Quantum mechanics without a quantization postulate

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Abstract
The one-particle Schrödinger and Dirac equations are derived, without making any quantization hypothesis, from the postulate that an elementary particle is a physical wave packet of dynamically varying form and size, rather than a pointlike object located somewhere within the support of a wavefunction that serves only as a mathematical probability amplitude. An isolated multiparticle system can, similarly, be described in principle as a set of interacting wave packets governed by coupled one-particle equations, a picture from which, in the nonrelativistic limit, the multiparticle Schrödinger equation can be obtained as a sufficiency condition for the system to have a conserved total energy equal to a particular value E.

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It has previously been shown [1] that, if the masses of free particles are defined absolutely as their rest-frame de Broglie frequencies, rather than in terms of the standard kilogram, then Planck's constant $\hbar$, which specifies the scale of the quantization rules and hence, supposedly, of 'quantum effects', in fact disappears from all quantum equations and their quantitative predictions. This suggests that it should be possible to develop a theory of quantum phenomena that does not make use of a quantization postulate to connect the two 'worlds' of classical and quantum physics but, instead, treats the two domains in a seamlessly unified manner. The present paper offers a quantization-free derivation of the key equations of the quantum mechanics of systems with a fixed number of particles from a handful of fundamental and empirically established principles: de Broglie's postulate of matter waves, Lorentz covariance, the existence of 'intrinsic spin', and the requirement of appropriate symmetry or antisymmetry under the exchange of indistinguishable particles.

1. The dispersion relation for matter waves

In 1923 de Broglie [2] postulated the existence of matter waves associated with material particles, using special relativity to develop an analogy with the photon/light wave duality and to show that such waves would have the unusual property that their wavelength would

be approximately inversely proportional to particle speed, becoming infinitely large in the particle's rest frame. A wave packet formed from these waves would then travel with a group velocity equal to the particle velocity, and so would always follow the motion of its point particle. Empirical evidence for matter waves and for this inverse dependence of wavelength on particle speed was soon obtained by Davisson and Germer [3] and Thomson [4] from electron diffraction by crystals, and subsequently by many other experiments.

We will take as our starting point de Broglie's picture of a packet of matter waves which, in a frame of reference in which the particle is at rest, is an oscillation synchronous over the finite volume of the packet, so that the mean wavelength becomes infinite; but we will drop the idea of a pointlike particle accompanying these waves and assume that the wave packet is, physically, the particle. Such an assumption requires, of course, the additional postulate (here treated as a working hypothesis, to be considered further in subsequent papers) that if and when the particle is detected the packet undergoes a physical collapse to one which is of much smaller size, and which is thus capable of producing well-defined tracks in such detectors as nuclear emulsions or bubble chambers.

Denoting the rest-frame de Broglie angular frequency by ω_R, we can use Lorentz transformation to find the 4-wavevector in any other frame, where the particle has velocity $\mathbf{v}$; $k_R^\alpha = (\omega_R/c, 0, 0, 0)$ transforms to $k^\alpha = (\omega/c, \mathbf{k})$ with

$$\omega = \omega_R \gamma, \qquad \mathbf{k} = \omega_R \gamma \mathbf{v}/c^2, \tag{1}$$

with $\gamma = [1 - \mathbf{v}^2/c^2]^{-\frac{1}{2}}$, giving the wavelength as $\lambda = 2\pi/|\mathbf{k}| = 2\pi c^2/(\omega_R \gamma |\mathbf{v}|)$ and displaying its inverse dependence on speed. The dispersion relation linking ω and $\mathbf{k}$ for free matter waves is therefore

$$\omega = \sqrt{\omega_R^2 + c^2 \mathbf{k}^2} \tag{2}$$

and, as de Broglie found, the group velocity $\mathbf{v}_g = \nabla_\mathbf{k} \omega = \mathbf{v}$.

We will define the free-particle rest-frame angular frequency ω_R, which is characteristic of the type of particle, as the 'absolute mass' [5] of the particle, and denote it by m:

$$m \equiv \frac{2\pi c^2}{\lambda \gamma |\mathbf{v}|}. \tag{3}$$

It is reasonable to refer to this quantity as a 'mass' because, comparing equation (3) with the usual expression $\lambda = 2\pi\hbar/(\bar{m}\gamma|\mathbf{v}|)$ for de Broglie wavelength in terms of the conventional particle mass $\bar{m}$ relative to the kilogram, we find

$$m = \frac{\bar{m}c^2}{\hbar}, \tag{4}$$

so that m is exactly proportional to $\bar{m}$, and in classical mechanics inertial masses are defined by the theory only up to a common scale factor. The angular frequency m is too high to be determined directly by frequency measurement, but can be obtained very accurately (to within an uncertainty, at present, of less than 70 parts per billion) for any microscopic particle by measuring λ for the particles via crystal diffraction when they have a precisely known speed [6] or by other means, such as measurement of atomic recoil velocities in the emission and absorption of photons [7]. From now on, we specify all masses by their absolute values and also, for convenience, choose units of length and time such that $c = 1$.

