

The Schrödinger Equation — 50 Years Later

A Survey of Current Research Problems

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Introduction

The Schrödinger equation is known to every physicist:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V(x,y,z,t) \Psi. \quad (1)$$

The durability of this equation after 50 years is truly remarkable. It is still the subject matter of intensive research, and its validity, new forms and faces, and its new applications continue. What is the fascination, the role and the significance of this equation today? Why is it going to be still of great import in spite of the advances in relativistic quantum theory and in quantum field theory? These are some of the questions we wish to discuss on the occasion of this anniversary.

Besides its profound physical significance and enormous range of applicability, the Schrödinger equation gave the impetus for the rapid development of whole new branches of modern mathematics, such as the Hilbert space theory and functional analysis, distribution theory and generalized functions, and the theory of group representations including the infinite-dimensional representations. We shall therefore touch some of these topics as well.

We discuss current research topics on some fundamental questions about and around the Schrödinger equation, leaving the status of research on its applications from atoms to nuclei, from simple molecules to DNA, from phonons to polarons, etc. to specialized text books and reviews. A jubileum volume dedicated to such applications appeared [“Wave Mechanics — The First 50 Years”, W. C. Price et al. editors (London, Butterworth, 1973)]. For mathematical problems we refer to a forthcoming issue of *Acta Physica Austriaca* also dedicated to the 50th anniversary of the Schrödinger equation.

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The present review takes an intermediary position between these two, and we put some emphasis on unsolved problems which delineate the border of knowledge around the Schrödinger equation.

Eigenvalues-Quantum Numbers

One of the most important features of the Schrödinger equation is its character as an eigenvalue equation giving the discrete values of certain physical quantities like energy and angular momentum. Schrödinger himself has entitled his original papers as “Quantization as an eigenvalue problem”¹. Eigenvalue problems were known in classical physics in the vibrations of strings, membranes and solids, for example. But the theoretical discovery of similar wave phenomena in atomic scale and the quantization of the periodic motions of electrons within an atom, with the occurrence of the Planck’s constant \hbar , was indeed revolutionary and had an immediate and farreaching effect. It was indeed a conceptual and theoretical discovery of “wave” phenomena after which the puzzling conglomerate of experimental information could be ordered and built into a single physical theory. Within a year or so, spectroscopy, chemistry and solid state physics was understood by physicists.

It is true that the Heisenberg-Jordan matrix mechanics preceded the Schrödinger equation by about six months². And the proof of equivalence of wave mechanics with the matrix mechanics has an important place in the history of physics and mathematics, and is also very interesting for the history of the personalities involved³. But the impact of wave mechanics was like that of an avalanche, it has accelerated the development of quantum mechanics, perhaps largely because of the familiarity of physicists with wave phenomena and the intuitive pictorial content of wave mechanics.

Now the discrete nature of physical quantities is not restricted to atomic, molecular and nuclear physics. The discrete masses of elementary particles, the discreteness of their spins and electric charges, and their various discrete “types” indicate that the same principle of “eigenvalue-problem” still operates in the domain of very small distances or much



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higher energies as compared to atomic phenomena. The general name for such properties of a system is “quantum numbers”: Quantum systems are characterized solely by quantum numbers and certain numerical parameters which set the scale. We hasten to note that not every physical quantity in quantum theory has discrete values; it is useful to treat, for example, energies and momenta of particles in a scattering experiment as continuous variables. The word “quantum number” is also used, by abuse of language, to denote all values of observables which label the state of the system, be it discrete, or, continuous. Thus we can write a general “eigenvalue equation” for an observable A having the value a for a system with wave function Ψ :

$$A \Psi = a \Psi, \quad (2)$$

and “the evolution equation”, generalizing Eq. (1),

$$i \hbar \partial \Psi / \partial t = H \Psi. \quad (3)$$

These are even valid for any quantum field theory, relativistic or nonrelativistic, and will be valid also in any foreseeable future. As is well-known, Eq. (3) reduces, for a stationary state, defined by $\Psi = u \exp \{-(i/\hbar) E t\}$ to (2): $H u = E u$. The evolution of an isolated system is then explicitly given by the equation

$$\Psi(t) = U(t) \Psi(0) \equiv \exp \{-(i/\hbar) H t\} \Psi(0). \quad (4)$$

In addition there are solutions which are non-stationary. But little direct use have been made so far of these more general solutions. They will be particularly important for time-dependent potentials.

Two Dilemmas

The Schrödinger equation as an eigenvalue problem solves one of the dilemmas for the solution of which the quantum mechanics was invented: the discrete atomic spectra. The other dilemma, the wave-particle duality of electrons in atomic phenomena, is actually also solved by the Schrödinger equation, because it accounts for the interference and diffraction phenomena with electrons, but at the expense of a new physical interpretation for the wave function Ψ , unusual from the point of view of classical physics: The wave function $\Psi(n, a; t)$ represents the probability amplitude for the system to have the values of the discrete quantum numbers n , and the continuous quantum numbers a (e. g. position or momentum) at time t . The debate over this interpretation and its philosophical, physical and mathematical ramifications still goes on and will continue until perhaps quantum mechanics is embedded in a more general physical theory.

Stochastic and Hydrodynamic Formulations

From almost the very beginning of wave mechanics physicists, including Schrödinger himself⁴ have tried to give a stochastic interpretation to the Schrödinger equation in the sense of Markov processes. The first question is: does the wave equation describe a collection of electrons in the statistical mechanics sense? The answer seems to be negative, as for example the fundamental double slit Gedanken-experiment show, where, in principle, one can send one electron after another. Next one could then ask: if the wave equation describes a single particle whose behavior is intrinsically probabilistic, does the particle move in an environment, a background “aether”, unseen or so far unknown, which causes the random behavior of particles? Or does the particle have an internal random mechanism? The analogy between the Schrödinger equation and the diffusion equation, or equations of fluid dynamics, is the basis for these considerations. Writing

$$\Psi = \Phi(\mathbf{r}, t) \times \exp \{i(m/\hbar) S(\mathbf{r}, t)\} \exp \{-i\Omega(t)\},$$

one can derive that $\varrho = \Phi^2$ is a density field satisfying a continuity equation $\partial \varrho / \partial t + \nabla \cdot \mathbf{n} \nabla S = 0$, and S satisfies the Euler equations of fluid dynamics with an additional quantum term proportional to \hbar^2 [Exercise 1]. If there is a kind of background, the quantum particle will perform a brownian motion.

