

QUANTIZATION OF NONLINEAR WAVE EQUATIONS

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ABSTRACT. We show that quantization of a nonrelativistic nonlinear wave equation is equivalent to the set of N -particle Schrödinger equations for all positive N . We compare the qualitative features of the quantized and unquantized field theory in a particular case, the cubic Schrödinger equation in one spatial dimension. We comment on the features of more general quantum field theories of interest in physics, and their possible relations to the properties of solutions of the corresponding classical field equations.

During the past three years there has been a growing interest among physicists in the quantization of soluble classical field theories (equivalent generally to systems of coupled nonlinear partial differential equations) [1], [4], [5]. It is the purpose of this review to sketch the quantization procedure as applied to relatively simple classical field theories, and to demonstrate that the resulting quantum field theories can be interpreted as describing an interesting physical system. Although the quantum field theory associated with a given classical field theory does not generally describe the same system as the classical theory, nonetheless solutions to the equations of motion of the classical theory give approximate information about physical observables in the quantized system.

1. The Quantization Procedure. In classical mechanics, the dynamics of a physical system is specified by a variational principle, Hamilton's principle:

$$\delta S = 0 \quad S = \int_{t_1}^{t_2} dt L$$

(1.1)

$$L = T(q_i, \dot{q}_i) - V(q_i)$$

where the action S is a time integral over the Lagrangian L . The potential energy V and kinetic energy T are expressed in terms of the system's coordinates $\{q_i\}$ and their first time derivatives $\{\dot{q}_i\}$. The variational condition $\delta S = 0$ is understood more precisely to mean that the actual ("allowed") motions of the system $\{q_i(t)\}$ correspond to the extrema of the functional S with the boundary conditions

$$q_i(t_1) = q_i^{(1)}$$
$$q_i(t_2) = q_i^{(2)}$$

(1.2)

fixed. The allowed motions expressed in terms of the Lagrangian are

$$(1.3) \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i},$$

which is generally a set of coupled second order nonlinear differential equations for the coordinates, one for each of the N q_i .

The Hamiltonian $H(p_i, q_i)$ is defined by the Legendre transformation

$$(1.4) \quad H = \sum_i p_i \dot{q}_i - L,$$

$$(1.5) \quad p_i \equiv \frac{\partial L}{\partial \dot{q}_i}, \quad i = 1, \dots, N$$

where p_i is called the i th *canonical momentum*. In terms of the Hamiltonian the equations of motion are

$$(1.6) \quad \begin{aligned} \frac{d}{dt} p_i &= - \frac{\partial H}{\partial q_i} \\ \frac{d}{dt} q_i &= \frac{\partial H}{\partial p_i} \end{aligned}$$

For $\partial V/\partial t = 0$, H is the total energy of the system, and is constant in time.

Canonical quantization is a set of rules by which the dynamics of the *quantized system* is associated with the dynamics of the classical system (1.6). In each case *dynamics* is defined to mean the time evolution of the system's *physical observables*. For the classical system the physical observables are the canonical coordinates and momenta, $\{q_i\}$ and $\{p_i\}$, which are the dependent variables in equation (1.6). The state of the classical system is specified at any time t by listing $q_i(t)$, $p_i(t)$, $i = 1, \dots, N$.

In the quantized system, the physical observables, still denoted $\{q_i\}$ and $\{p_i\}$, are Hermitian operators on the vectors ψ of a Hilbert space \mathcal{H} , and distinct states of the system correspond to distinct rays (sometimes called *state vectors*) in \mathcal{H} . The physical observables are constrained to obey the algebra

$$(1.7) \quad p_i q_j - q_j p_i \equiv [p_i, q_j] = -i\hbar \delta_{ij},$$

where $\hbar = 1.054 \times 10^{-27}$ erg-sec is related to Planck's constant. We will henceforth measure the p 's and q 's in units where $\hbar = 1$. Equation (1.7) is understood to mean

$$(1.8) \quad (\alpha, [p_i, q_j]\beta) = (\alpha, -i\hbar \delta_{ij}\beta) \quad \text{for all } \alpha, \beta$$

where α and β are vectors of \mathcal{H} , and (\cdot, \cdot) is the inner product on \mathcal{H} . [Since in quantum mechanics one is usually concerned with Hermitian operators \mathcal{O} , for which $(\alpha, \mathcal{O} \beta) = (\beta, \mathcal{O} \alpha)^*$, the notation $\langle \alpha | \mathcal{O} | \beta \rangle \equiv (\alpha, \mathcal{O} \beta)$ (introduced by Dirac) is commonly used. In this notation, vectors of \mathcal{H} are denoted $|\alpha\rangle$, their Hermitian conjugates $\langle \alpha|$, and the inner product $\langle \alpha | \beta \rangle = (\alpha, \beta)$.] It is immediately evident that no vector of \mathcal{H} can simultaneously be an eigenvector of two operators A and B unless $[A, B] = 0$. If $\{A_i\}$ is a set of mutually commuting observables, all functions of the p 's and q 's, and assumed functionally independent, then $\{A_i\}$ is called *complete* if there exists no operator $B(\{p_i\}, \{q_i\})$ which is functionally independent of the A_i satisfying $[B, A_i] = 0$ for all i . The simultaneous eigenvectors of a complete set of (mutually) commuting observables span \mathcal{H} . Such a basis vector ψ , satisfying

$$(1.9) \quad A_i \psi = a_i \psi$$

corresponds to a physical state where a measurement of the observable corresponding to A_i is certain to yield the numerical result a_i . A general physical state need not be an eigenvector of *any* of a particular complete set of commuting observables.