It can be shown [1, 8] that the absolute mass m, as a frequency, has the physical property of inertia. Consider the behaviour of a wave packet bearing charge q accelerated by an external electromagnetic field, and so executing a curved path in spacetime, in the 'classical limit' where the packet size is small compared with the distance of the packet from the source of the field. The occurrence of such a curved path requires a distortion of the wave pattern

which corresponds to local shifts of the mean 4-wavevector k^α off the mass shell, that is, to values such that $k^\alpha k_\alpha \equiv \omega^2 - \mathbf{k}^2$ is not equal to m^2. The distortion can be covariantly quantified by specifying that the local k^α has to be replaced by $(k^\alpha - qA^\alpha)$, thus defining a spacetime-dependent 4-vector $A^\alpha(x) = A^\alpha(\mathbf{x}, t) = (\phi(\mathbf{x}, t), \mathbf{A}(\mathbf{x}, t))$, which we refer to as the '4-potential'; in other words, we can generalize equation (1) to

$$k^\alpha = mU^\alpha + qA^\alpha \tag{5}$$

where U^α is the velocity 4-vector $(\gamma, \gamma\mathbf{v})$. Consideration of the spacetime geometry of the distorted wave pattern then implies that the packet's 4-velocity changes with its proper time τ according to $dU^\alpha/d\tau = (q/m)(\partial^\alpha A^\beta - \partial^\beta A^\alpha)U_\beta$, demonstrating the inertial property of m and, in fact, deriving Newton's second law with a force of Lorentz form.

We can, finally, derive the dispersion relation for matter waves subject to an arbitrary prescribed electromagnetic potential A^α; using equations (2) and (5) we can write $m^2 = m^2\gamma^2(1 - \mathbf{v}^2) = (\omega - q\phi)^2 - (\mathbf{k} - q\mathbf{A})^2$, or

$$\omega = \sqrt{m^2 + (\mathbf{k} - q\mathbf{A})^2} + q\phi, \tag{6}$$

reducing for a low-speed particle to

$$\omega \approx m + \frac{1}{2m}(\mathbf{k} - q\mathbf{A})^2 + q\phi. \tag{7}$$

2. The one-particle Schrödinger equation

The dispersion relation for any kind of wave is of limited applicability because it refers only to the relationship between ω and $\mathbf{k}$ for the idealized case of a single monochromatic plane wave; a wave equation describing the detailed point-to-point spacetime behaviour of the wave's 'displacement' $F(\mathbf{x}, t)$ is required to treat wave packet evolution and to solve boundary value problems involving the waves. Such a wave equation can be obtained by considering a typical plane wave with displacement $F = F_0 \cos(\mathbf{k} \cdot \mathbf{x} - \omega t)$ and replacing the ω and $\mathbf{k}$ in the dispersion relation by appropriate time and space derivatives. This is very simple for classical nondispersive waves, such as sound, seismic waves, light *in vacuo* or shallow water waves [9], where the phase speed v_p is independent of frequency and the dispersion relation is $\omega = v_p|\mathbf{k}|$, with v_p a constant; we can write

$$\frac{\partial^2 F}{\partial t^2} = -\omega^2 F = -v_p^2 \mathbf{k}^2 F = v_p^2 \nabla^2 F, \tag{8}$$

which, being a linear wave equation, also applies to the superpositions of plane waves in a wave packet or of special functions with symmetries appropriate to a particular boundary geometry.

Matter waves are, however, dispersive, and so this procedure requires modification. Let us consider the case of a slow charged particle subject to an electrostatic potential ϕ, with dispersion relation $\omega \approx m + (1/2m)\mathbf{k}^2 + q\phi$. If we multiply both sides of this by the 'displacement' associated with matter waves, denoted by Ψ, and let Ψ be a typical plane wave $\Psi_0 \cos(\mathbf{k} \cdot \mathbf{x} - \omega t)$, which we will call $\Psi^{(1)}$, there is the problem that, while the $\mathbf{k}^2 \Psi^{(1)}$ on the right-hand side becomes $-\nabla^2 \Psi^{(1)}$, $\omega\Psi^{(1)}$ is minus the first time derivative of a different function $\Psi^{(2)} = \Psi_0 \sin(\mathbf{k} \cdot \mathbf{x} - \omega t)$. It appears that in order to represent matter waves we must use two wavefunctions, $\Psi^{(1)}$ and $\Psi^{(2)}$, coupled together according to

$$-\frac{\partial \Psi^{(2)}}{\partial t} = -\frac{1}{2m}\nabla^2 \Psi^{(1)} + (m + q\phi)\Psi^{(1)} \tag{9}$$

and, similarly,

$$\frac{\partial \Psi^{(1)}}{\partial t} = -\frac{1}{2m}\nabla^2 \Psi^{(2)} + (m + q\phi)\Psi^{(2)}. \tag{10}$$

We can, however, try a representation in terms of a single function which is a linear combination of these two functions, $\Psi = \Psi^{(1)} + C\Psi^{(2)}$, where C is a constant. If we add equation (9) to C times equation (10), the right-hand side of the resulting equation will just be $[-(1/2m)\nabla^2\Psi + (m + q\phi)\Psi]$ whereas the left-hand side can be written as $C[\partial\Psi^{(1)}/\partial t - (1/C)\partial\Psi^{(2)}/\partial t]$, and can be made proportional to $\partial\Psi/\partial t$ if we choose C such that $-1/C = C$, or $C^2 = -1$; so we need to make C equal to i, and our linear combination is the complex function

$$\Psi = \Psi^{(1)} + i\Psi^{(2)}. \tag{11}$$

The pair of coupled equations can then be written as the single equation

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2m}\nabla^2\Psi + (m + q\phi)\Psi. \tag{12}$$

The occurrence in the dispersion relation of an odd power (1) of ω but even powers (0, 2) of **k** thus forces us to use a complex wavefunction if matter waves are to be represented by a single symbol, and the form of the dispersion relation leads to the one-particle Schrödinger equation [10]. Equation (12) differs from its usually quoted form in two ways. It does not contain Planck's constant, not because $\hbar$ has been set to 1 ($\hbar$ still has its usual SI value) but because $\hbar$ is irrelevant here since we are not assuming any quantization rules; and there is an extra term $m\Psi$, which could easily be removed by using the new wavefunction $\Psi' = e^{imt}\Psi$, but is retained to emphasize the fact that the Schrödinger equation describes quite small departures of the angular frequency from the dominant free rest-frame value m, changes which arise from particle motion and the effect of external potentials.