Hidden Variables

These questions touch right one of the central problems of quantum theory in general, namely the existence of hidden variables, i. e. is Ψ a complete description of a system, or an incomplete one? Mathematically, the observables in quantum theory on a given state cannot be represented by random variables, unless they commute (von Neumann theorem)⁵. Thus the mathematical form of quantum theory and stochastic theories are completely different, but in some cases they may yield the same observable predictions⁶.

It is interesting that the Einstein-Podolski and Rosen Gedankenexperiment can now be formulated in such a way that quantum theory can be compared experimentally with a theory admitting hidden variables: Two particles are emitted from a point in a correlated way, say in a singlet state. The measurement of the spin component on one particle predicts in principle, with certainty (probability one) the spin component of the other particle-separated space-like from the first particle-before making any measurement on it. Thus, one obtains different spin-correlation results for the two theories. Experiments

have and are being indeed performed to test certain inequalities separating the two theories; but unfortunately the results are still not completely conclusive⁷. A very recent experiment⁸ seems to show a very strong correlation of linear polarization of two photons emitted from an atomic $J=1$ state in agreement with quantum mechanics. The existence of local hidden variables would make the correlation much weaker.

The Concept of Potential

In its simplest and best known form, Eq. (1), the Schrödinger equation may represent the wave behavior of a single electron: $\Psi(\mathbf{x}, t)$ is the probability amplitude of the particle moving in a potential $V(\mathbf{r}, t)$ which is taken over from classical mechanics. It is remarkable that in atomic and molecular physics we get along fine with classical potentials; we have only to represent the particles by a wave function. The concept of potential is a very powerful tool in physics, even in quantum field theory, for treating the bound state problems, where the perturbation theory is rather useless. It has played a most essential role in all the stationary problems of atomic, nuclear, molecular and solid state physics, and it will continue to do so in many other problems. Thus, the quantization rules for non-relativistic mechanics

$$[\text{e. g. } q \rightarrow q, p \rightarrow -i \partial / \partial q, \therefore V(q) \rightarrow V(q)]$$

are very well verified.

We shall come back to a geometric interpretation of potential in later Sections.

Many Particle Wave Equation

The passage from the wave function of a single particle $\Psi(\mathbf{x}, t)$ to the wave function $\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N, t)$ describing N particles, with the same time parameter, is by no means trivial both from conceptual and mathematical point of view. It was indeed a miracle that the Schrödinger equation developed first for a single particle also worked admirable for two or more particles, like the He-atom. Note now that the “wave” of many particles is not a wave in the ordinary space R^3 , but in the abstract configuration space $R^3 \times R^3 \times \dots \times R^3$ (N -times). The wave Eq. (1), which we shall write simply as $i \Psi_t = (-\Delta + V) \Psi$ in the units $\hbar = 1, 1/2m = 1$ goes over now to

$$i \Psi_t = [-\Delta_1 - \Delta_2 - \dots - \Delta_N + V(\mathbf{x}_1, \dots, \mathbf{x}_N, t)] \Psi, \quad (5)$$

and there is no simple relation between

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N, t)$$

and the N single particle wave functions

$$\Psi_i(\mathbf{x}_i, t), i = 1, \dots, N$$

satisfying coupled equations (Hartree-Fock-type equations). Further work in this direction is very desirable.

One immediate consequence of the many-body wave function was that a new symmetry, namely the exchange of two identical coordinates, could now be represented on the space of wave functions: The two functions $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ and $\Psi(\mathbf{x}_2, \mathbf{x}_1)$ obtained from each other by the exchange of \mathbf{x}_1 and \mathbf{x}_2 can now be the same or different, i. e. negative of each other. As a result we can understand why in the two electron systems of He, the triplet state $1s 2s^3S$ lies lower than the singlet state $1s 2s^1S$ (Heisenberg, June 1926) [exercise 2], or why two neutral H-atoms could bind to form the H_2 -molecule by van der Waals forces (Heitler-London, June 1927) [exercise 3] which was the beginning of quantum chemistry and physicists had finally understood chemistry, where old quantum theory had failed.

The separation of center of mass variables from (5), even in the case of $N=2$, is only possible for very simple interactions. For example, the Zeemann potential (constant external magnetic field) for atoms cannot be simply added to Eq. (1), contrary to many textbooks, but must be added to each term in (5), and the center of mass motion is only approximately separable [exercise 4]. Thus also radiation problems, for example the Lamb Shift in H-atom, should be formulated in the two-body form, and not as a one-body in an external Coulomb field. The fixing of the force center strongly effects radiation and renormalization problems.

Space of States — Hilbert Space

Although physical phenomena take place in the ordinary three-dimensional space around us, and time, physicists and mathematicians introduce all sorts of other, abstract, spaces whose points represent different states of the physical reality and in which the image of the change or evolution of a system can be followed. The phase-space of analytical mechanics, a $2n$ -dimensional abstract, and in general non-euclidian, space of n -coordinates $q_1 \dots q_n$ and n -momenta $p_1 \dots p_n$, is such a space. Similarly, all possible solutions Ψ, Φ, \dots of the Schrödinger equation (1) at fixed time t , form a space \mathcal{H} of functions. Since (1) is linear \mathcal{H} is a linear space. The integral $\|\Psi\|^2 \equiv \int |\Psi(\mathbf{x})|^2 d^3x$ represents the

total probability and hence can be taken to be unity, and the integral $|(\Psi, \Phi)|^2 \equiv \int \Psi^*(\mathbf{x}) \Phi(\mathbf{x}) d^3x$ is the conditional probability of finding the state Φ if the system is in the state Ψ , hence for mutually exclusive states $|(\Phi, \Psi)|^2 = 0$, i.e. Ψ and Φ are “orthogonal”. With this scalar product \mathcal{H} becomes a projective Hilbert space. This means that $e^{i\alpha} \Psi$ for all α , $\alpha = \text{real}$, represents the same physical state: a phase does not matter because only $|\Psi|^2$ characterizes a state. Thus in the superposition of two states $(\Psi_1 + \Psi_2)$ an overall phase is immaterial but the relative phase between Ψ_1 and Ψ_2 remains measurable and important. For example, a beam of spin 1/2 particles can be split into two, and one undergoing an interaction and then brought together again to interfere, produces a relative phase -1 which is observable (exercise 5).