It is easy to prove the *uncertainty principle*, which says that for any state ψ , if $[p, q] = -iI$

$$(1.10) \quad (\psi, (p - \bar{p})^2 \psi)(\psi, (q - \bar{q})^2 \psi) \geq \frac{1}{4} (\psi, \psi)^2$$

where $\bar{p} = (\psi, p\psi)$ and $\bar{q} = (\psi, q\psi)$. For let $\alpha = (p - \bar{p})\psi$ and $\beta = (q - \bar{q})\psi$. By Schwarz's inequality, $(\alpha, \alpha)(\beta, \beta) \geq |(\alpha, \beta)|^2$, and thus with $\hat{p} = p - \bar{p}$, $\hat{q} = q - \bar{q}$

$$(1.11) \quad \begin{aligned} (\psi, \hat{p}^2 \psi)(\psi, \hat{q}^2 \psi) &\geq |(\psi, \hat{p}\hat{q}\psi)|^2 \\ &= |(\psi, \{\frac{1}{2}[\hat{p}, \hat{q}] + \frac{1}{2}(\hat{p}\hat{q} + \hat{q}\hat{p})\}\psi)|^2 \\ &= |(\psi, -i/2 \psi)|^2 + |(\psi, \frac{1}{2}[\hat{p}\hat{z} \hat{q}\hat{p}]\psi)|^2 \\ &\geq \frac{1}{4} (\psi, \psi)^2 \end{aligned}$$

where in the second from the last step we have used the commutator condition and the Hermiticity of p and q .

The dynamics of the quantum system is specified by (1.6), where the p 's and q 's are now regarded as Hermitian operators. Using (1.7) the operator equations of motion can be rewritten

$$(1.12) \quad \begin{aligned} \frac{d}{dt} p_i &= i[H, p_i] \\ \frac{d}{dt} q_i &= i[H, q_i], \end{aligned}$$

where $\hbar = 1$. The system (1.12) is understood more rigorously to mean

$$(1.13) \quad \begin{aligned} \frac{d}{dt} (\alpha, p_i \beta) &= (\alpha, i[H, p_i] \beta) \\ \frac{d}{dt} (\alpha, q_i \beta) &= (\alpha, i[H, q_i] \beta). \end{aligned}$$

Note that equations (1.12) have the form

$$(1.14) \quad \frac{d}{dt} \mathcal{O} = i[H, \mathcal{O}].$$

This is true more generally of any operator \mathcal{O} which is a function of the p 's and q 's, and which does not depend explicitly on time. An immediate consequence is that if $[H, \mathcal{O}] = 0$, \mathcal{O} corresponds to a *conserved quantity* of the quantized system, and eigenvectors of the Hamiltonian can be chosen to be eigenvectors of \mathcal{O} as well.

It is apparent from the form of (1.13) that one is free to assign the time dependence either to the state vectors or to the operators. In the *Schrödinger picture*, the operators are taken to be time independent and the state vectors time dependent, so that as the system develops in time it is described by a sequence of different state vectors. As a consequence (1.13) becomes the Schrödinger equation

$$(1.15) \quad H_s(p, q) \beta_s(t) = i \frac{\partial}{\partial t} \beta_s(t),$$

which is formally integrated to yield

$$(1.16) \quad \beta_s(t) = e^{-iHt} \beta_s(0).$$

In the Schrödinger picture, for a finite number of p 's and q 's, the commutation relations (1.7) can be represented by

$$(1.17) \quad p_i = -i \frac{\partial}{\partial q_i}$$

and the state vector by a function of the q 's and time

$$(1.18) \quad \psi(q_1, \dots, q_N; t).$$

Then (1.13) are equivalent to

$$(1.19) \quad \begin{aligned} & i \frac{\partial}{\partial t} \psi(q_1, \dots, q_N; t) \\ &= H \left(p_i = -i \frac{\partial}{\partial q_i}, q_i \right) \psi(q_1, \dots, q_N; t), \end{aligned}$$

which is the usual Schrödinger equation.

In the *Heisenberg picture*, all the time dependence is assigned to the operators. The Heisenberg picture state vectors are related to those in the Schrödinger picture by the unitary transformation

$$(1.20) \quad \beta_s(t) = e^{-iHt} \beta_H \Rightarrow \beta_H = \beta_s(0).$$

When the operators in the two pictures are related

$$(1.21) \quad \mathcal{O}_s = e^{-iHt} \mathcal{O}_H e^{iHt}$$

it is apparent that the inner products (called *matrix elements* in quantum mechanical language) are the same in the two pictures:

$$(1.22) \quad (\alpha_s, \mathcal{O}_s \beta_s) = (\alpha_H, \mathcal{O}_H \beta_H).$$

The choice between the Schrödinger and Heisenberg pictures is dictated by convenience. [In some applications it is convenient to put part of the time dependence in the state vectors and the remainder in the operators. This is called the *interaction picture*.]