The real quantity $|\Psi|^2$ was originally interpreted by Schrödinger as proportional to charge density, but this was soon replaced by Born's postulate [11] that $|\Psi|^2$ gives the probability of finding the supposedly pointlike particle at a given location at a given time, so its integral over all space must be unity at all times. Here we can continue to think of it provisionally in terms of a charge density, with 'charge' extended to include all the additive entities (electric charge, baryon number, hypercharge, etc) that can be carried by a particle, but operationally we treat it as a probability density, although expressed somewhat differently from Born's statement. We extend our working hypothesis by postulating that, if the particle is detected at time t, the probability of its packet collapsing to a smaller one contained within a small (finite) volume ΔV centred on the point **x** is $|\Psi(\mathbf{x}, t)|^2\Delta V$.

For a particle trapped in some fixed external potential $\phi(\mathbf{x})$ and so forming a standing wave with, say, a frequency E, the time dependence can be factored out by writing $\Psi(\mathbf{x}, t) = \psi(\mathbf{x})e^{-iEt}$, where $\psi(\mathbf{x})$ is a real spatial function; Ψ then satisfies the time-independent Schrödinger equation

$$\left[m - \frac{1}{2m}\nabla^2 + V(\mathbf{x}) - E\right]\Psi = 0 \tag{13}$$

where $V(\mathbf{x}) \equiv q\phi(\mathbf{x})$.

The case of a particle subject to both electric and magnetic potentials can be treated by a similar procedure applied to the dispersion relation in equation (7) and leads to the modified Schrödinger equation

$$i\frac{\partial \Psi}{\partial t} = m\Psi + \frac{1}{2m}(i\nabla + q\mathbf{A})^2\Psi + q\phi\Psi. \tag{14}$$

For a steady, spatially uniform magnetic field $\mathbf{B}$ one can rewrite this equation, as shown in many quantum textbooks, in the form

$$i\frac{\partial \Psi}{\partial t} = m\Psi - \frac{1}{2m}\nabla^2\Psi - \frac{q}{2m}\mathbf{B}\cdot\mathbf{L}\Psi + q\phi\Psi, \tag{15}$$

where $\mathbf{L}$ is the orbital angular momentum operator $\mathbf{r}\times(-i\nabla)$]. The new $\mathbf{B}$-dependent term in this equation can be thought of as due to the interaction with the external magnetic field of a magnetic moment $(q/2m)\mathbf{L}$ associated with the orbital motion.

A further correction is, however, required in the dispersion relation for an electron or other material particle in a magnetic field: a double-valuedness in the particle energy which is conventionally described as 'intrinsic spin' [12], although it differs fundamentally from orbital angular momentum in that the 'spin' has a single magnitude and generates twice the magnetic moment per unit of angular momentum. Here we do not try to picture a spinning wave packet, but merely formalize the double-valuedness by allowing for the particle to exist in one of, or a superposition of, two states Ψ_1 and Ψ_2, with frequencies $\omega_{1,2} = m + (1/2m)(\mathbf{k} - q\mathbf{A})^2 + q\phi \mp (q/2m)B^3$ in a magnetic field oriented along the x^3 axis. Writing the two states as components of a column vector denoted by Ψ, this can be written as

$$\begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \left[\left(m + \frac{1}{2m}(\mathbf{k} - q\mathbf{A})^2 + q\phi\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{q}{2m}B^3\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}. \tag{16}$$

The last term can be written formally in rotation-covariant form as $[-(q/2m)\vec{\sigma}\cdot\mathbf{B}\Psi]$, where we introduce a set of three frame-invariant matrices σ^1, σ^2 and σ^3, with σ^3 equal to the last matrix in equation (16); covariance under rotation can be ensured if we choose σ^1 and σ^2 *and* the rule for transformation of Ψ such that $[-(q/2m)\vec{\sigma}\cdot\mathbf{B}\Psi]$ transforms in the same way as Ψ itself. It can be shown [13] that this can be achieved if Ψ transforms as a 'Pauli spinor'

$$\Psi \to \Psi' = \exp\left(i\frac{\theta}{2}\mathbf{n}\cdot\vec{\sigma}\right)\Psi, \tag{17}$$

under rotation by angle θ about direction $\mathbf{n}$, and

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{18}$$

so that the σ^i satisfy the commutation and anticommutation relations

$$[\sigma^i, \sigma^j] = 2i\epsilon_{ijk}\sigma^k, \qquad \{\sigma^i, \sigma^j\} = 2\delta_{ij}I, \tag{19}$$

with I denoting the (2×2) unit matrix. These equations have been derived, not from the application of postulated quantization rules, similar to those for orbital angular momentum, to some imagined spinning motion of the particle, but merely from the double-valuedness of the energy in a magnetic field plus rotational covariance.

Finally, writing the time dependence of Ψ_1 and Ψ_2 as $e^{-i\omega_1 t}$ and $e^{-i\omega_2 t}$ and using the previous method to eliminate ω_1, ω_2 and $\mathbf{k}$ in the dispersion relations, we obtain Pauli's generalization [14] of the Schrödinger equation,

$$i\frac{\partial \Psi}{\partial t} = \left[m + \frac{1}{2m}(i\nabla + q\mathbf{A})^2 + q\phi - \frac{q}{2m}\vec{\sigma}\cdot\mathbf{B}\right]\Psi. \tag{20}$$

3. The Dirac equation

If we try to extend this approach to finding a Lorentz covariant wave equation, we run into the problem that, even for a free particle, we have to deal with a term $\sqrt{m^2 + \mathbf{k}^2}$ in the dispersion relation (6) and hence with a difficult operator $\sqrt{m^2 - \nabla^2}$. But Dirac realized that if one regards the wavefunction as a multicomponent object represented by a column vector, as in Pauli's treatment of spin, the dispersion relation can be taken as a matrix equation which, on squaring, gives the correct relation $\omega^2 = m^2 + \mathbf{k}^2$ [15].