As we vary the time t we obtain a family of Hilbert spaces \mathcal{H}_t . We cannot take superpositions of states at different times. If two states cannot be added to form another state (i.e. another solution) we say that they are separated by a superselection rule. Thus time t can be viewed as a continuous superselection parameter. The electric charge e is another example: Two states with different values of e , $e = 1$ and $e = -1$, for example, cannot be superposed; such states do not occur in nature, or every state we can prepare always has a definite value of e , as in classical physics. Otherwise relative phase between two states with different charges would be observable which by gauge symmetry cannot be (exercise 6).

The differential operators in the Schrödinger equation (1), $\partial/\partial t$, $\partial^2/\partial x^2, \dots$ are linear operators on the Hilbert space \mathcal{H} , because they map one element Ψ of \mathcal{H} into another element Ψ' . For a rigorous mathematical treatment we have to be careful that an operation does not take a state outside the Hilbert space. Most operators of quantum mechanics are defined only for a subset of elements. The problem of domain for unbounded operators, like d/dx or the wave operator \square, \dots is one of the most interesting and difficult parts of functional analysis. For example, the operator d/dx is not hermitian on the half line $0 < x < \infty$, although it is on the full-line $-\infty < x < +\infty$ (exercise 7).

An instructive and important example is the much discussed⁹ conjugate pair of variables

$$L_z = -i\hbar \partial/\partial \varphi, \text{ and } \varphi,$$

the third component of the angular momentum and the azimuthal angle φ . It is clear and has been recognized early by Jordan¹⁰ that the commutation relation $[L_z, \varphi] = -i\hbar$, is meaningless (exercise 8: Take the matrix elements of both sides in states

$|jm\rangle$). This is because L_z is hermitian on the space Ω of periodic functions $f(\varphi) = f(\varphi + 2\pi)$, but multiplication with φ is not defined in Ω .

Self-adjointness and Extensions

An important area of research around the Schrödinger equation is therefore the study of self-adjointness and spectral theory for the differential operator¹¹ $H = -\Delta + V$. In physical terms, this is the study of solubility and the nature of solutions (eigenvalues) for the stationary states of the system given by the eigenvalue equation $H\Psi = E\Psi$. Exactly soluble cases, in terms of known functions, are few. The problem is to find the largest class of potentials $V(\mathbf{r})$ for which the Schrödinger equation is in principle soluble, and for each potential to specify the nature of discrete and continuous spectra. It is clear that there are potentials, for example, attractive singular potentials $V(r) \sim r^{-a}$, $a > 2$, for which the Schrödinger equation is not a well posed problem: the solutions are overcomplete and one cannot — without further input — choose the correct solution. In mathematical language, the operator $-\Delta + V$ in this case is not a self-adjoint operator. This example even occurs in physics, e.g. in the radial equation of the relativistic Coulomb problem for large Z , the charge of the nucleus, a problem which will regain interest in view of the possible existence of superheavy stable elements with $Z = 124, 126$. To this problem we shall come back later again in another context. Often one can make a self-adjoint extension of an operator, like $-\Delta + V$. If this is possible, the operator is called essentially self-adjoint (e.s.a.), but in general there are many such extensions, and the correct extension is really a physical problem, not mathematical. It means to find correct boundary conditions in the domain of the operator so that the problem is well-defined, for example, correct boundary conditions at the origin for a highly singular attractive potential.

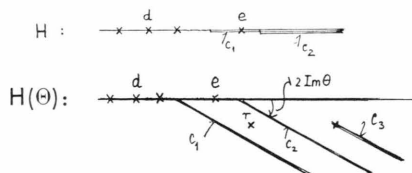
Discrete and Continuous Spectra

The spectrum of a self-adjoint operator consists of discrete points and continuous line segments (and possibly of a singular part), interpreted physically as bound states and scattering states. (It is hard to give a physical meaning to singular spectrum: it would be a state describing a particle going to infinity infinitely slowly, or going back or forth to and from infinity, for example). A discrete spectral point can be embedded on the continuous spectrum. For example, in the atom, neglecting the interelec-

tronic interactions, one electron in a scattering state, the other in a discrete state, represents such a situation.

Resonances

Along the continuous spectrum we have to single out resonance states by further properties. The existence and the description of resonances is of fundamental theoretical and experimental importance in the whole of physics, and it is remarkable that the Schrödinger equation carries also the information on resonances¹². But it is a delicate problem as shown by the great abundance of continued research papers on unstable particles and resonances. Intuitively, the particle goes around the force center or is captured for a while before going to infinity; in other words the wave function is concentrated, in a stationary description, almost like that of a bound state but with a small leakage, an oscillatory tail of small amplitude. One could introduce further structure along the continuous spectrum, such as the notion of spectral concentration at the position of the resonance. Another way is to exhibit resonances as discrete points again, but in the complex plane of the eigenvalues. An interesting new form of the second method, called analytic dilatation, consists in making the transformation $\mathbf{x} \rightarrow e^{i\Theta} \mathbf{x}$, $\Theta = \text{complex}$. The Hamiltonian H (of a general many body system) transforms into a new Hamiltonian $H(\Theta)$ and the spectrum of H goes over to (exercise 8)



- d = discrete eigenvalues
- e = embedded eigenvalues
- r = resonance eigenvalues
- c_1 = first threshold (real) cut
- c_2 = a higher real threshold cut
- c_3 = a complex threshold determined by bound states of subsystems.

Because the continuous spectra are now rotated by an angle $2 \text{Im } \Theta$, resonances are now seen as isolated discrete complex eigenvalues of $H(\Theta)$ with normalizable eigenvectors. This method can also be used numerically in practical calculations.

Generalized Eigenvectors

The states belonging to the continuous spectra are properly called “generalized eigenvectors”; they do not strictly belong to the Hilbert space, because

they are not normalizable. One can however, either use distribution theory (e.g. Dirac’s δ -functions), or more physically, wave packets to deal with this problem. The use of unrenormalizable plane waves is very common. Quantum mechanics may then be formulated in a more general linear space (linearity is essential for superposition principle) consisting of the so-called Gel’fand triplet of spaces $\Phi \subset \mathcal{H} \subset \Phi'$, where Φ' is the linear space including unrenormalizable states, \mathcal{H} the Hilbert space, and Φ a nice subspace of \mathcal{H} , dual to Φ' . This triplet is also called the rigged Hilbert space¹³.