2. The Harmonic Oscillator. We now demonstrate the utility of the Heisenberg picture by solving perhaps the most fundamental quantum mechanical system, the harmonic oscillator. The Lagrangian

$$(2.1) \quad L = \frac{1}{2} (\dot{x}^2 - x^2)$$

leads to

$$(2.2) \quad H = \frac{1}{2} (p^2 + q^2),$$

and from (1.6) to the equations of motion

$$(2.3) \quad \begin{aligned} p(t) &= \frac{dq(t)}{dt} \equiv \dot{q}(t) \\ q(t) &= - \frac{dp(t)}{dt} \equiv -\dot{p}(t). \end{aligned}$$

Defining the new operators

$$(2.4) \quad \begin{aligned} a &= \frac{1}{2^{1/2}} (q + ip) \\ a^\dagger &= \frac{1}{2^{1/2}} (q - ip), \end{aligned}$$

we find that (2.3) becomes

$$(2.5) \quad \dot{a}(t) = -ia(t); \quad \dot{a}^\dagger(t) = ia^\dagger(t),$$

which is immediately integrated. From the commutation relations (1.7),

$$(2.6) \quad \begin{aligned} [a(t), a^\dagger(t)] &= 1 \\ [a(t), a(t)] &= [a^\dagger(t), a^\dagger(t)] = 0. \end{aligned}$$

In terms of a and a^\dagger

$$(2.7) \quad H = \frac{1}{2} (a^\dagger a + a a^\dagger)$$

and it is readily computed that

$$(2.8) \quad [H, a] = -a, \quad [H, a^\dagger] = a^\dagger$$

Eigenstates of H are states of definite energy. If ψ_n is an eigenstate with energy ω_n , $H\psi_n = \omega_n\psi_n$, we find from (2.8) that

$$(2.9) \quad \begin{aligned} H(a^\dagger\psi_n) &= a^\dagger H\psi_n + [H, a^\dagger]\psi_n \\ &= (\omega_n + 1)a^\dagger\psi_n \end{aligned}$$

and similarly

$$(2.10) \quad H(a\psi_n) = (\omega_n - 1)a\psi_n.$$

Thus, starting from ψ_n we can generate an infinite series of other eigenstates by repeated application of a and a^\dagger .

$$(2.11) \quad \begin{aligned} \psi_{n+r} &= (a^\dagger)^r \psi_n & H\psi_{n+r} &= (\omega_n + r)\psi_{n+r} \\ \psi_{n-r} &= (a)^r \psi_n & H\psi_{n-r} &= (\omega_n - r)\psi_{n-r} \end{aligned}$$

However the spectrum of H is bounded below since H is a sum of squares of Hermitian operators, and consequently there must be a state of lowest energy ψ_0 such that

$$(2.12) \quad a\psi_0 = 0.$$

This state has energy E_0 given by

$$(2.13) \quad \begin{aligned} E_0\psi_0 &= H\psi_0 = \frac{1}{2} a a^\dagger \psi_0 \\ &= \frac{1}{2} [a, a^\dagger] \psi_0 = \frac{1}{2} \psi_0 \end{aligned}$$

Thus we know the entire spectrum of H :

$$(2.14) \quad H\psi_n = (n + \frac{1}{2})\psi_n, \quad n = 0, 1, 2, \dots$$

[In the Schrödinger picture the Hamiltonian is the differential operator $H = (-\partial^2/\partial x^2 + x^2)/2$, and finding its eigenvalues involves considerably more labor.]

The interpretation of the discrete spectrum of H is that the quantized harmonic oscillator has only certain allowed energies, in contrast with the classical harmonic oscillator. This is typical of quantized sys-

tems. [Normally in addition to a countable number of discrete states there is a continuous portion of the spectrum, higher in energy [6].] We say the harmonic oscillator, which might represent one of the normal modes of oscillation of a complicated system, is *occupied by n quanta*, $n = 0, 1, 2, \dots$, where n is called the *occupation number* (or later, the *occupation number* for this mode of oscillation).

It is possible to construct an operator N which corresponds to a conserved quantity of the oscillator,

$$(2.15) \quad N = a^\dagger a, \quad [H, N] = 0.$$

Clearly $N\psi_0 = 0$ since $a\psi_0 = 0$, and if $N\psi_n = \tilde{n}\psi_n$,

$$(2.16) \quad \begin{aligned} N\psi_{n+1} &= na^\dagger\psi_n = a^\dagger N\psi_n + [N, a^\dagger]\psi_n \\ &= (\tilde{n} + 1)a^\dagger\psi_n = (\tilde{n} + 1)\psi_{n+1}. \end{aligned}$$

Thus $N\psi_n = n\psi_n$ and N , which extracts the occupation number of any state ψ_n , is called the *number operator*.

Finally we note that if we define normalized state vectors $\tilde{\psi}_n$ so that $(\tilde{\psi}_n, \tilde{\psi}_n) = 1$, it can be shown that

$$(2.17) \quad \begin{aligned} a\tilde{\psi}_n &= (n)^{1/2}\tilde{\psi}_{n-1} \\ a^\dagger\tilde{\psi}_n &= (n + 1)^{1/2}\tilde{\psi}_{n+1}. \end{aligned}$$

3. Quantum Field Theory. Some physical systems are essentially continuous in nature (that is, have essentially an infinite number of observables) and yet display unmistakable signs of quantum behavior, such as permitting only discrete values of the total energy. An example is electrons in a crystalline solid. In any macroscopic sample there are on the order of 10^{22} quasi-free electrons (quasi-free in that they are not bound to a particular atom, but, of course, can't leave the sample).

