WHERE DOES SCHRODINGER'S EQUATION REALLY COME FROM?

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ABSTRACT

We begin by summarising a conventional view of Schrödinger's Equation. Questions are asked and this view is criticised. There follows a mathematical experiment wherein an hierarchy of identities is quantized. These identities apply to arbitrary, differentiable functions of the coordinates that are themselves differentiable functions of time; such functions appear in classical dynamics. It turns out that the quantizations are not identities unless we restrict the form of the Hamiltonian operator. The Schrödinger and Dirac forms satisfy whereas arbitrary choices do not. The Dirac form is a better approximation in that it satisfies higher level identities than the Schrödinger form.

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1. The Schrödinger Equation

(1) $H\phi = ih\dfrac{\partial \phi}{\partial t}; \quad h \equiv \text{(Plank's constant)}/(2\pi)$

where t is time (treated as a scalar that commutes with all operators), ϕ represents the state and H is the energy operator; H is usually taken to have the same structure as the Hamiltonian of the corresponding classical model (if there is one).

(2) $\phi \equiv \phi(\underline{q}, t)$

is taken to be a complex, normed, continuous , differentiable function of the (scalar) coordinates

(3) $\underline{q} \equiv \{q_1, q_2, \ldots. q_n\}$

and is defined on an Hilbert space with the $\underline{q}$ as arguments; t is treated as a label.

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1.1 The Eigenvalue Equation

The first step, in finding an eigenvalue E of H with eigenfunction ϕ, is to note that

$$(5) \quad H\phi = ih\frac{\partial\phi}{\partial t} = E\phi \Rightarrow \phi = \psi(\underline{q})\exp(-itE/h)$$

where the eigenfunction $\psi(\underline{q})$ satisfies

(6) $H\psi = E\psi$; also sometimes called Schrödinger's equation

To make further progress we need to specify H as an operator function of other operators with known properties. Typically, when dealing with a particle or system of particles, the operator arguments are the coordinates $\underline{Q}$ and their conjugate momenta $\underline{P}$ with the correspondence (from classical scalars to operators)

$$(7) \quad \underline{p} \to \underline{P}; \quad \underline{q} \to \underline{Q}$$

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1.2 The Original Problem

The original Schrödinger problem (the hydrogen atom) considers the Hamiltonian operator

$$(9) \quad H \equiv \frac{1}{2m}\sum_{j=1}^{n} P_j^2 + V(\underline{Q}); \quad n = 3; \quad m \text{ is the scalar mass}$$

with representations

$$(10) \quad Q_j \equiv q_j I; \quad P_j \equiv -ih\frac{\partial}{\partial q_j}; \quad I \text{ is the unit operator}$$

which corresponds to a single Newtonian particle in a scalar field $V(\underline{q})$. Here the coordinates are Cartesian; and the representation (10) is suitable only to such coordinates.

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2. Criticisms

2.1 Standard Explanations

By integrating Newton's laws, in the context of Euclid's geometry, we arrive at Hamiltonian mechanics; and (9) is simply the operator form of an important Hamiltonian. Whether or not the eigenvalue problem (6) turns out to be useful in QM is a matter for theory and experiment. Another form for the Hamiltonian is obtained from SR (special relativity) mechanics; here Euclid's geometry and Newton's universal time are replaced by Einstein's space-time. The corresponding eigenvalue equation (6) is Dirac's equation.

2.2 Objections

These ‘standard’ explanations, for the importance of certain Hamiltonian forms, seem to me to be unsatisfactory; we need a deeper insight.

- The efficacy of Newton’s laws is profoundly mysterious.
- On the face of it, there is no obvious reason why only some models work both, in the large, as a basis for CM and, in the small, as a basis for QM.
- The structure of space-time, which we all take for granted, is just as mysterious as Newton’s laws!