Let us take Ψ as an n-component object and write the free-particle dispersion relation in the form

$$\omega = \alpha^i k^i + \beta m = \vec{\alpha} \cdot \mathbf{k} + \beta m, \tag{21}$$

where ω is an $(n \times n)$ diagonal matrix with elements $(\omega_1, \omega_2, \ldots, \omega_n)$, and $\alpha^1, \alpha^2, \alpha^3$ and β are Hermitian $(n \times n)$ matrices chosen so that the square of the right-hand side of equation (21) is $(m^2 + \mathbf{k}^2)$ times the n-dimensional unit matrix (not shown explicitly in the matrix equations that follow). One can then easily show that Dirac's matrices must satisfy the relations

$$\{\alpha^i, \alpha^j\} = 2\delta_{ij}, \qquad \{\alpha^i, \beta\} = 0, \qquad \beta^2 = 1. \tag{22}$$

The Pauli matrices $\{\sigma^i\}$ satisfy the first set of anticommutation relations but there is no nonzero (2×2) Hermitian matrix β satisfying the second set since, as is well known, any Hermitian (2×2) matrix can be expressed as a linear superposition of the Pauli matrices and the (2×2) unit matrix I. So we increase n from 2 to 4, choose β as the simplest nontrivial matrix satisfying $\beta^2 = 1$ and construct the Hermitian $(4 \times 4)\{\alpha^i\}$ from the $\{\sigma^i\}$

$$\alpha^i = \begin{pmatrix} a\sigma^i & b\sigma^i \\ b^*\sigma^i & d\sigma^i \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{23}$$

where a, b and d are complex constants to be determined. It is then readily shown from the anticommutation relations in equation (19) that equations (22) are satisfied if a and d vanish and $|b| = 1$, so a possible choice of Dirac matrices is

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{24}$$

the so-called 'standard' representation; we could, of course, use any other set $(U\alpha^i U^{-1}, U\beta U^{-1})$, with U a unitary (4×4) matrix, which would also satisfy equation (22), without altering the physics.

Following the path of what was done in the previous section in deriving the Pauli equation, we consider a plane wave in which the four components $(\Psi_1, \Psi_2, \Psi_3, \Psi_4)$ of the Dirac spinor Ψ are given the time dependences $(e^{-i\omega_1 t}, \ldots, e^{-i\omega_4 t})$ and multiply Ψ on the left by both sides of the matrix dispersion relation equation (21). The introduction of time and space derivatives of Ψ then leads to the free-particle Dirac equation

$$i\frac{\partial \Psi}{\partial t} = -i\vec{\alpha} \cdot \nabla\Psi + \beta m \Psi \tag{25}$$

which, being linear and independent of frequency and wave vector, applies also to a relativistic wave packet. The Dirac equation can be written in manifestly Lorentz covariant form: if we define $\gamma^0 \equiv \beta$ and $\gamma^i \equiv \beta\alpha^i$, equation (25) becomes

$$(i\gamma^\alpha \partial_\alpha - m)\Psi = 0. \tag{26}$$

For a charged particle in an external electromagnetic field we make the same replacements $(\omega \to \omega - q\phi, \mathbf{k} \to \mathbf{k} - q\mathbf{A})$ as in the previous section, obtaining a dispersion relation

$$\omega = \vec{\alpha} \cdot (\mathbf{k} - q\mathbf{A}) + \beta m + q\phi \tag{27}$$

and the generalized Dirac equation

$$i \frac{\partial \Psi}{\partial t} = [-\vec{\alpha} \cdot (i\nabla + q\mathbf{A}) + \beta m + q\phi]\Psi, \tag{28}$$

or, in manifestly Lorentz covariant form,

$$[\gamma^{\alpha}(i\partial_{\alpha} - qA_{\alpha}) - m]\Psi = 0. \tag{29}$$

The Dirac equation is the simplest Lorentz covariant evolution equation for a multicomponent Ψ function capable of taking into account the phenomenon of 'intrinsic spin'. The detailed interpretation of the equation is given in many textbooks [16, 17], and need not be repeated here, except for a few general comments. First, it turns out that only two of the four complex components of a Dirac spinor are independent, corresponding to the existence of a two-valued energy in an external magnetic field. In the nonrelativistic limit and the standard representation, the components Ψ_1 and Ψ_2 become much larger than Ψ_3 and Ψ_4 and it can be shown that they form a 2-spinor satisfying the Pauli equation (20), with the factor multiplying the $(\vec{\sigma} \cdot \mathbf{B}\Psi)$ term now not needing to be put in by hand but automatically having the correct value (apart from small QED corrections). The next order of approximation leads to an 'improved Pauli equation' incorporating a spin–orbit coupling term proportional to $(\vec{\sigma} \cdot \mathbf{L}\Psi)$, as observed experimentally in atomic states.

The other outcome of the Dirac equation is that it has solutions with negative frequencies, as is clear from the dispersion relation (27) using the standard representation, because the $(-I)$ in the β matrix multiplying the mass m gives rise to negative values of ω_3 and ω_4. In the nonrelativistic limit these solutions have values of Ψ_3 and Ψ_4 much larger than those of Ψ_1 and Ψ_2, and it is easily shown that in an external electric field they represent waves accelerated in a direction opposite to that of positive frequency waves and are thus interpreted as antiparticles bearing an opposite value of electric charge.