From Discrete to Continuous Spectra. “A Paradox”

A perturbation can change a discrete spectrum into a continuous one. A simple example is the Stark effect in Hydrogen atom, i.e. a constant external electric field. It can be seen that the new Hamiltonian has only continuous spectrum. Yet, if the external potential energy is treated as a perturbation in the Schrödinger equation, one can evaluate the energy shift ΔE_n of each discrete level of the atom in agreement with experiment (exercise 9). The solution of this “paradox” is as follows: Experimentally due to the presence of other atoms the external field does not extend to infinity; there are finite boundary conditions, otherwise the energy would be infinite. Hence, either we have to impose new boundary conditions with the perturbation, i.e. a new space of functions; or consider a self-adjoint extension of the Hamiltonian. We see again the importance of self-adjointness and spectral theory in this example. Moreover, it must be shown that in the external field all levels of the atom become actually resonances.

Rigorous Bounds on the Numbers of Bound States

Short of the explicit solution of the eigenvalue problem another set of results that can be proved rigorously are the various general bounds on the number of energy levels, on the minimum of energy, etc. For example, the number of discrete energy levels of a given angular momentum l in the central potential $V(r)$ is bounded by

$$n_l(V) \leq (2l+1)^{-1} \int_0^\infty r |V(r)| dr$$

(Bargmann) [not counting the $(2l+1)$ -orbital multiplicity].

Another bound on the number of total energy-levels is¹⁴

$$N(V) \leq (4\pi)^{-2} \int \frac{|V(\mathbf{x})| |V(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^2} d\mathbf{x} d\mathbf{y} \quad (6)$$

(Birman-Schwinger) .

There seems to be so far no bounds on the number of resonance levels. This would be an interesting problem to attempt.

Stability of Matter

The problem of the stability of matter is related to the lower bound on the ground state energy of the Hamiltonian $-\Delta + V = H$. Given a set of nuclear positions we consider a number of electrons interacting with the nuclei and among themselves. Then the expectation value of H in the ground state is less or equal to a negative number $-E_0$. This was first shown by Dyson and Lenard¹⁵ and the value of E_0 was considerably improved recently¹⁶. The motion of the nuclei, assumed above to be fixed, would only increase the energy. These bounds do not take into account magnetic and possible other forces at shorter distances and relativistic effects, so that further work in the area of stability matter (also of nuclear matter) is desirable.

Variational Principles — Resonances Again

Stationary bound and resonance states can also be treated from the point of view of variational principles. Variational principles have almost universal validity in physics and offer great generality and simplicity. Stationary states maybe defined as states $|\varphi\rangle$ whose probability as time goes on in stationary $\delta\langle\varphi|U_t|\varphi\rangle=0$, where $U(t)$ is the time evolution operator (4). The eigenvalue problem (1) follows from here. A weaker condition is the stationarity of the probability amplitude rather than probability:

$$\delta|\langle\varphi|U_t|\varphi\rangle|^2=0.$$

This weaker condition has more solutions, and may contain also resonances. But a very clean-cut formulation applicable only to resonances would be important. Earlier we have discussed the method of complex dilatations to locate the resonances. In potential theory a resonance with a complex eigenvalue may also be formulated by suitable boundary conditions: To find a solution u_c of the equation

$$u_c'' + (k_c^2 - V(r))u_c = 0,$$

for example, with complex eigenvalue k_c^2 such that

$$u_c(r=0)=0 \quad \text{and} \quad u_c'/u_c|_{r=a}=i k_c.$$

This formulation is applicable for short-range potentials and one has to show that the results are independent of the cut-off distance $r=a$.

Group Theory and Group Representations

The invariance of the Schrödinger equation under a group of transformations shows us a new way of realizing symmetries in nature, much different than in classical mechanics. For example, under a rotation of the coordinates $\mathbf{x}'=R\mathbf{x}$, we obtain a new wave function $\Psi'(\mathbf{x})=\Psi(R\mathbf{x})=U(R)\Psi(\mathbf{x})$. Thus to the symmetry operation R in ordinary space, there corresponds the symmetry operation $U(R)$ in the Hilbert space of states. In a symmetric theory physical results are the same after and before the symmetry operation. Hence all subsets of states of the form $\{U(R)\Psi\}$, when R varies, are physically equivalent. How can we then observe an exact symmetry at all? (Paradox of Curie.) We can know about the existence of such equivalent states only if we can break the symmetry, or if we prepare initially a particular state. The operator $U(R)$ is called the representative of R in the Hilbert space, and all $\{U(R), R\in G\}$, satisfying the group properties and preserving the scalar products form a unitary representation $U(G)$ of the group G . Given a group G there is then a well-defined (and largely solved for compact groups G) mathematical problem, to determine all possible unitary representations $U(G)$ and their dimensions; the corresponding spaces on which $U(G)$ act, are then the physical states spaces. Thus symmetry helps to find and label possible quantum states of a system, if we do not have the corresponding wave equation, or if we cannot solve it.

This principle may be first applied to the symmetry group of space-time. In non-relativistic theory, an isolated system can be viewed from any inertial frame, the results of physical observations being independent of the frame, and the family of all such frames are related to each other by the group G of galilean transformations. Thus the unitary representations $U(G)$ of G determine equivalent quantum states of isolated systems. The irreducible components of $U(G)$ may be taken to define elementary systems, and we have as many distinct elementary systems, as there are inequivalent irreducible representations of G , i.e. the so-called dual space. The Hilbert space of each irreducible representation span the equivalent states of a given elementary system.

Actually it is more convenient to start from the conformal group of space-time which includes dilatations and scale-changes from point to point, in addition to galilean transformations. The non-relativistic limit of the conformal group yields the quantum mechanical version of the Galilei group, as well as additional invariance transformations. It can be verified that the Schrödinger Eq. (1) is invariant under galilean transformations only if the wave

function $\Psi(\mathbf{x}, t)$ is multiplied by a suitable phase factor in addition to the transformations of the arguments (exercise 10). This is meant by the quantum mechanical version of the Galilei transformations.

The same idea when applied to the transformations between inertial frames of the special theory of relativity, namely the group of inhomogeneous Lorentz transformations (i.e. the Poincaré group) gives a specification of relativistic elementary systems. In the absence of a complete relativistic quantum mechanics, the group representation theory has been a powerful and essential element of many relativistic considerations in quantum theory¹⁷. There is of course a well defined process, called the nonrelativistic limit, to go from the Poincaré group to the Galilean group.