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3. The Identities

3.1 The First Three

Let $\theta(\underline{q})$ be *any* real, continuous, differentiable function that does not depend explicitly on t. Then, by regarding the coordinates $\underline{q}$ as differentiable functions of time, we have

(11) $\dot{\theta} = \dot{q}^j \theta_{,j}$; $\theta_{,j} \equiv \dfrac{\partial \theta}{\partial q^j}$; Einstein summation convention in force

where suffices on the coordinates have been raised to implement the summation convention. The identity (11) can be differentiated, with respect to time, to give further 'higher level' identities. Thus

(12) $\ddot{\theta} = \ddot{q}^j \theta_{,j} + \dot{q}^j \dot{q}^k \theta_{,j,k}$

(13) $\dddot{\theta} = \dddot{q}^j \theta_{,j} + 3\ddot{q}^j \dot{q}^k \theta_{,j,k} + \dot{q}^j \dot{q}^k \dot{q}^l \theta_{,j,k,l}$

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3.2 $\theta(\underline{q})$ Interpreted as Classical

Because the $\underline{q}$ are taken to be functions of t we can interpret these differential identities as equations in *classical mechanics*. If (11), (12) and (13) are equations in CM then $\theta(\underline{q})$ must be a variable within a system and, as such, has a physical meaning; but, if we are not prepared to specify either which system or which variable, then $\theta(\underline{q})$ is , for most intents and purposes, arbitrary. That the system is classical is consistent with our assertion that both the $\underline{q}(t)$ and $\theta(\underline{q})$ are differentiable.

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4. Quantization of the First Level Identity (11)

4.1 Correspondences

Suppose, first, that we choose $\theta(\underline{q})$ to be arbitrary within its class; and suppose, second, that we attempt to 'quantize' (i.e., provide an operator form for) the classical equation (11) according to the usual QM recipes. The correspondence between classical variables and quantum operators is:

(15) $a \to A; \quad f(a) \to F(A); \quad \dot{a} \to \dot{A}$

where $\dot{A}$ is defined by

(16) $\dot{A} \equiv \frac{i}{h}(HA - AH)$; see (4) ; $\frac{\partial A}{\partial t} = O$; null operator

(20) $\alpha a + \beta b \to \alpha A + \beta B; \quad ab \to (AB + BA)/2; \quad \alpha, \beta$ are real scalar constants

(17)
$$\frac{\partial a}{\partial q^j} \to -\frac{i}{h}(AP_j - P_j A) \equiv \frac{\partial A}{\partial Q^j} \equiv A_{,j}; \quad a(\underline{p}, \underline{q}) \to A(\underline{P}, \underline{Q})$$
$$\frac{\partial a}{\partial p_j} \to \frac{i}{h}(AQ^j - Q^j A) \equiv \frac{\partial A}{\partial P_j} \equiv A^{;j}$$

where the PD notation suggests the algorithm required to perform calculations.

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4.2 The Operator Equation Corresponding to (11)

All the above operators are either Hermitian or self adjoint (representing real observables). Notice that we have used the Schrödinger representation in which none of the operators depend on t.

With the above definitions we can express the operator equation that corresponds to (11):

$$(21) \quad \dot{\Theta} = \frac{i}{h}(H\Theta - \Theta H) = \tfrac{1}{2}(H^{;j}\Theta_{,j} + \Theta_{,j}H^{;j})$$

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5. The Quantization Restricts H But Allows the Schrödinger Form (9)

Because the function $\theta(\underline{q})$ is arbitrary so is the operator $\Theta(\underline{Q})$. Therefore, because (11) is an identity that holds for arbitrary $\theta(\underline{q})$, (21) should also be an identity that holds for arbitrary $\Theta(\underline{Q})$; but, as it turns out, (21) is an identity *only for certain forms of* H. For example suppose that

$$(22) \quad H \equiv P^3; \quad \Theta = \Theta(Q)$$

then (21) becomes

$$(27) \quad \Theta''' = O; \quad \Theta' \equiv \frac{i}{h}(P\Theta - \Theta P) = \frac{\partial \Theta}{\partial Q}$$

which is not true for arbitrary Θ. So the form (22) is disallowed. But, the forms

$$(28) \quad H \equiv P; \quad H \equiv P^2 \text{ and } (9)$$

satisfy (21).

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6. Quantization of the Second Level Identity (12)- The Schrödinger Form (9) is an Approximation

We may use the rules of Section 5 to quantize the second level identity (12). We obtain

(33)

$$\ddot{\Theta} = \frac{-1}{h^2}[H(H\Theta - \Theta H) - (H\Theta - \Theta H)H]$$
$$= \frac{i}{2h}[(HH^{:j} - H^{:j}H)\Theta_{,j} + \Theta_{,j}(HH^{:j} - H^{:j}H)]$$
$$+[(H^{:j}H^{:k} + H^{:k}H^{:j})\Theta_{,j,k} + \Theta_{,j,k}(H^{:j}H^{:k} + H^{:k}H^{:j})]/4$$

The first of the choices (28) satisfies (33) exactly; but, when we substitute (9), (33) gives

(34) $$-\frac{h^2}{4m^2}\sum_{j,k}\Theta_{,j,j,k,k} = O$$

Given that, for (9), $n = 3$ the operator equation (34) corresponds to the scalar PDE

(35) $$-\frac{h^2}{4m^2}\nabla^2(\nabla^2\theta(\underline{q})) = 0$$

where, we recall, the $\underline{q}$ are the Cartesian coordinates of a single particle.