The requirement that matter waves have a Lorentz covariant dispersion relation which is of first order in both angular frequency and 3-wavevector thus forces the wavefunction Ψ to have a surprisingly complicated mathematical nature; it has four complex components which not only embody the property of intrinsic spin but also imply the existence of an antiparticle corresponding to each type of 'charge'-bearing particle.

4. Multiparticle quantum mechanics

In the previous sections of this paper we have derived the one-particle equations of quantum mechanics from various forms of the dispersion relation for matter waves, which in turn follow from de Broglie's picture of synchronous oscillation in the rest frame plus Lorentz transformation and the introduction of potentials as measures of off-mass-shell shifts. There are a number of other ways of deriving the one-particle equations: for example, the Schrödinger equation from the algebra of the generators of Galilean transformations [18] and the Dirac equation from the simplest nontrivial multicomponent representation of the Lorentz group [19–21]. But there does not appear to be any such simple derivation from first principles of the quantum evolution equation for a system of two or more interacting particles.

The conventional approach to such a system is centred on the multiparticle Schrödinger equation, whose origins lie more in the matrix mechanics of Born, Heisenberg and Jordan [22] than in Schrödinger wave mechanics. It retains some of the formalism of classical point-particle mechanics [23], making use of the Hamiltonian function $H(q_1, \ldots, q_N; p_1, \ldots, p_N)$ from which the Newtonian equations of motion can be obtained via Hamilton's equations, but regarding the $\{q_n\}$ and $\{p_n\}$ as operators satisfying the quantization rules $[q_n, p_m] = i\hbar\delta_{nm}$;

it is then postulated that the state vector Ψ of the system evolves in time according to $i\hbar\partial\Psi/\partial t = H\Psi$.

If we express this formalism in the position representation, Ψ becomes a function in configuration space $(q_1, \ldots, q_N)$ and time, a nonseparable, entangled function which, according to the orthodox view, cannot be regarded as the product of N separate wave packet functions evolving in ordinary spacetime. This entanglement is a property of great importance in treating not only the dynamical interparticle correlations in bound systems, but also, more recently, the observed nonlocal correlations between particles formerly in interaction which have subsequently become separated by large distances.

For the case of one particle in an external prescribed potential, this formalism leads to the one-particle Schrödinger equation derived in section 2, and it is thus a reasonable generalization of that equation to multiparticle systems—one which leads to comprehensive and accurate predictions in thousands of different physical systems. But it is still just a postulate. And there is still the problem, as in the one-particle case, that if the absolute masses of particles are used then $\hbar$, the characteristic scale factor of the quantization rules that make quantum-mechanical quantities different from classical quantities, vanishes from all the quantitative predictions of the multiparticle Schrödinger equation [1].

Moreover, it is not possible to formulate a Lorentz covariant extension of the equation; there is a 'no-interaction theorem' [24], according to which the only classical multiparticle system for which one can give a fully covariant Hamiltonian formulation is one in which the particles do not interact with each other. It is possible to make low-order relativistic corrections to the Schrödinger equation [25], but the fundamental problem of combining special relativity with multiparticle quantum mechanics still eludes us; most of present-day quantum mechanics is covariant only under Galilean transformations, in which the speed of light is taken to be infinite—an assumption that is particularly worrisome if one tries to 'explain' quantum nonlocal correlations merely by appeal to the entanglement of the multiparticle wavefunction in configuration space.

Can the multiparticle Schrödinger equation be in some sense derived from the one-particle equations? Let us try to formulate the N-particle problem as a set of coupled one-particle equations describing N interacting wave packets, with each particle evolving in a way governed by the rapidly changing potential due to all its similarly evolving neighbours.

Most of what we will do in this section is restricted to the nonrelativistic case of low particle speeds, but we can at least start with Lorentz covariant equations. Consider a set of N spin-$\frac{1}{2}$ particles with masses m_r and charges q_r $(r = 1, 2, \ldots, N)$ interacting electromagnetically with each other and forming a closed system isolated from external fields. The spacetime evolution of the rth wave packet $\Psi_r(x) = \Psi_r(\mathbf{x}, t)$ (supposed normalized to unity) should be given by the Dirac equation

$$\left[i\gamma^\alpha \frac{\partial}{\partial x^\alpha} - m_r - q_r \gamma_\alpha A_r^\alpha(x) \right] \Psi_r(x) = 0, \tag{30}$$

but with $A_r^\alpha(x)$ the rapidly varying retarded potential due to the other $(N-1)$ particles:

$$A_r^\alpha(x) = \sum_{s=1(s \neq r)}^{N} \int d^4 x_s D_R^{\alpha\beta}(x - x_s) q_s \Psi_s^\dagger(x_s) \gamma_0 \gamma_\beta \Psi_s(x_s) \tag{31}$$

where $D_R^{\alpha\beta}(x) = \eta^{\alpha\beta}\theta(x^0)\delta(x^2)/2\pi = \eta^{\alpha\beta}\delta(x^0 - |\mathbf{x}|)/(4\pi|\mathbf{x}|)$ is the standard electromagnetic retarded Green function [26] and $\Psi_s^\dagger(x)\gamma^0\gamma^\alpha\Psi_s(x)$ is the 4-current density of the sth particle. Substitution of equation (31) into equation (30) then gives a set of N coupled nonlinear integrodifferential equations for the $\Psi_r(x)$ in ordinary spacetime. These equations are Lorentz

covariant and ought to be valid up to the level where higher QED effects such as pair creation, self-interaction or vacuum polarization need to be taken into account.