Dynamical Groups

The application of kinematical symmetry groups, such as rotations, galilean transformations, as well as permutations of identical particles, which we have mentioned earlier (i.e. fermions and bosons), is rather well understood. For example, for rotations $U(R) = \exp(i\alpha_k J_k)$ and the infinitesimal generators (angular momenta) J_k are operator on Hilbert space with commutation relations (exercise 11)

$$[J_1, J_2] = iJ_3, \quad [J_2, J_3] = iJ_1, \quad [J_3, J_1] = iJ_2. \quad (7)$$

It is remarkable that the dynamical problems can also be solved by the representations of groups which are now called dynamical groups¹⁸. We consider here the case of Schrödinger equation of the type (1). Typically, such an equation with potential arises from a two-body problem ($\mathbf{r}_1, \mathbf{r}_2$) when the center of mass motion \mathbf{R} is separated. The two-body system is galilean invariant, hence the system as a whole realizes a reducible representation of the galilean group. In the center of mass system the system still has infinitely many degrees of freedom, namely with respect to the relative coordinates $\mathbf{q} = \mathbf{r}_1 - \mathbf{r}_2$. For spherically symmetric potentials the Lie algebra of angular momentum, \mathbf{J} , commutes with Hamiltonian H . But there are other Lie algebras of dynamical importance. The simplest is the Heisenberg Lie algebra consisting of \mathbf{p} , \mathbf{q} and I with $[p_i, q_j] = i\delta_{ij}$ ($\hbar = 1$). The corresponding group is called the Weyl group. In the enveloping field of $(\mathbf{p}, \mathbf{q}, I)$ (i.e. functions of \mathbf{p}, \mathbf{q}) there are other Lie algebras besides $\mathbf{J} = \mathbf{r} \times \mathbf{p}$. The Schrödinger equation can easily be solved if it can be written linearly in the generators of a dynamical group. For

example, the quantities

$$I_0 = -\frac{1}{8a}p^2 - \frac{a}{2}q^2 - \frac{b}{q^2}, \quad (8)$$

$$I_4 = -\frac{1}{8a}p^2 + \frac{a}{2}q^2 - \frac{b}{q^2}, \quad T = \frac{1}{2}\mathbf{q} \cdot \mathbf{p} - \frac{3}{4}i,$$

or, the quantities

$$I_0 = \frac{1}{2}\left(qp^2 + \frac{a}{q} + q\right), \quad (8')$$

$$I_4 = \frac{1}{2}\left(qp^2 + \frac{a}{q} - q\right), \quad T = \mathbf{q} \cdot \mathbf{p} - i$$

satisfy the commutation relations (exercise 11)

$$[I_0, I_4] = iT, \quad [I_4, T] = -iI_0, \quad (9)$$

$$[T, I_0] = iI_4,$$

which are almost like those of the components of the angular momentum J_i , i.e. generators of $SO(3)$, Eq. (7), except the minus sign in the second term. They are the generators of the group $SO(2, 1)$. The stationary Schrödinger equation for an oscillator (plus a $1/r^2$ -potential), or for Kepler problem (plus a $1/r^2$ -potential) can therefore be written as

$$(I_0 + \beta I_4 + \gamma)\Psi = 0, \quad (10)$$

where β and γ are functions of the parameters of the Schrödinger equation and E only (exercise 12). Because the unitary irreducible representations of the dynamical algebra and the spectra of the operators I_0, I_4, T are known, the solution space of the Schrödinger equation is identical with the representation space, and the problem is explicitly solved in terms of quantum numbers. We have thus a way to give a group theoretical (hence geometrical) foundation to quantum dynamics analogous to quantum kinematics: space-time groups are the analogs of dynamical groups. Quantization consists then in determining the representation of both symmetry and dynamical groups. The operators (8'), \mathbf{J} and others complete to a full dynamical algebra $O(4, 2)$ with 15 parameters which describe the complete degeneracy of the problem.

It is interesting that Eq. (10) is the rest frame form of a covariant equation of the form

$$(I_\mu P^\mu - M)\Psi = 0, \quad (11)$$

where I_μ and M are operators (i.e. infinite-dimensional matrices) and P_μ the total energy-momentum vector of the composite atom. Thus we have a generalization of the Dirac equation for the electron (where $I_\mu = \gamma_\mu$ is a 4×4 -matrix and $M = m$, a number) to a system with many more internal degrees of freedom; it treats the atom globally as

though it were an “elementary particle” — the interparticle potentials do not occur explicitly. Such equations are called *infinite component wave equations* and have been widely used also in hadron physics.

Given a system with dynamical variables (p_i, q_i) , the construction of all Lie algebras of the type (8) – (8') is a mathematical problem, largely unsolved. But we can also inquire into the geometric significance of dynamical groups. According to an old and ingenuous idea of Heinrich Hertz¹⁹ a motion in a potential field can be represented by a free geodesic motion in a higher dimensional space. It is possible that the concept of force or potential is due to the existence of cyclic (or ignorable) hidden coordinates and constraints, the elimination of which yields the potential terms in the Lagrangian. Indeed the nonrelativistic Kepler problem is a geodesic motion in a curved four-dimensional Riemannian space which is embedded in a 6 dimensional pseudo-euclidian space. If we start from a two-body problem and impose suitable restrictions we may arrive at the same manifold. Now the groups of motions in 6-dimensions, like $O(4, 2)$, act on the manifold of geodesics, which then shows the appearance of dynamical groups.

Geometric Quantization

While we are discussing mathematical problems we should mention the recent surge of interest among mathematicians to understand quantum theory from the point of view of group representations and symplectic structure of classical mechanics. This theory, called “geometric quantization” was initiated by Souriau and Kostant²⁰. The purposes of these efforts are first to formulate the quantization rules for arbitrary curvilinear coordinates, or better, in a coordinate independent way, and secondly to have a rigorous correspondance between the phase-space $(p_1, \dots; q_1, \dots)$ of analytical mechanics, and the wave function $\Psi(q)$ of quantum mechanics; as a result mathematicians will finally reformulate quantum mechanics. For a quantization starting from the phase-space one may also attempt to define suitable operators acting on the space of functions over the phase space with suitable scalar products. This type of quantization has been discussed early by Weyl²¹ and Wigner²²; it has been reintroduced again recently using the Moyal brackets²³.