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7. The Dirac Form (42) is Exact Up to Level Two

The solutions of (35) can approximate many functions; but in no sense are they arbitrary. So, except for a limited class of operators $\Theta(\underline{Q})$, (9) does not satisfy (33). The question arises: can we modify (9) so as still to satisfy (21) while, at the same time, eliminating the error term (see the LHS of (34))?

The Hamiltonian (9) is a low momentum approximation to a classical relativistic Hamiltonian given by

(38) $$(H(\underline{p},\underline{q})-V(\underline{q}))^2 = \sum_{j=1}^{3} c^2 p_j^2 + m^2c^4;$$ c is the light speed

Quantizing (38) and taking the square root of (41) in the manner of Dirac

(42) $$H(\underline{P},\underline{Q}) = \sum_{j=1}^{3} c\sigma_j P_j + \sigma_0 mc^2 + V(\underline{Q})$$

(42a) $$\sigma_\alpha \sigma_\beta + \sigma_\beta \sigma_\alpha = 2\delta_{\alpha\beta} I; \quad \alpha,\beta = 0,1,2,3$$

where the σ_α are Hermitian operators that commute with both the $\underline{P}$ and the $\underline{Q}$. H, defined by (42) and (42a), satisfies both (21) and (33) exactly.

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8. The Dirac Form is Exact At Least Up to Level Three

A further calculation shows that, given the linear form

(45) $H(\underline{P},\underline{Q}) \equiv \sigma^j P_j + \sigma + V(\underline{Q});$ Einstein in force

and provided that the σ^α ($\sigma^0 \equiv \sigma; \quad \alpha = 0,1,2,3$) commute with both the $\underline{P}$ and the $\underline{Q}$, (21) and (33) are *always* identities whatever mutual commutation rules govern the σ^α. But a calculation at level three (i.e., beginning with (13)) shows that we must have

(46)
$$(\sigma^j\sigma^k + \sigma^k\sigma^j)\sigma^l = \sigma^j(\sigma^j\sigma^k + \sigma^k\sigma^j) \Rightarrow (\sigma^j)^2\sigma^k = \sigma^k(\sigma^j)^2; \quad \forall\, l.j.k$$

and

(47)
$$(\sigma^j\sigma^k + \sigma^k\sigma^j)\sigma = \sigma(\sigma^j\sigma^k + \sigma^k\sigma^j) \Rightarrow (\sigma^j)^2\sigma = \sigma(\sigma^j)^2; \quad \forall\, j.k$$

These conditions are satisfied by any set of operators σ^j and σ that satisfy (see (42a)

(48) $\sigma^\alpha\sigma^\beta + \sigma^\beta\sigma^\alpha = 2\delta^{\alpha\beta} I; \quad \alpha, \beta = 0,1,2,3; \quad \sigma^0 \equiv \sigma$

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9. Conclusions

Two alternative views can be taken of these calculations:

(a) The operator forms of the differential identities themselves fail to be identities for all $\Theta(\underline{Q})$ and all H because the quantization recipe is at fault.

(b) The insistence that $\theta(\underline{q})$ is a continuous, differential function of the coordinates $\underline{q}$ and, further, that the $\underline{q}$ are continuous, differential functions of the time t identifies $\theta(\underline{q})$, although otherwise arbitrary, as belonging to a classical system. The restrictions placed on H, to ensure that the operator forms remain identities for arbitrary $\Theta(\underline{Q})$, therefore characterise classical systems.

It is shown that the Schrödinger form of H can only approximate the higher level identities. The Dirac form is exact at least up to level 3.

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$$\dot{f}(\underline{p},\underline{q}) = \sum_j \left(\frac{\partial f}{\partial p_j}\dot{p}_j + \frac{\partial f}{\partial q_j}\dot{q}_j \right) = \sum_j \left(\frac{\partial f}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial f}{\partial p_j}\frac{\partial H}{\partial q_j} \right) \equiv \{f, H\}_{p,q}$$

$$\rightarrow \dot{F} \equiv \frac{i}{h}(HF - FH)$$

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