's and p 's are the coordinates and conjugate momenta of the system. We restrict ourselves to problems in which the integrals are not explicit functions of the time t .

⁴ H. A. Kramers, Proc. Amsterdam Acad. **33**, 959 (1930). E. Wigner, *Göttingen Nachrichten, Mathematisch-Physikalische Klasse* (1932), p. 546.

⁵ Cf., E. T. Whittaker, *Analytical Dynamics* (Cambridge Press, third edition), Chapters 10, 11, 12.

Having such an integral we define an infinitesimal contact-transformation

$$Q_k = q_k + \delta q_k; \quad P_k = p_k + \delta p_k, \quad (2)$$

where

$$\delta q_k = \epsilon(F, q_k); \quad \delta p_k = \epsilon(F, p_k). \quad (3)$$

The symbol (A, B) designates the Poisson-bracket

$$(A, B) = \sum \left(\frac{\partial A}{\partial q_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial q_k} \right)$$

and ϵ is the parameter of the transformation. Such a transformation takes one orbit in phase space (coordinates q, p) into an infinitely near orbit lying on the same energy surface.⁶

Suppose now that we have found a set of independent integrals F_1, F_2, \dots, F_r . Each of these integrals can be used to generate a one-parameter group of contact-transformations by the above procedure. It follows from the Lie theory of continuous transformation groups that these transformations will form a group if the set of integrals satisfy conditions of the form⁷

$$(F_k, F_m) = \sum C_{km}^g F_g, \quad (4)$$

where the coefficients C_{km}^g are constants, or are at most functions of the total energy. The problem of finding the continuous groups of symmetry transformations of a given dynamical problem is thus reduced to the search for integrals by means of which one can specify the infinitesimal elements of the group. For our purpose it is not necessary to find the finite transformations of the group.

CONTINUOUS GROUPS OF CONTACT-TRANSFORMATIONS IN QUANTUM MECHANICS

The general procedure for adapting these considerations to quantum-mechanical theory is known, but certain necessary alterations must be made.⁸ The integrals must be represented by

⁶ Reference 5, Section 144.

⁷ S. Lie and F. Engel, *Theorie der Transformationsgruppen* (Teubner). G. Vivanti, *Leçons élémentaires sur la Théorie des Groupes de Transformations* (Gauthier-Villars, Paris, 1904). L. P. Eisenhart, *Continuous Groups of Transformations* (Princeton University Press, 1933).

⁸ For the quantum-mechanical transformation theory see P. A. M. Dirac, *Quantum Mechanics* (Oxford Press, second edition, 1935), or E. C. Kemble, *Fundamental Principles of Quantum Mechanics* (McGraw-Hill, New York, 1937).

Hermitian operators, so that it may be necessary to symmetrize them in the p 's and q 's. In our actual examples we use the Cartesian coordinates and momenta as usual, but we suppose here merely that they obey the ordinary commutation rules. The integral property of the F 's is expressed by their commutation with the Hamiltonian.

The transition to quantum mechanics is based on the correspondence

Poisson-bracket $\rightarrow (1/i\hbar)$ commutator.

For our purposes we require this correspondence to be an algebraic equivalence such that the commutators of the F operators satisfy the operator relations

$$[F_k, F_m] = i\hbar \sum C_{km} F_g. \quad (5)$$

Here the C 's must be constants, or at most operators depending on the Hamiltonian alone. Although in principle they need not be the coefficients appearing in Eq. (4), it is to be anticipated that they will be the same.

The formal proof that the operators satisfying Eq. (5) define a group of transformations (in Hilbert space) is easily supplied, and will not be given here. From a formal point of view the finite transformations of the group can be considered to be generated by the unitary operators

$$U(\lambda_1, \dots, \lambda_r) = e^{i(\lambda_1 F_1 + \dots + \lambda_r F_r)}, \quad (6)$$

the λ 's being the finite parameters of the group.

The further statement of our problem is now identical with that employed in the study of the geometrical groups. The matrices for the operators of Eq. (6) form a unitary representation of the group with the eigenfunctions of each energy level as basis. We shall suppose each of these representations irreducible. In our examples the irreducibility has been proved by direct computation of the matrices. The degree of each representation is the degree of degeneracy of the energy level in question. Naturally all possible unitary representations of the group in question may not occur in a given problem, due primarily to secondary restrictions which are placed on the allowable eigenfunctions; i.e., single-valuedness, quadratic integrability, etc.

Before passing to the discussion of the examples, a few further remarks on the preceding theory seem called for.

As we have developed it, the procedure is frankly exploratory, and arises directly out of the well-known similarities between classical and quantum dynamics. The essential point is to find suitable integral operators satisfying Eq. (5), and it is here that the classical theory furnishes valuable guidance. When the classical integrals fail to go over properly into quantum operators the method fails (e.g., 2-dimensional anisotropic oscillator).