There is of course still no satisfactory solution of the problem of ordering of noncommuting operators when passing from classical to quantum mechanics. It should be stressed that even in the case of the simplest problem the linear oscillator, the

Hamiltonian is not unique: the family of operators $H_\lambda = \frac{1}{2}(p^2 + q^2) + \lambda[p, q]$ all correspond to the same classical Hamiltonian since $[p, q]$ vanishes in the classical limit. The question can be settled by experimental consequences of the zero-point energy. It is, however, interesting that dynamical group quantization picks up a definite ordering, because only in one ordering will the commutation relations of the operators close to a Lie algebra as in the examples (8) and (8').

Quantum mechanics when properly formulated is equivalent to group representations. This is most evident for symmetry groups. More generally, if we know the states of a quantum system in its rest frame as a representation of a dynamical group we may pass to the states of the moving system by the mathematical process of induced representations²⁴, or by writing a wave equation of the type (11). The remaining problem is to choose, in the rest frame, among all canonical transformations, those corresponding to the dynamical group of the system.

There is also the inverse problem of going from quantum theory to classical theory. The quantum mechanical pure states are quite different than the classical ones. However, from the infinite superpositions of pure states one can construct the so-called coherent states in which the dispersion of various physical quantities takes its minimum value, e. g. $\Delta p \Delta q = \hbar/2$, or $\Delta J_x \Delta J_y = |\langle J_z \rangle| \hbar/2$. Such states come closest to the classical states in such a way that one can actually follow the classical elliptical orbits of the Kepler problem, for example²⁵.

Nonlinear Schrödinger Equation

The simplest realistic example of a non-linear Schrödinger equation has the form

$$i \hbar \frac{\partial \Psi}{\partial t} = - \frac{\hbar^2}{2m} \Delta \Psi + g^2 (\Psi^* \Psi) \Psi. \quad (12)$$

when compared with Eq. (1), the potential V is now proportional to the density of the solution. In an iterative process, one may assume a solution Ψ_0 , evaluate $V = g^2 (\Psi_0^* \Psi_0)$, and then solve the Schrödinger equation with this potential, etc. Equation (12) occurs in non-linear optics and in plasma physics. It does not come as a surprise, because the coupled Schrödinger and Maxwell equations ($c = \hbar = 1$)

$$i \frac{\partial \Psi}{\partial t} = \left[- \frac{1}{2m} (\nabla + i e \mathbf{A})^2 + A_0 \right] \Psi, \quad (13)$$

$$\square A_0 = e \Psi^* \Psi,$$

$$\square \mathbf{A} = - \frac{i e}{2m} [\Psi^* \nabla \Psi - (\nabla \Psi)^* \Psi]$$

lead, when we eliminate A_0 and \mathbf{A} , to even non-local, non-linear integro-differential equations. Compared to this, (12) is only a local nonlinear equation. Up to now little attention was given to the study of non-linear systems, but at present there is a growing interest, for non-linear equations possess many properties which are not present in the linear case²⁶. A striking case is the existence of particle-like solutions of non-linear classical equations called solitons. These represent a wave packet whose form does not change with time, even if two or more of them pass each other. The non-linear Schrödinger equation will be an important research field in the near future.

For example, for Eq. (12), there are spherically symmetric stationary solutions of the form $\Psi = f(r)e^{-i\omega t}$, where f satisfies the equation

$$Af + (2m\omega/\hbar)f - 2m(g/\hbar)^2 f^3 = 0.$$

In one-dimension, for example, there are periodic solutions, but in addition one “solution” (in this case better a one kink) solution of the form

$$f = \pm (\hbar^{1/2}/g) \tanh[\pm (m\omega/\hbar)^{1/2}(x - x_0)],$$

which carries a finite total field energy.

The Schrödinger Field

One can view the Schrödinger Eq. (1), or the non-linear Schrödinger equation (12) as classical field equations, or wave equations in analogy to the classical electromagnetic waves or water waves. It is not known whether a classical beam of very large number of particles (neglecting spin) would obey the Schrödinger field equation, as beam of a large number of photons do obey the macroscopic Maxwell field equations. If so the appearance of a macroscopic complex field Ψ and i is remarkable; if not, what is the macroscopic classical field of a beam of particles? Of course, in our daily experience we meet easily with classical electromagnetic fields, and single electrons, but the question is an important one. The quantization of Maxwell field gives us the collection of photons; the quantization of the Schrödinger field, called second quantization, gives the collection of one, two, ... many particle states. For photon field we have quantization only once, and if the Schrödinger field is a classical field there would be also only one quantization for the matter field. The coupling of the Maxwell field and the Schrödinger field governs the radiation problems of free or bound electrons. The method of second quantization and the corresponding perturbation theory diagrams have been extensively used in solid state, nuclear and statistical physics as well²⁷.

Eigenvalue Problems from Relativistic Theories

The Dirac equation of the electron

$$(-i\gamma^\mu \partial_\mu - m)\Psi = 0$$

is modelled after the Schrödinger equation (1). It is first order in time-derivatives and can be put in the form of Eq. (3): $i\partial\Psi/\partial t = H_D\Psi$. The difference is that Ψ is now a spinor with four-components, Ψ_α , and H_D is a 4×4 -matrix, hence we have a set of four coupled linear first order differential equations. Similar equations are valid for other relativistic systems of different masses and spins. After separating the angular part, the radial equation can be brought into the form (exercise 13)

$$[d^2/dr^2 + (E^2 - m^2) - V(r, E)]U(r) = 0, \quad (14)$$

i. e. a one-dimensional stationary Schrödinger equation in the “effective” potential $V(r, E)$, which is now energy dependent. A particularly instructive and rich example is provided by an electron with its anomalous magnetic moment moving in the Coulomb field of a positron. Here we see several phenomena that we have discussed. The potential in the reduced equation is shown in Figure 1. For low

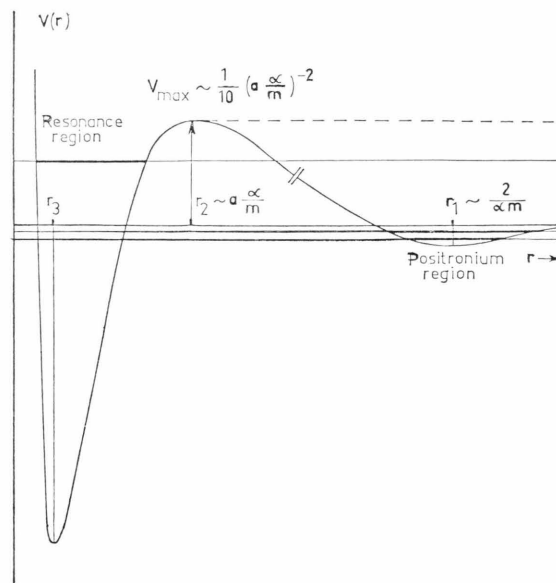


Fig. 1

negative energies we have the bound states corresponding to positronium. For positive high energies there are resonance states (called superpositronium); these are metastable states with very narrow-width which decay via barrier penetration²⁸. The poten-

tial shape of Fig. 1 is typical for all resonance phenomena in atomic, molecular and nuclear physics. It is possible that even the unstable elementary particles, neutron above all, or μ , π , K , ... mesons and baryons, decay, due to their internal constitution, via a barrier penetration. But this we do not know yet. At present the unstability of “elementary” particles are described by a new phenomenological interaction, called the weak interactions.