It is then natural to extend the quantization procedure to continuous systems. For continuous systems (1.1) becomes

$$(3.1) \quad \delta S = 0 \quad S = \int_{t_1}^{t_2} dt \int d^3x \mathcal{L}$$

$$\mathcal{L} = \mathcal{F}(\varphi, \dot{\varphi}) - \mathcal{V}(\varphi, t).$$

\mathcal{L} , the *Lagrangian density*, is now the difference of the kinetic and potential energy *densities*, written in terms of the *field* $\varphi(x, t)$ and its first time derivative and first spatial derivative (we consider only the case of a single field). Here x is really just an index, differing from i in (1.1) only in that it can take on a continuous set of values. Defining the canonical momentum

$$(3.2) \quad \pi(x, t) = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}(x, t)},$$

we may define the *Hamiltonian density* by the Legendre transformation

$$(3.3) \quad \mathcal{H} = \int d^3x \pi(x, t) \dot{\varphi}(x, t) - \mathcal{L}$$

and the Hamiltonian

$$(3.4) \quad H = \int d^3x \mathcal{H}.$$

In the transcription to continuum systems, the quantization procedure generalizes straightforwardly [7]. The field variables become *field operators* on a Hilbert space of state vectors, and satisfy the *equal time commutation relations* (ETCR)

$$(3.5) \quad [\pi(x, t), \varphi(x', t)] = -i(\hbar)\delta^3(x - x').$$

The equations of motion transcribe to

$$(3.6) \quad \frac{d}{dt} \pi = i[H, \pi], \quad \frac{d}{dt} \varphi = i[H, \varphi].$$

We now embark on the demonstration that the non-relativistic quantized system whose classical Hamiltonian density is

$$(3.7) \quad \mathcal{H}(x) = -(\vec{\nabla} \varphi(x))^2 + \frac{1}{2} \int d^3y |\varphi(x)|^2 V(x - y) |\varphi(y)|^2$$

is equivalent to the Schrödinger equation for N identical bosons,

$$(3.8) \quad i \frac{\partial}{\partial t} \psi(q_1 \cdots q_N; t) = \left[\sum_{j=1}^N -\frac{d^2}{dq_j^2} + \sum_{i,j} V(q_i - q_j) \right] \psi(q_1 \cdots q_N; t)$$

for all N . In other words, to a quantized system of N particles interacting pairwise via the potential $V(x - y)$, for any N . The development below follows that of Fetter and Walecka [8].

The equivalence of (3.7) and (3.8) is most easily demonstrated by rewriting both in terms of creation and annihilation operators for the normal modes of oscillation in each case.

Let us begin with (3.8). The Schrödinger wavefunction $\psi(q_1 \cdots q_N; t)$ may be expanded

$$(3.9) \quad \psi(q_1 \cdots q_N; t) = \sum_{k_1 \cdots k_N} C(k_1 \cdots k_N; t) \psi_{k_1}(q_1) \cdots \psi_{k_N}(q_N),$$

where the $\{\psi_k(x)\}$ constitute a complete orthonormal set. Thus the normalization $\int |(q_1 \cdots q_N; t)|^2 d^N q = 1$ means that $\sum_{k_1, \dots, k_N} |C(k_1 \cdots k_N; t)|^2 = 1$. Typically the $\{\psi_k(x)\}$ are chosen to be plane waves $\psi_k(x) = e^{ikx}$ for convenience. Substituting this expression in (3.8) and using the orthonormality of the $\{\psi_k(x)\}$ we obtain

$$\begin{aligned}
 & i \frac{\partial}{\partial t} C(k_i \cdots k_N; t) \\
 &= \sum_{j=1}^N \sum_k \int dq_j \psi_{k_j}^\dagger(q_j) \\
 & \quad \left(- \frac{\partial^2}{\partial q_j^2} \right) \psi_k(q_j) C(k_1 \cdots k_{j-1} k k_{j+1} \cdots k_N; t) \\
 (3.10) \quad & + \frac{1}{2} \sum_{i \neq j=1}^N \sum_k \sum_{k'} \int \int dq_i dq_j \psi_{k_i}^\dagger \\
 & \quad (q_i) \psi_{k_j}^\dagger(q_j) V(q_i - q_j) \psi_k(q_i) \psi_{k'}(q_j) \\
 & \quad \times C(k_i \cdots k_{i-1} k k_{i+1} \cdots k_{j-1} k' k_{j+1} \cdots k_N; t).
 \end{aligned}$$

We may streamline the notation somewhat by letting

$$(3.11) \quad \int dq_j \psi_{k_j}^\dagger(q_j) \left(- \frac{\partial^2}{\partial q_j^2} \right) \psi_k(q_j) \equiv \langle k_j | T | k \rangle$$

and

$$\begin{aligned}
 (3.12) \quad & \int \int dq_i dq_j \psi_{k_i}^\dagger(q_i) \psi_{k_j}^\dagger(q_j) \\
 & \quad V(q_i - q_j) \psi_k(q_i) \psi_{k'}(q_j) \equiv \langle k_i k_j | V | k k' \rangle.
 \end{aligned}$$

We now make use of our assumption that the N particles described by (3.10) are identical bosons. This is equivalent to the physical assumption of the indistinguishability of identical particles, which says that in our system of N particles we are not allowed to talk, for example, about states with particle 2 at position x , but only about states with a particle at position x , since no one particle can be distinguished from any of the others. Mathematically this is expressed by specifying that the space of state vectors $\psi(q_1 \cdots q_N; t)$ is the *completely symmetrized* tensor product of the "one particle spaces" $\{\psi_k(x)\}$. Consequently we may take the C coefficients to be completely symmetric in the arguments k_1, \dots, k_N . (For identical particles obeying Fermi statistics, the space of state vectors is the *completely antisymmetrized* tensor product of the one-particle spaces, and the C coefficients are completely *anti-*

symmetric in their arguments.) Thus there is a large redundancy in the C 's.