One can imagine trying to solve these equations by a quest for 'self-consistency' in which one starts with a plausible set of Ψ_r's and iterates between successive approximations to the A_r^α's and Ψ_r's using equations (30) and (31)—something like the Hartree method [27], but much more difficult because the A_r^α's are dynamically varying with time rather than being mere time averages. This would, of course, be an extremely complicated mathematical task; can we say something about the N-particle system, given our picture of it as a set of interacting wave packets, but avoiding the almost impossible labour of actually calculating the individual Ψ_r's?

Let us simplify things by assuming that the wave packets are moving at such low speeds that we can use nonrelativistic kinematics and ignore retardation and magnetic effects, including dynamical effects due to spin; that is, we take the wavefunction for the rth particle as a single normalized complex function $\Psi_r(\mathbf{x}, t)$ of position and time multiplied by a constant Pauli spinor, and assume only electrostatic interactions. Our system of particles is then governed by the simpler, but still formidable, set of N coupled equations for the Ψ_r in ordinary spacetime

$$\mathrm{i}\frac{\partial}{\partial t}\Psi_r(\mathbf{x}, t) = \left\{ m_r - \frac{1}{2m_r}\nabla^2 + q_r \sum_{s=1(s\neq r)}^{N} \int \mathrm{d}^3 x_s \frac{q_s |\Psi_s(\mathbf{x}_s, t)|^2}{4\pi |\mathbf{x} - \mathbf{x}_s|} \right\} \Psi_r(\mathbf{x}, t), \tag{32}$$

with $r = 1, 2, \ldots, N$.

The main difficulty in the solution of problems in multiparticle mechanics—classical or quantum—comes from the fact that the potential energy of a system is inseparably shared by all its particles. In the classical case we can, however, write an expression for the total energy E of the system and know that, in the kind of isolated system we are concerned with here, E is conserved in time—even if the system displays deterministic chaos [28]. For an isolated classical system of pointlike particles governed by electrostatic interparticle forces, the momentum $\mathbf{p}_r = m_r \mathbf{v}_r = m_r \, \mathrm{d}\mathbf{x}_r/\mathrm{d}t$ of the rth particle satisfies the Newtonian equation of motion $\mathrm{d}\mathbf{p}_r/\mathrm{d}t = -\nabla_r \sum_{s\neq r} V_{rs}$, where $V_{rs} = Q_r Q_s e^2/(4\pi |\mathbf{x}_r - \mathbf{x}_s|)$ and, as is well known, it can be shown [23] from these equations that the total energy

$$E \equiv \sum_r \left(m_r + \mathbf{p}_r^2/2m_r \right) + \sum_{r,s;r<s} V_{rs} \tag{33}$$

is constant in time; the restriction $r < s$ in the double summation of V_{rs} comes from the successive buildup of the potential energy as particles are imagined to be added one at a time, avoiding self-interaction and double counting.

We can readily write a similar equation for the quantum case, guided by the simple expression for the conserved energy E of a single particle in a prescribed external potential, obtained from the time-independent Schrödinger equation (13) and the normalization of Ψ to unity,

$$E = \int \mathrm{d}^3 x\, \Psi^*(\mathbf{x}, t) \left[m - \frac{1}{2m}\nabla^2 + V(\mathbf{x}) \right] \Psi(\mathbf{x}, t), \tag{34}$$

which expresses the kinetic energy as the $|\Psi|^2$-weighted average of $(-1/(2m\Psi)\nabla^2\Psi)$ over the wave packet and the potential energy as the $|\Psi|^2$-weighted average of V. For N mutually

interacting wave packets we may thus write the conserved total energy as

$$E = \sum_{r=1}^{N} \int d^3 x_r\, \Psi_r^*(\mathbf{x}_r, t) \left(m_r - \frac{1}{2m_r} \nabla_r^2 \right) \Psi_r(\mathbf{x}_r, t)$$

$$+ \sum_{r<s} \int d^3 x_r\, d^3 x_s\, \Psi_r^*(\mathbf{x}_r, t) \Psi_s^*(\mathbf{x}_s, t) V_{rs}(|\mathbf{x}_r - \mathbf{x}_s|) \Psi_r(\mathbf{x}_r, t) \Psi_s(\mathbf{x}_s, t). \quad (35)$$

The final term is the sum of the pairwise mutual electrostatic potential energies of charge distributions (possibly overlapping each other) having charge densities proportional to $|\Psi_r|^2$, $|\Psi_s|^2$. (The $\mathbf{x}_r$ and $\mathbf{x}_s$ are just dummy variables ranging over the supports of the rth and sth wave packets, and have nothing to do with the positions of imagined pointlike particles.)

This energy equation is not in itself of much use to us for calculating possible values of E because of course we do not know the rapidly varying $\Psi_r(\mathbf{x}, t)$ functions corresponding to each of the N wave packets. Suppose, however, that we invent the product function

$$\Phi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N; t) \equiv \Psi_1(\mathbf{x}_1, t), \Psi_2(\mathbf{x}_2, t), \ldots, \Psi_N(\mathbf{x}_N, t) \chi(1, 2, \ldots, N), \quad (36)$$

where χ is a direct product of the constant Pauli spinors for the N particles, and rewrite equation (35) in terms of Φ by inserting the normalization condition $[1 = \int d^3 x\, \Psi_q^*(\mathbf{x}, t) \Psi_q(\mathbf{x}, t)$ for the qth wave packet] $(N-1)$ times in each of the rest plus kinetic energy integrals and $(N-2)$ times in each of the potential energy integrals. The energy equation then takes the more compact form

$$\int d^3 x_1\, d^3 x_2 \cdots d^3 x_N\, \Phi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N; t) \left[\sum_r \left(m_r - \frac{1}{2m_r} \nabla_r^2 \right) + \sum_{r<s} V_{rs} - E \right]$$

$$\times \Phi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N; t) = 0. \quad (37)$$

This equation will hold if the invented function Φ and the energy E together satisfy the equation

$$\left[\sum_r \left(m_r - \frac{1}{2m_r} \nabla_r^2 \right) + \sum_{r<s} V_{rs} - E \right] \Phi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N; t) = 0, \quad (38)$$

that is, the time-independent form of the multiparticle Schrödinger equation, arising here as a sufficiency condition for the total energy of the system to be conserved and equal to the constant E.