The inclusion of the magnetic interactions has the further effect that the centrifugal term

$$[j(j+1) - Z^2 \alpha^2]/r^2$$

of the Dirac equation is no longer the dominant potential as $r \rightarrow 0$. This term changes sign, hence the Dirac equation loses its validity for

$$Z \geq (\sqrt{3}/2) 137 \cong 118$$

(the Hamiltonian ceases to be self-adjoint — as we have discussed earlier), but Eq. (14) is now valid for all Z .

Just on this example of high Z Coulomb problem it is important to emphasize that the correct self-adjoint-extension of the Hamiltonian is a physical problem. Mathematically there may be many possible extensions none of which may be physical. It really depends what happens physically at $r \rightarrow 0$ when the potential is singular. We might put a cut-off to the potential at $r = r_0$ (corresponding roughly to nuclear size) and forbid the particle to penetrate into the region $r < r_0$, or the particle may really be spiralling into the singular center for a while and escape again. The dynamical group approach discussed earlier provides an extension which maybe of the second type. The spectra of high Z elements may give some clue to this problem.

Schrödinger Equation in Curved Space-time

The Schrödinger equation in the form (1) is valid only for cartesian coordinates. If we use generalized or curvilinear coordinates, or if the particle is in a Riemannian space, Eq. (1), must be modified. Already in 1927 physicists began to study such equations. It is clear that the Laplacian Δ must be replaced by the corresponding Laplace-Beltrami differential operator appropriate for a space with metric g_{ab} . But in addition there is a new term proportional to the scalar curvature R of the space which was missed in some of the early papers. Thus, the general form of the Schrödinger equation is ²⁹

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^a} \left(\sqrt{g} g^{ab} \frac{\partial \Psi}{\partial q^b} \right) - \frac{\hbar^2}{6} R \Psi, \quad (15)$$

where q^1, q^2, \dots are the generalized coordinates, g_{ab} metric in this configuration space, $g = \det |g_{ab}|$, $R = \text{curvature}$, and $\Psi(q^1, q^2, \dots; t)$ the wave function. This equation can be used in problems with constraints, for example, or as a matter of principle if the world is curved in the large (or possibly in the very small). It would be interesting to find physical examples of (15) to solve them in order to verify the quantization rules for arbitrary coordinates. An interesting example would be the motion of a quantum particle near a Schwarzschild singularity.

Coming back to the forceless mechanics of Hertz and Eisenhart²⁹, the trajectory of a particle in a potential V can be formulated as a geodesic in a higher dimensional Riemann space. This precisely gives us a possibility to verify the quantum Eq. (15), because the same problem, say the Coulomb problem, can either be formulated as a Schrödinger equation (1) in flat space with potential, or as a curved space Eq. (15) but without potential.

There is, in fact a curious discrepancy on the sign of the last term in Eq. (15) proportional to the scalar curvature between canonical quantization method and the Feynman path integral quantization, which contrary to some claims, has not been resolved³⁰.

Particle Coordinates versus Collective Degrees of Freedom

In Eqs. (1), (4) or (15) we have interpreted the variables x_i or q^a as the coordinates of particles. It is important to realize that exactly the same type of equations hold for the quantized collective degrees of freedom of complicated systems or fields. Consider an extended object, say a spherical shell, which, under appropriate forces, performs periodic radial oscillations. If such oscillations are quantized, each quantum carrying an energy $\hbar\omega$, where ω is the frequency of the oscillations, we will obtain a Schrödinger equation of the form

$$i\hbar \partial \Psi / \partial t = H(p, q) \Psi,$$

where now q is the radius of the shell (and not a particle coordinate), and p the conjugate variable to the radius. Thus the quantized oscillations of a deformable extended object can have discrete energy eigenvalues.

Collective motions of atoms and nuclei, rotations and deformations of a nucleus can be treated in this manner. It is possible that these considerations also apply to elementary particles in a fundamental way, especially to hadrons, which appear as objects with internal degrees of freedom, with internal charge

and magnetic moment distributions, but do not seem to split into constituents. Hence an extensible model would be a natural model. The motions of the extended continua can be formulated relativistically. For example the deformation vector $a_\mu(x)$ of an elastic medium may satisfy a field equation of the type

$$\square a_\mu(x) = -\partial V/\partial a^\mu, \quad (16)$$

where $V = V(a^\mu)$ is the potential energy as a function of deformations. If we ask for special solutions of these field equations depending on one single degree of freedom $\tau = (1/k^2) k^\mu x_\mu$ we arrive at $\ddot{a}_\mu = -\partial V/\partial a^\mu$, the quantization of which, in the rest frame, gives a Schrödinger equation³¹

$$[-\frac{1}{2}\Delta + V(a)]\Psi = M\Psi, \quad (17)$$

where the independent variables are the deformations and M the “mass” of the quantized deformations. We learn two lessons: (i) Nonrelativistic Schrödinger-like equations have a rigorous place in relativistic theories; (ii) A Schrödinger-like equation for the masses of a system does not necessarily represent particle-like constituents (which in particle physics may correspond to “quarks”), but may represent degrees of freedom for deformations. This would explain why quark-like “constituents” are not seen as free-particles and would solve automatically the problem of “quark-confinement”.

The Schrödinger equations which arise here have to be solved in a finite domain $0 \leq q \leq R$, where R can be itself a dynamical variable. This contrasts the standard boundary conditions at $q \rightarrow \infty$, and represents a novel mathematical feature: dynamical boundary conditions.