Suppose the complete orthonormal set $\{\psi_k(x)\}$ is labeled by $k = k^{(1)}, k^{(2)}, \dots$. (For systems of infinite volume, the complete orthonormal set will generally have a continuous index. In the interest of notational simplicity, we will pretend that the index is discrete.) Then a C coefficient (and all its brothers obtained by permuting the arguments) may be specified by listing the number of arguments n_i among the k_j that take on the value $k^{(i)}$. n_i is called the *occupation number of the i^{th} one particle mode*. Obviously

$$(3.13) \quad 0 \leq n_i \leq N; \sum_i n_i = N.$$

Now define a new set of coefficients

$$(3.14) \quad f(n_1, n_2, \dots; t) \equiv \left(\frac{N!}{n_1!n_2! \dots} \right)^{1/2} C(\dots; t)$$

$$0! \equiv 1$$

where $C(\dots; t)$ is any of the C coefficients among whose arguments each $k^{(i)}$ appears n_i times. These have the normalization

$$(3.15) \quad \sum_{n_1 n_2 \dots} |f(n_1 n_2 \dots; t)|^2 = 1.$$

Now we insert (3.14) into (3.10) and convert the sums over indices k, k' , etc. to sums over the occupation numbers n_1, n_2, \dots . After considerable algebra and combinatorics [6] we obtain

$$(3.16) \quad i \frac{\partial}{\partial t} f(n_1 n_2 \dots; t) = \sum_i \langle i|T|i \rangle n_i f(n_1 n_2 \dots; t)$$

$$+ \sum_{i \neq j} \langle i|T|j \rangle (n_i)^{1/2} (n_j + 1)^{1/2}$$

$$f(n_1 \dots n_i - 1 \dots n_j + 1 \dots; t)$$

$$+ \sum_{i \neq j \neq k \neq l} \langle ij|V|kl \rangle \frac{1}{2} (n_i)^{1/2} (n_j)^{1/2} (n_k + 1)^{1/2} (n_l + 1)^{1/2}$$

$$f(n_1 \dots n_i - 1 \dots n_j - 1 \dots n_k + 1 \dots n_l + 1 \dots; t)$$

$$+ \sum_{i \neq j \neq k \neq l} \langle ij|V|kl \rangle \frac{1}{2} (n_i)^{1/2} (n_i - 1)^{1/2} (n_k + 1)^{1/2} (n_l + 1)^{1/2}$$

$$f(n_1 \dots n_i - 2 \dots n_k + 1 \dots n_l + 1 \dots; t).$$

The Schrödinger wavefunction $\psi(q_1 \cdots q_N; t)$ may be written in terms of *time independent abstract state vectors* $|n_1 n_2 \cdots\rangle$:

$$(3.17) \quad |\psi(t)\rangle \equiv \psi(q_1 \cdots q_N; t) = \sum_{n_1 n_2 \cdots} f(n_1 n_2 \cdots; t) |n_1 n_2 \cdots\rangle.$$

Note that all the time dependence of ψ is contained in the f coefficients. In terms of the one particle basis vectors

$$(3.18) \quad |n_1 n_2 \cdots\rangle \doteq \left(\frac{n_1! n_2! \cdots}{N!} \right)^{1/2} \sum_{\substack{k_1 \cdots k_N \\ \leftrightarrow (n_1 n_2 \cdots)}} \psi_{k_1}(q_1) \cdots \psi_{k_N}(q_N),$$

where the sum is over all sets $\{k_i\}$ consistent with the occupation numbers $\{n_i\}$, and equality is understood in the sense of denoting the same vector in \mathcal{H} . The abstract state vector is just the tensor product

$$(3.19) \quad |n_1 n_2 \cdots\rangle = |n_1\rangle_1 |n_2\rangle_2 \cdots,$$

where $|n_i\rangle_i$ is a state vector in the space where the single mode $\psi_{k_i}(x)$ can be occupied by any non-negative number of particles $n_i = 0, 1, 2, \cdots$ (in practice $n_i \leq N$, but we need not restrict the space on this account). We define creation and annihilation operators on these spaces in exact analogy to those for the harmonic oscillator

$$(3.20) \quad \begin{aligned} [b_i, b_j^\dagger] &= \delta_{ij} [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0, \\ N_i |n_i\rangle_i &\equiv b_i^\dagger b_i |n_i\rangle_i = n_i |n_i\rangle_i, \\ b_i |n_i\rangle_i &= (n_i)^{1/2} |n_i - 1\rangle_i, \\ b_i^\dagger |n_i\rangle_i &= (n_i + 1)^{1/2} |n_i + 1\rangle_i. \end{aligned}$$

Here N_i is the number operator in the i^{th} space.