In the search for classical integrals we are guided by the knowledge that for our type of problem there exist $(2n-1)$ time-independent integrals. However, these integrals exist in principle only *im kleinen*; i.e., over small and suitably restricted ranges of the variables. For our purposes it is apparently necessary that they exist over a whole energy surface.⁹ On the other hand, the classical problems which lend themselves to the quantization procedure are very limited in number. It appears quite possible that the problem of quantization in quantum mechanics and the existence of transformation groups on the orbits in the corresponding classical problem are intimately related.

Another point concerns the number of parameters in the group. When we have found $(2n-1)$ suitable classical integrals, their Poisson-brackets may still not satisfy Eq. (4). In this case we can continue to form new integrals using Poisson's theorem.¹⁰ In this manner we proceed until we have completed a set satisfying Eq. (5), if possible. We are confronted with two questions: (1) Under what conditions will the process terminate so that we obtain a group, and (2) if it does terminate shall we stop there, or shall we seek further integrals to generate a still larger group of transformations? Possibly questions of this sort can be answered in terms of the general theory of transformation groups. Our present view is that we have found everything requisite if $r \geq (2n-1)$ so that the classical group is transitive with respect to transformations on an energy surface in phase space. The analogous criterion in quantum mechanics seems to be the *irreducibility* of the representations.

EXAMPLES

A. The hydrogenic atom (3-dimensional)

As this problem has been discussed in detail by Fock² and Bargmann,³ we shall confine ourselves to a statement of the results. The symmetry group is built up on the integrals

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}; \quad \mathbf{A} = (1/2mZe^2)(\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) + \mathbf{r}/r.$$

\mathbf{L} is the ordinary angular momentum operator, and \mathbf{A} is the Lenz-Pauli vector integral. The commutation rules of these six integrals and their explicit reduction to the 4-dimensional rotation group are given in detail by Bargmann. The

⁹ We are indebted to Dr. W. Kaplan for discussion and correspondence on this point.

¹⁰ Reference 5, Section 145.

results can be readily verified by considering the solutions in the momentum space where corresponding operators can be found.¹¹ This second procedure is equivalent to that of Fock.

B. The Kepler problem in two dimensions

The Hamiltonian is

$$H = (1/2m)(p_1^2 + p_2^2) - Ze^2/(q_1^2 + q_2^2)^{1/2}.$$

We find the three integrals

$$L_3 = q_1 p_2 - q_2 p_1,$$

$$A_1 = -(1/2mZe^2)(L_3 p_2 + p_2 L_3) + q_1/r,$$

$$A_2 = +(1/2mZe^2)(L_3 p_1 + p_1 L_3) + q_2/r,$$

having the commutation relations

$$[L_3, A_1] = i\hbar A_2; \quad [L_3, A_2] = -i\hbar A_1,$$

$$[A_1, A_2] = (i\hbar/mZ^2e^4)(-2H)L_3.$$

If we define

$$A_1 = (i\hbar/m^3Ze^2)(2|E|)^{1/2}F_1,$$

$$A_2 = (i\hbar/m^3Ze^2)(2|E|)^{1/2}F_2,$$

$$L_3 = i\hbar F_3,$$

where E is the total energy eigenvalue, we find for $E < 0$;

$$[F_1, F_2] = F_3; \quad [F_3, F_1] = F_2; \quad [F_2, F_3] = F_1,$$

which are the commutation rules for the 3-dimensional rotation group. For $E > 0$:

$$[F_1, F_2] = -F_3; \quad [F_3, F_1] = F_2; \quad [F_2, F_3] = F_1,$$

which are the commutation rules for the group of linear transformations on three real variables with the invariant form $(x_1^2 + x_2^2 - x_3^2)$, which we may call the 3-dimensional Lorentz group.

For the bound energy states the energy values are

$$E_{\lambda, \nu} = -(mZ^2e^4/2\hbar^2)/(\lambda + \nu + \frac{1}{2})^2. \\ (\lambda, \nu = 0, 1, 2, \dots).$$

Using plane polar coordinates the wave functions have the form

$$\psi_{\pm \lambda, \nu} = f_{\lambda \nu}(r)e^{\pm i\lambda \varphi}.$$

¹¹ E. Hylleraas, *Zeits. f. Physik* **74**, 216 (1932). B. Podolsky and L. Pauling, *Phys. Rev.* **34**, 109 (1929). In line 6 of page 115 of this reference one should put $\zeta = nP/Zp_0$.

For $\lambda > 0$ there exists a doubling due to the subgroup of rotations associated with F_3 , while all states for which $\lambda + \nu = N = \text{const.}$ form a degenerate set. The matrix of F_3 is diagonal, and the direct computation of the matrices for F_1 and F_2 leads to the customary representations D_N , the degree of degeneracy being $g(N) = 2N + 1$, N integral.