The Inverse Schrödinger Equation for Nonlinear Waves

The Schrödinger equation has occurred recently, in an unexpected way, in the solution of non-linear partial differential equations. Let $u(x, t)$ be a solution of a non-linear equation, for example, the Korteweg-de Fries equation

$$\frac{\partial u}{\partial t} - 6u \frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0, \quad 0 < x < \infty, t < 0, \quad (18)$$

then there exists an associated Schrödinger equation in which $u(x) \equiv u(x, 0)$ acts as a potential:

$$\partial^2 \Psi / \partial x^2 - [u(x) - \lambda] \Psi = 0. \quad (19)$$

The appearance of Ψ is only intermediary; the correspondence is, we repeat, between nonlinear classical wave u and the potential in the associated linear Schrödinger equation. The inverse scattering problem in wave mechanics is the determination of

the potential from the knowledge of its bound states and phase shifts, e. g. via the Gel'fand-Levitan equation³². Hence the solution of (18) can be expressed in terms of a discrete set of bound state parameters and phase-shifts $\delta(k)$, whose time-evolution is known. This is then an important method of exact solution of non-linear equations³³. For example, for (18), if the initial condition is $u(x, 0) = -2 \operatorname{sech}^2 x$, Eq. (19) is an exactly soluble Schrödinger equation with one bound state only and the Gelfand-Levitan equation gives

$$u(x, t) = -2 \operatorname{sech}^2(x - 4t) \quad (19)$$

which is the famous soliton solution of (18), a solitary wave with velocity 4 and fixed amplitude 2 (in proper units).

Let $\hat{L} = -d^2/dx^2 + u(x, t)$. Introducing an operator

$$B = -4 \frac{d^3}{dx^3} + 6u \frac{d}{dx} + 3 \frac{du}{dx} + ic.$$

we can rewrite the non-linear Eq. (18) as

$$\partial L / \partial t = [B, L(t)].$$

This is the Heisenberg equation for the “associated” problem: B plays the role of the “Hamiltonian” and $L(t)$ of an observable. Consequently, the eigenvalues λ of $L(t)$ are independent of time, and we can write $L(t) = U(t) L(0) U^{-1}(t)$ with $U(t) = e^{Bt}$. Thus, it is sufficient to consider $L(0) = -d^2/dx^2 + u(x, 0)$ as we did above.

Theory of Forces

The Schrödinger equation (1) still contains an arbitrary potential V within certain limits discussed. A physical theory is not complete unless we specify besides the equations of motion, also precisely the form of the forces or potentials which actually occur in nature. Not every function V is physical. This is true in mechanics, wave mechanics and in field theories. The theory should not contain no more or no less than those interactions which can occur in nature. The form of interactions is determined from a model of matter which complements the laws of motions, and together makes physics possible.

Thus at the fundamental level we must have principles which uniquely determines the potential between the particles existing in nature, or the coupling between two fields. The Maxwell equations coupled via the principle of minimal electromagnetic interactions to the Schrödinger equation, Eqs. (13), solve this problem for non-relativistic problems. But the principle of minimal interactions although elegant from a geometric point of view is rather mys-

terious and the underlying physics is not easily expressible intuitively. It would be desirable to have more compelling principles, for example, of geometrical nature. Or to have a “unitary” theory in which matter occurs as singularities of fields.

Wave Functions with Non-integrable Phase Factors

Usually Schrödinger’s concept of wave function $\Psi(x, t)$ is represented by a standard complex function. It was noted early by Weyl³⁴ and Dirac³⁵ that more general mathematical objects may represent new fundamental phenomena. The general principles of quantum mechanics are not violated, if the wave function Ψ has a phase which depends on a path in space time. Let

$$\Psi = \Psi_1 \exp(i\beta), \quad (20)$$

where Ψ_1 has a definite phase and β is not an ordinary local function, but its value at the point $P = (x, t)$ depends on the path $C(P_0 P)$ from a fixed point P_0 . But β is the same for all wave functions of the system in order to satisfy the superposition principle. Assuming the derivatives of β are local functions, we can write

$$\beta = \frac{e}{\hbar} \int_{P_0}^P A_\mu(x) dx^\mu, \quad \mu = 0, 1, 2, 3, \quad (21)$$

where $A_\mu(x, t)$ are local functions, which are not gradient of some scalar function $\varphi(x, t)$.

If now Ψ is the basic wave concept and satisfies a wave equation of the Schrödinger (or Dirac) type, then Ψ_1 will satisfy the equation

$$i\hbar \left(\frac{\partial}{\partial t} + i \frac{e}{\hbar} A_0 \right) \Psi_1 = - \frac{\hbar^2}{2m} \left(\nabla + i \frac{e}{\hbar} \mathbf{A} \right)^2 \Psi_1, \quad (22)$$

which is precisely the first of Equations (13). It is remarkable, that the very fundamental, and some-

what mysterious concept of “minimal coupling” has such a geometrical significance.

A further consequence of the phase factor in (20) and (21) is the following. The phase factor is undetermined by an additive term $2\pi n$. By continuity arguments this can happen if the wave function vanishes inside a small closed path along which the phase (21) is evaluated. We have then using Stokes theorem

$$\begin{aligned} (e/\hbar) \oint A_\mu dx^\mu &= (e/\hbar) \int F_{\mu\nu} dx^\mu dx^\nu \\ &= (e/\hbar) \int \mathbf{B} \cdot d\mathbf{f} = 2\pi n. \end{aligned}$$

Thus, if there is an indeterminacy in the phase by an amount $2\pi n$, the magnetic flux $\int \mathbf{B} \cdot d\mathbf{f} = 2\pi n \hbar/e = n h/e$ is not only different from zero, but also quantized in units of h/e . This phenomenon occurs in superconductivity as well as in the theory of magnetic monopoles. In fact Dirac²³ introduced magnetic charges by this procedure. For if the flux $\oint \mathbf{B} \cdot d\mathbf{f}$ is due to a magnetic pole, we have $\oint \mathbf{B} \cdot d\mathbf{f} = 4\pi g = n h/e$, or $eg = \frac{1}{2} n \hbar$, which is the charge quantization condition.

It is interesting that the Schrödinger equation is exactly soluble for two interacting pair of dyons (dyon = particle having both an electric charge e and a magnetic charge g) both by functional and dynamical group methods³⁶. A great deal of our knowledge about models of hadrons with magnetic monopoles is derived from such exact solutions, as was the case in atomic models for the exact solution of the Schrödinger equation with Coulomb potential. This by the way is now a special case of the former.

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I confine myself to references of historical importance and to appropriate reviews where other references can be found.

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