We have not yet taken into account another important ingredient of quantum theory arising in the treatment of multiparticle systems: the need to symmetrize or antisymmetrize Φ for any set or sets of particles in the system which are indistinguishable. Suppose for simplicity that there is just one set of indistinguishable particles in the system, represented by the first N' factors in equation (36) (for example, the electrons in an atom). Clearly, because of the symmetry of the operator in square brackets in equation (38) under interchange of particle labels 1 and 2, it will still hold if we replace Φ by

$$\Phi'(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N; t) \equiv \pm \Psi_1(\mathbf{x}_2, t), \Psi_2(\mathbf{x}_1, t), \ldots, \Psi_N(\mathbf{x}_N, t) \chi(2, 1, \ldots, N) \quad (39)$$

or by any function resulting from the permutation of position variables and spin labels of one or more pairs among the N' particles; or, since equation (38) is linear in Φ, by any linear combination of such permuted Φ's. We postulate the additional condition, required by experiment, that the Φ in equation (38) must possess the correct symmetrization or antisymmetrization property—for example, in the case of electrons in an atom, the

antisymmetrization required for the spin-$\frac{1}{2}$ electrons, obtainable by expressing Φ not by a simple product as in equation (36) but by a Slater determinant [29].

The approach in this section is somewhat limited in that, strictly speaking, the multiparticle Schrödinger equation has not been derived, since equation (38) has not been rigorously shown to be a necessary condition for equation (35) to hold, and the method applies only to an isolated system of particles. However, it suggests that there is a significant difference in status between the one-particle and multiparticle Schrödinger equations: whereas the former provides a complete account of the dynamical evolution of the particle wave packet, the latter seems to be more a statement about the energy E of the multiparticle system, and provides a way of calculating the allowed eigenvalues of E without trying to follow in detail the very complicated evolution of N mutually interacting wave packets.

One further simplification comes from separating out the global centre-of-mass evolution of the isolated system [30]. If we re-express the Φ for a bound system as a function of relative coordinates $\mathbf{x}_{Rr}$ and c.m. coordinates $\mathbf{x}_{Cr}$ by the sequences

$$\mathbf{x}_{Rr} \equiv \mathbf{x}_r - \mathbf{x}_{C,r-1}, \qquad \mathbf{x}_{Cr} \equiv \frac{m_r \mathbf{x}_r + (m_1 + m_2 + \cdots + m_{r-1})\mathbf{x}_{C,r-1}}{m_1 + m_2 + \cdots + m_r} \quad (40)$$

and define reduced masses by

$$\frac{1}{\mu_r} \equiv \frac{1}{m_r} + \frac{1}{m_1 + m_2 + \cdots + m_{r-1}} \quad (41)$$

the multiparticle Schrödinger equation becomes

$$\left[m' - \frac{1}{2m'}\nabla_{CN}^2 - \sum_{r=2}^N \left(\frac{1}{2\mu_r}\nabla_{Rr}^2\right) + \sum_{r<s} V_{rs}(\mathbf{x}_{R2}, \ldots, \mathbf{x}_{RN}) - E \right]$$
$$\times \Phi(\mathbf{x}_{CN}, \mathbf{x}_{R2}, \ldots, \mathbf{x}_{RN}; t) = 0, \quad (42)$$

where $m' \equiv \sum_{r=1}^N m_r$. This can be satisfied by a product of the form $\Phi = \Phi_C(\mathbf{x}_{CN}, t) \Phi_R(\mathbf{x}_{R2}, \ldots, \mathbf{x}_{RN})$. If we can find functions Φ_R and corresponding constants $\mathcal{E}$ such that

$$\left[-\sum_{r=2}^N \left(\frac{1}{2\mu_r}\nabla_{Rr}^2\right) + \sum_{r<s} V_{rs}(\mathbf{x}_{R2}, \ldots, \mathbf{x}_{RN}) - \mathcal{E} \right] \Phi_R(\mathbf{x}_{R2}, \ldots, \mathbf{x}_{RN}) = 0, \quad (43)$$

which is the Schrödinger equation for $(N-1)$ particles of masses $(\mu_2, \ldots, \mu_N)$, with a discrete set of negative eigenvalues $\mathcal{E}$, the other factor must satisfy

$$\left[m' + \mathcal{E} - \frac{1}{2m'}\nabla_{CN}^2 - E \right] \Phi_C(\mathbf{x}_{CN}, t) = 0, \quad (44)$$

which has simple solutions of the form $\Phi_C(\mathbf{x}_{CN}, t) = A_{\mathbf{K}}\, e^{i\mathbf{K}\cdot\mathbf{x}_{CN}} f(t)$ (where the function $f(t)$ remains to be determined), provided that the energy of the system has the value

$$E = m' + \mathcal{E} + \frac{\mathbf{K}^2}{2m'} \cong m' + \mathcal{E} + \frac{\mathbf{K}^2}{2(m' + \mathcal{E})} \quad (45)$$

(since $\mathcal{E} \ll m'$).