C. The 2-dimensional isotropic harmonic oscillator

The Hamiltonian is

$$H = (p_1^2 + p_2^2)/2m + k(q_1^2 + q_2^2)/2,$$

for which the following are integrals

$$F_1 = (1/2i\hbar)(q_1 p_2 - q_2 p_1),$$

$$F_2 = (1/4i\hbar)\{(1/m^3k^{1/2})(p_1^2 - p_2^2) + m^3k^{1/2}(q_1^2 - q_2^2)\},$$

$$F_3 = (1/2i\hbar)\{(1/m^3k^{1/2})p_1 p_2 + m^3k^{1/2}q_1 q_2\}.$$

The first arises from the angular momentum, and the second from the energy difference of the two separate oscillators, while the third has no obvious physical significance. The commutation rules are

$$[F_i, F_k] = F_l,$$

the indices forming a cyclic permutation on (1, 2, 3). If we build the representation on the usual oscillator functions obtained by separation of the variables, the matrix of F_2 will be diagonal, with the matrix elements

$$(N_1, N_2 | F_2 | N_1, N_2) = i(\frac{1}{2}N - N_1),$$

where N_1 and N_2 are the quantum numbers of the two oscillators, and $N = N_1 + N_2 = \text{const.}$

The abstract group is therefore the same as that of the 2-dimensional Kepler problem, with the degree of degeneracy $g(N) = N + 1$. However, since N can assume all positive integral values, the representations include the half-integral as well as the integral cases. To our knowledge this is the first instance in which the half-integral representations of the rotation group have been known to appear in physical problems other than those connected with relativistic or spin theory.

However, for the purposes of generalization to higher dimensions we prefer to interpret the

group which appears here as the unitary unimodular group on two complex variables, which is doubly-isomorphic to the 3-dimensional rotation group.

D. The n -dimensional isotropic oscillator

The treatment of the preceding example can be generalized readily to any number of dimensions. We give only the result of the calculation.

Considering the problem as a collection of n one-dimensional oscillators it is always possible to find (n^2-1) linearly independent integrals, namely, the $\binom{n}{2}$ angular momenta, the $(n-1)$ differences of the energy of the separate oscillators, and the $\binom{n}{2}$ combinations of the form $q_1q_2 + p_1p_2$. It has been verified that the group generated by these infinitesimal transformations is isomorphic to the unimodular unitary group in n dimensions, which has (n^2-1) parameters.

Under the transformations of this group the eigenspaces of the Hamiltonian transform according to the representations by symmetric tensors. The dimensions of the representations are

$$g(N) = \binom{N+n-1}{n-1},$$

where $N = \sum N_i$, the N_i 's being the quantum numbers of the individual oscillators. This is then the degree of degeneracy of the energy levels, as can be checked directly.

It may be noted that there exist further representations of this group built on tensors which are not wholly symmetric,¹² but they do not occur in this physical application.

E. The 2-dimensional anisotropic oscillator

As remarked in the introduction, this problem presents certain peculiarities. The Hamiltonian can be written as

$$H = (p_1^2/2M_1 + M_1\omega_1^2q_1^2/2) + (p_2^2/2M_2 + M_2\omega_2^2q_2^2/2).$$

If the ratio of the two frequencies ω_1/ω_2 is rational, the energy levels are degenerate. Let us write

$$n\omega_1 = m\omega_2 = \tau; \quad \alpha = M\omega,$$

where n and m are positive integers, and introduce the new variables

$$b = (p - i\alpha q)/(2\alpha)^{\frac{1}{2}}; \quad b^* = (p + i\alpha q)/(2\alpha)^{\frac{1}{2}}.$$

It is easily verified that in both classical and quantum mechanics the following expressions are integrals

$$F_1 = \frac{1}{2}(b_1^n b_2^{*m} + b_1^{*n} b_2^m), \\ F_2 = -(i/2)(b_1^n b_2^{*m} - b_1^{*n} b_2^m).$$

For the classical mechanics we can define the integrals

$$B_1 = \frac{(\omega_1\omega_2)^{\frac{1}{2}}}{\tau} \cdot F_1 \cdot (b_1 b_1^*)^{-\frac{1}{2}(n-1)} \cdot (b_2 b_2^*)^{-\frac{1}{2}(m-1)}, \\ B_2 = \frac{(\omega_1\omega_2)^{\frac{1}{2}}}{\tau} \cdot F_2 \cdot (b_1 b_1^*)^{-\frac{1}{2}(n-1)} \cdot (b_2 b_2^*)^{-\frac{1}{2}(m-1)}, \\ B_3 = (1/2\tau)(b_2 b_2^* - b_1 b_1^*),$$

which have the Poisson-bracket relations

$$(B_1, B_2) = B_3 \dots$$

with cyclic permutations of the indices. We can thus conclude that there exists a group of contact-transformations in phase space which leaves the system of orbits of given energy invariant. This group is isomorphic to the 3-dimensional rotation group.

We have tried various expedients for carrying these results over to the quantum-mechanical problem, but so far have not found it possible to do so. In view of the negative results, it would scarcely be profitable to elaborate on them here. We feel, however, that the difficulties encountered in this relatively simple problem throw question on the true interpretation of classical multiply-periodic motions in quantum mechanics.

We are very much indebted to Professors Fock and Podolsky for correspondence relative to their work on the hydrogen atom.

¹² H. Weyl, *The Classical Groups* (Princeton University Press, 1939), p. 201.