It is now a simple matter to rewrite the vector version of (3.16) (recall we arrived at (3.16) by taking inner products with the vector equation (3.8)) to obtain an expression for the Hamiltonian in terms of operators on the space of abstract state vectors $|n_1 n_2 \cdots\rangle$. Take the second term on the right hand side of (3.16) as an example. Using (3.17) it becomes

$$\begin{aligned}
& \sum_{n_1 n_2 \dots} \sum_{i \neq j} \langle i|T|j \rangle f(\dots n_i - 1 \dots n_j + 1 \dots) \\
& \quad (n_i)^{1/2} (n_j + 1)^{1/2} |n_1 n_2 \dots \rangle \\
& \quad = \left\{ \sum_{n_1 n_2 \dots} \sum_{i \neq j} \langle i|T|j \rangle f(\dots n_i' \dots n_j' \dots) \right\} \\
(3.21) \quad & (n_i' + 1)^{1/2} (n_j')^{1/2} |n_1 n_2 \dots \rangle \\
& \quad = \{ \quad \} b_i^\dagger b_j |n_1 n_2 \dots \rangle \\
& \quad = \sum_{i \neq j} \langle i|T|j \rangle b_i^\dagger b_j |\psi(t)\rangle.
\end{aligned}$$

After similar manipulations on the other terms, the Schrödinger equation becomes

$$\begin{aligned}
(3.22) \quad & i \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \\
& \hat{H} = \sum_{ij} b_i^\dagger \langle i|T|j \rangle b_j \\
& \quad + \frac{1}{2} \sum_{ijkl} b_i^\dagger b_j^\dagger \langle ij|V|kl \rangle b_k b_l.
\end{aligned}$$

Defining the total number operator

$$(3.23) \quad \hat{N} = \sum_i N_i$$

we find that

$$[H, \hat{N}] = 0,$$

so that by (1.14), the total number of particles is conserved in time, as expected.

Bringing (3.7) into the form (3.22) is almost a trivial task. When quantized, the system (3.7) has the Hamiltonian

$$\begin{aligned}
(3.24) \quad & H = \int d^3x \hat{\psi}^\dagger(x) T(x) \hat{\psi}(x) \\
& \quad + \frac{1}{2} \int \int d^3x d^3y \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) V(x-y) \hat{\psi}(y) \hat{\psi}(x) \\
& T = - \frac{\partial^2}{\partial x^2},
\end{aligned}$$

where the hat reminds us that ψ and ψ^\dagger become operators. If we expand $\hat{\psi}$ and $\hat{\psi}^\dagger$ in terms of the operators c_k and c_k^\dagger , we have

$$\begin{aligned} \hat{\psi}(x) &= \sum_k \psi_k(x) C_k \\ \hat{\psi}^\dagger(x) &= \sum_k \psi_k^\dagger(x) C_k^\dagger \end{aligned} \tag{3.25}$$

where $\{\psi_k(x)\}$ are the *same functions* as in (3.9), and find that the ETCR (3.5) require that c and c^\dagger obey

$$[C_i, C_j^\dagger] = \delta_{ij}, \quad [C_i, C_j] = [C_i^\dagger, C_j^\dagger] = 0. \tag{3.26}$$

The state vectors are once again $|\psi(t)\rangle = \sum f(n_1 n_2 \dots; t) |n_1 \dots\rangle$ as in (3.17), and using (3.11), (3.12), and (3.25), the Hamiltonian becomes

$$\begin{aligned} H &= \sum_{i,j} C_i^\dagger \langle i|T|j\rangle C_j \\ &+ \frac{1}{2} \sum_{ijkl} C_i^\dagger C_j^\dagger \langle ij|V|kl\rangle C_k C_l \end{aligned} \tag{3.27}$$

Thus equivalence is established.

Several remarks are appropriate.

The system with the Hamiltonian (3.27) has no restriction on the total number of particles. It is easy to check that the total number operator \hat{N} commutes with the Hamiltonian

$$\begin{aligned} [\hat{N}, H] &= 0, \\ \hat{N} &= \sum_i d_i^\dagger C_i = \int d^3x \hat{\psi}^\dagger(x) T(x) \hat{\psi}(x) \end{aligned} \tag{3.28}$$

Thus if we start with N particles in the system, there will always be N particles. However, N is arbitrary, and consequently the quantized form of (3.7) is equivalent to an infinite set of equations (3.8) with $N = 1, 2, \dots$

The quantization of (3.7) is sometimes referred to as “second quantization,” since one begins with a Schrödinger-like equation. This is confusing terminology and should be avoided. Equation (3.7) describes the dynamics of a *classical* system, and it is only to classical systems that the quantization procedure may be applied.

In the special case $V(x - y) = \delta(x - y)$ in one space dimension, (3.7) becomes the Hamiltonian for the cubic (“nonlinear”) Schrödinger equation. Consequently, its quantized version prescribes the dynamics of a system of N identical bosons interacting pairwise via delta function potentials, for arbitrary N .

The cubic Schrödinger equation is particularly interesting because it is one of a handful of systems (until recently, the *only* system) which can be solved exactly in both their quantized and un-quantized forms. The properties of these solutions are discussed in the next section.

3. **The Cubic Schrödinger Equation.** The classical cubic Schrödinger equation

$$(4.1) \quad i \frac{\partial}{\partial t} \varphi + \frac{\partial^2}{\partial x^2} \varphi + K|\varphi|^2\varphi = 0$$

has been solved by Zakharov and Shabat [5] for $K > 0$ using inverse scattering techniques. Qualitative features of the solutions are typical of solutions of soliton equations: solutions asymptotically break into well-separated solitons of arbitrary amplitude and velocity, which suffer only a time delay in scattering.