This is the energy, or frequency, of a free particle with mass $(m' + \mathcal{E})$ moving with 3-wavevector, or 3-momentum, $\mathbf{K}$. In particular, the rest-frame frequency, or absolute mass, of a bound state with binding energy $B = -\mathcal{E} > 0$ is

$$m = \sum_{r=1}^N m_r - B. \quad (46)$$

This demonstrates the additivity of what we have called absolute mass: a composite system such as an atom or molecule possesses an overall de Broglie frequency corresponding to its total mass (minus B) and a corresponding de Broglie wavelength which can be measured in interference or diffraction experiments.

The N-particle Schrödinger equation, equation (38), can be generalized by noting that the factor $f(t)$, being the time dependence of a free wave Φ_C with 3-wavenumber $\mathbf{K}$ and rest-frame frequency m, must according to the Lorentz transformation have the form $e^{-i\omega t}$, with $\omega = m\gamma = \sqrt{m^2 + \mathbf{K}^2} \cong m + (1/2m)\mathbf{K}^2$; this is equal to the E appearing in equation (45), so that $E\Phi(t) = E\Phi_C(t)\Phi_R$ can be replaced by $i\partial\Phi(t)/\partial t$ to give the time-dependent multiparticle Schrödinger equation for an isolated system

$$i\frac{\partial\Phi}{\partial t} = \left[\sum_r \left(m_r - \frac{1}{2m_r}\nabla_r^2\right) + \sum_{r<s} V_{rs}\right]\Phi. \tag{47}$$

This form can be used, for example, in the more general situation where Φ_C takes the form of a wave packet, a superposition of plane waves with different $\mathbf{K}$'s and E's.

5. Discussion

In the earlier part of this paper we have derived the one-particle equations of quantum mechanics, the Schrödinger and Dirac equations, without any use of $\hbar$-dependent quantization rules applied to the behaviour of a supposedly pointlike object—using instead the picture of an elementary particle as a wave packet of dynamically varying form and size, with the frequency of the de Broglie oscillation in the rest frame defined absolutely as the particle's inertial mass. We have then seen that the N-particle Schrödinger equation can be arrived at as a sufficiency condition for an isolated system, viewed as a complicated assemblage of N interacting wave packets, to have a conserved total energy equal to a particular value E. Furthermore, the defined function Φ satisfying this equation can be expressed as the product of a free centre-of-mass wavefunction Φ_C, with a rest-frame de Broglie frequency equal to the sum of the absolute masses of the constituents (minus a binding correction), and a time-independent function Φ_R, expressing the internal evolution of the system, which satisfies an $(N-1)$-particle Schrödinger equation. The reduced problem is still, except for the $N = 2$ case, quite formidable, but it can be tackled by various approximation methods such as perturbation theory or, if that fails, the variational method.

This talk of an N-particle system consisting of N separate wave packets evolving in ordinary spacetime runs against the current orthodoxy, which dates from the downfall of Schrödinger's early interpretation of his wave equation in the mid-1920s. But it is difficult to find arguments against it. Why should we expect the Dirac (or one-particle Schrödinger) equation to break down just because the source of the potential acting on the rth particle is itself changing due to the dynamically correlated evolution of neighbour wave packets? It is true that the multi-packet picture as it stands is not useful for calculation because of its mathematical complexity; but by the procedure outlined in the previous section one obtains for the nonrelativistic case an eigenvalue equation for the total energy which can be solved—exactly for $N = 2$ and by approximate means for higher N. The nonseparability, or entanglement, of the defined Φ function satisfying the multiparticle Schrödinger equation arises as a mathematical consequence of the 'burying' of the very complicated individual time dependences in the overall e^{-iEt} factor appearing in Φ; the effect of interparticle correlations is retained in the form of the complicated standing wave described by the reduced $(N-1)$-particle equation. (The nonlocal kind of entanglement displayed in the detection of pairs

of spacelike-separated particles formerly in interaction is quite another question, and will be discussed in a future paper.)

This picture throws light on a number of other awkward questions. One is to understand what happens when a free composite system undergoes dispersive spreading; for example, how is it that the electron and proton wave packets in a spreading hydrogen atom can evolve in such a way as to ensure that the composite packet still has the properties of being hydrogen—for example in its electromagnetic emission and absorption spectra? The answer here would be that the individual behaviour of the constituents is too complicated to be pictured; it is the overall Φ_C packet that spreads, carrying with it a complex of interacting packets characterized by the Φ_R equation, maintaining the energy $\mathcal{E}$ of whatever internal state that complex happens to have, and therefore displaying the right spectral properties.

A more widely discussed question is the apparent difference between the unpredictable behaviour of an isolated nonlinear system which, treated by classical mechanics, would display chaos [28], and the smooth and systematic behaviour governed by the linear Schrödinger equation obtained when such a system is 'quantized'. This seeming contradiction can be resolved if one regards the multiparticle Schrödinger equation, in contrast to the one-particle equation, not as a complete dynamical description of a system but, rather, an energy equation; the time dependence is the quite predictable e^{-iEt} contributed by the Φ_C factor, while the Φ_R factor for the case $N \geqslant 3$, where deterministic chaos can classically occur, already involves very complicated behaviour even in the reduced system—reflecting, perhaps, the behaviour one would expect if the system were to be treated by the quantum Heisenberg picture.

Further work is needed to extend this approach to a broader domain—for example, to the effects of dynamical spin dependence or of external forces acting on the system. A much bigger challenge is to apply the energy equation method to relativistic particle systems, starting from N coupled Dirac equations and somehow tackling the problem of the retardation of the potentials. Even so, this would not be the last word on the quantum treatment of multiparticle systems, because it would not yet be taking into account QED effects which cannot be adequately treated by using a potential description of interaction, such as pair creation and self-interaction—and which, perhaps, may eventually throw light on the nonlocal phenomena involved in particle detection.

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