The corresponding quantized system was solved by McGuire [10], who integrated the N -particle Schrödinger equation (3.8) for arbitrary N . McGuire's solution is too involved to present here, but it may be remarked that the particularly simple form of the interaction potential is essential to its success.

McGuire finds that in addition to the elementary bosons, the system possesses a single bound state of N bosons for each value of $N = 2, 3, \dots$ with binding energy

$$(4.2) \quad E_b = -\frac{K^2}{48}(N^3 - N).$$

One of the more remarkable features of the quantized theory is that for collisions of N particles with initial velocities v_1, v_2, \dots, v_N , the final velocities are always the same as the initial velocities even though for $N > 2$ they are not kinematically restricted to be so. Finally, for collisions of bound states with single particles or other bound states, there are no inelastic processes. That is, if in the initial state there are n_1 single particles, and n_j bound states of j particles, there will be n_1 single particles and n_j bound states of j particles in the final state. Of course, when we consider indistinguishable particles, it is not legitimate to ask whether the particles have rearranged themselves among the various bound and free particle states. If the particles *are* distinguishable, McGuire finds that such rearrangements can occur, so that an initial state of three particles with particles 1 and 2 bound together *can* result in a final state with particles 2 and 3 bound.

5. **Other Field Theories.** The quantized cubic Schrödinger equation is probably the simplest of all quantum field theories. While certain of its qualitative features are characteristic of all interesting quantum field theories, others are peculiar to it and result from the restrictions to point interactions, nonrelativistic kinematics, Bose statistics, and one spatial dimension. In this section we systematically remove these restrictions, noting the change in the character of the quantum field theory, and eventually arrive at relativistic gauge theories in three space dimensions, which are expected by physicists to describe the dynamics of elementary particles.

Two of the features of the cubic Schrödinger theory, the existence of bound and continuum (scattering) states, are general. In theories where all interactions are repulsive, we expect no bound states on intuitive grounds. For theories with attractive interactions, there may or may not exist bound states.

If we allow a general interaction potential $V(q_i - q_j)$, we find that inelastic processes are no longer prohibited. For example, if in the initial state there are two bound states of two particles each, there is a finite probability that the final state will contain (1) no bound state (four free particles, or (2) a bound state of two particles and two free particles, or (3) a bound state of three particles and one free particle, or (4) two bound states of two particles each. Note that there are always four particles in the final state because the number operator obeys $[\hat{N}, H] = 0$.

When we make a quantum field theory consistent with the kinematics of special relativity by requiring that the action S be Lorentz-invariant, there is a much more drastic consequence. The number operator no longer commutes with the Hamiltonian: $[\hat{N}, H] \neq 0$. Thus if there are n_i particles in the initial state, there may be any number of particles n_f in the final state, subject only to the kinematical constraints that the total energy and total momentum be conserved. A relativistic quantum field theory is inherently a theory with an indefinite number of particles, and description of its dynamics by a Schrödinger-like equation is not tenable. The occupation number formalism (closely related, as we have seen, to the canonical quantization procedure) provides a natural description. It should also be mentioned that the concept of interaction via a potential is not easily incorporated into relativistic theories; in relativistic quantum theories, interactions are mediated by the exchange of particles.

As noted earlier, it is possible to quantize a field theory with *anti-commutation* relations rather than commutation relations, leading to particles which obey Fermi statistics. To do this self-consistently for a

relativistic theory requires that one introduce a set of fields which, acting on the ground state, produce a single-particle state which transforms under spatial rotations according to an even-dimensional representation of $SU(2)$, the covering group of the rotation group. This set collectively is called a *Fermi field*. The Lagrangian density is constructed to be invariant under rotations. A non-obvious consequence is that for each type of particle there is automatically a type of *antiparticle* with equal mass and opposite charge. The number of particles minus the number of antiparticles is conserved. A set of fields which produce single-particle states transforming under odd-dimensional representations of $SU(2)$ for spatial rotations is consistently quantized with *commutation* relations, and collectively is called a *Bose field*. One is by no means limited to theories with a single Bose or Fermi field. (The above statements are correct, but somewhat misleading, since really the connection between internal symmetry under spatial rotations and the statistics of identical particles arises through the full Lorentz group. For a thorough explication, see [11].)

The application of relativistic quantum field theory in which physicists are most interested is to elementary particle phenomena, which occur in three spatial dimensions. Removing the restriction to one space dimension leads to field theories where the kinematics is much less restrictive. When particles scatter they may change their directions. The allowed new directions form a continuum.

To summarize, a relativistic quantum field theory in three space dimensions may generally be expected to have the following qualitative features: bound and continuum states, inelastic processes, indefinite numbers of particles, fermion-antifermion pairs, and scattering with nontrivial kinematics.

What sort of quantum field theory are physicists interested in? A popular model for strongly interacting particles (*hadrons*) is one in which the observed hadrons are bound states of either two or three "quarks," much as atomic nuclei are bound states of neutrons and protons. The quarks are taken to be fermions, and are bound together by exchanging "gluons" (which are a generalization of the photon), so that as a consequence, two-quark bound states are bosons and three-quark bound states are fermions. In one version of this model, the Lagrangian density is

$$\begin{aligned}
 \mathcal{L} = & -\frac{1}{4}(\partial_\mu B_\nu^a - \partial_\nu B_\mu^a \\
 (5.1) \quad & - C_{bc}^a B_\mu^b B_\nu^c)(\partial^\mu B^{a\nu} - \partial^\nu B^{a\mu} - C_{bc}^a B^{b\mu} B^{c\nu}) \\
 & + \psi_{ij}^\dagger \gamma^0 [i\gamma^\mu (\delta_{im} \partial_\mu - ig B_\mu^a T_{im}^a)] \psi_{mj}
 \end{aligned}$$

where

- the ψ 's are Fermi fields and the B^a 's are Bose fields
- each ψ_{bj} is a Dirac spinor. The ψ 's transform under the fundamental representation of $SU(3)$ in their first indices and under the fundamental representation of $SU(N)$ in their second indices.
- the γ 's are Dirac matrices,
- Greek indices are Lorentz indices and Latin indices are group indices; repeated indices are summed over: $\mu, \nu = 0, 1, 2, 3$; $a, b, c = 1, \dots, 8$; $l, m = 1, 2, 3$; $j = 1, \dots, N$,
- the C_{bc}^a are the structure constants of $SU(3)$,
- the $T_m^{(a)}$ are the matrix generators of $SU(3)$, three by three, eight in all,
- g is a coupling constant.

The Fermi fields ψ_{bj} represent the different varieties of quarks (three colors and N flavors), and the Bose fields B^a_μ represent the gluons exchanged by the quarks to bind themselves into hadrons. The number of flavors, N , is not agreed upon, but is at least four.

This quark model has not been solved for two reasons: (1) bound states (which are the only states really of interest) are very difficult to find in relativistic quantum field theories, and (2) the usual perturbative calculational techniques cannot be applied, since the coupling constant g is large. In addition there is a conceptual problem: no particles observed in nature correspond to the quarks themselves, so we require that the field theory possess no states with free quarks. It is not clear how this will happen.

6. The Role of Classical Solutions. Recently a number of groups [1], [4], [5] have showed how, knowing solutions to a classical field theory, one can obtain approximate information about the states of the quantized theory. One of the more attractive schemes, proposed by Dashen, Hasslacher, and Neveu, and described elsewhere in this volume by Hasslacher and Neveu, is a generalization of the WKB method of ordinary quantum mechanics, via functional integrals. The method is valid for strong coupling (where perturbation theory isn't) and gives good results for the energies of bound states when the number of bound states is large. It has been tested on model field theories in one space dimension where the spectrum of states is known exactly by other means, and is found to give good results [12], [13].

The meaning of a classical solution in the quantized theory is that it approximately equals the matrix element of the field operator between two bound states. Loosely speaking, to each localized, stable solution of the classical equations of motion there corresponds a series of bound states in the quantum theory.

It must be stressed that before these approximate quantization schemes can be carried out, classical solutions must be known. Theories such as (5.1) are extremely complex and one cannot expect to find analytic solutions to them in the near future. However there are much simpler quantum field theories in three space dimensions which have important physical applications, for example, in the structure of atomic nuclei. The exact solution of *any* classical field theory in more than one space dimension must be regarded as a significant step toward the solution of these more difficult problems.

A few comments are appropriate on the general features of solutions of classical field theories in three space dimensions, as they relate to the phenomenology of quantized theories.

A two line calculation called Derrick's theorem shows that there can be no *time independent* solitary waves in Hamiltonian systems of relativistic scalar fields in three space dimensions. For let $\varphi(x)$ be a hypothetical such solution. Then $\varphi(\lambda x)$ must minimize the Hamiltonian for $\lambda = 1$, where

$$(6.1) \quad H(\varphi(x)) = \int d^3x (\vec{\nabla}_x \varphi(x))^2 + V(\varphi(x)), \quad V(\varphi) \geq 0.$$

But

$$(6.2) \quad \begin{aligned} H(\varphi(\lambda x)) &= \frac{1}{\lambda^3} \int d^3(\lambda x) \lambda^2 (\vec{\nabla}_{\lambda x} \varphi(\lambda x))^2 + V(\varphi(\lambda x)) \\ &= \frac{1}{\lambda} T + \frac{1}{\lambda^3} V, \end{aligned}$$

which has no minimum for any λ . Friedberg, Lee, and Sirlin [14] have showed that for a trivial time dependence $\varphi \sim e^{-i\omega t}$ it is possible in certain cases to construct energetically stable solitary waves. Another possibility is to stabilize the solitary waves topologically, by requiring the map from the sphere at spatial infinity into the space of an internal symmetry group of the fields be nontrivial (see [15]).

It is difficult to see the correspondence between classical field theory and the quantum phenomena of inelasticity and particle decay. It could turn out that these features are purely quantum mechanical in origin, and that the classical theory is a true soliton equation, with a different kind of soliton for each fundamental particle and its excitations in the quantum theory. Or the classical theory might have no true solitons, but merely energetically stable solitary waves, into which the asymptotic $|t| \rightarrow \infty$ scattering states form themselves. In such an event, it would be interesting to find that classical theories can have asymptotic states with *only* solitary waves (and no dissipative excitations).

These important questions will only be resolved by a systematic investigation of solutions to higher dimensional classical field theories.

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