A Two-Page Derivation of Schrödinger’s Equation

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We give an exceptionally short derivation of Schrödinger’s equation by replacing the idealization of a point particle by a density distribution.

I. INTRODUCTION

There is strong reason to believe that Nature works according to mathematical laws. All the substantial progress of science supports this view.

– P.A.M. Dirac

Contrary to a common textbook view that the Schrödinger equation (SEQ) cannot possibly be derived [2, 3], the number of published papers that either present derivations of the SEQ and/or (semi-) classical perspectives on the SEQ, increases continuously [1]. We shall present yet another derivation of the SEQ based mostly on formal mathematical considerations.

Classical mechanics is often identified with the mechanics of “point particles” or “mass points”. There is no classical theory of extended continuous microscopic objects, despite the fact that “natural philosophy” defined material objects as res extensa. But since classical physics identifies matter by its position in space and time, it seems unclear how to assign a common identity to the volume elements of extended objects. Newton tried to circumvent the problem by the involvement of a supernatural power [51]:

[...], it seems probable to me, that God in the Beginning form’d Matter in solid, massy, hard, impenetrable, movable Particles, of such Sizes and Figures, and with such other Properties, and in such Proportion to Space, as most conduced to the End for which he form’d them; and that these primitive Particles being Solids, are incomparably harder than any porous Bodies compounded of them; even so very hard, as never to wear or break in pieces; no ordinary Power being able to divide what God himself made one in the first Creation.

Boscovich [52], an influential Serbian Jesuit scientist, suggested a different approach by the invention of point particles in the strict mathematical sense [53]:

According to Boscovich an atom is an indivisible point, having position in space, capable of motion, and possessing mass. [...] It has no parts or dimensions: it is a mere geometrical point without extension in space: it has not the property of impenetrability, for two atoms can, it is supposed, exist at the same point.

But though Boscovich’ position seems to have prevailed in modern textbooks on analytical mechanics, a survey of textbooks on mechanics of the 19th century, before the advent of quantum theory, provides evidence that the “classical” point particle never was accepted as an undisputable and self-consistent idea [54]. Also James Clerk Maxwell, to give just one example, disagreed with Boscovich [53]:

We make no assumption with respect to the nature of the small parts – whether they are all of one magnitude. We do not even assume them to have extension and figure. Each of them must be measured by its mass, and any two of them must, like visible bodies, have the power of acting on one another when they come near enough to do so. The properties of the body or medium are determined by the configuration of its parts.

Rohrlich critically reviewed the idealization of the classical point particle [55]. He wrote that “in the point limit, classical physics cannot be expected to make sense at all”. As he explains, a point charge, regarded from the standpoint of classical electrodynamics, implies infinite self-energy. Hence, according to Rohrlich, “the concept of a ”classical point particle” is, in view of quantum mechanics, an oxymoron. Quantum mechanics tells us that below a certain magnitude of distance, usually characterized by a Compton wavelength, classical physics ceases to be reliable; predictions made by classical mechanics or classical electrodynamics must be replaced by quantum mechanical predictions.”

As our derivation will demonstrate, the SEQ implicitly suggests yet another solution to the problem of extended objects, namely it transforms the problem of the “parts” of extended objects into Fourier space: The extended particle is then not an ensemble of “material points” in space, but an ensemble of waves in Fourier space. The question whether we interpret the “extended object” as a probability distribution or directly as a mat-

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1 See Refs. [4–9], [10–16], [17–21], [22–27], [28–33], [34–39], [40–44], [45–48], [49, 50]. This list, though rather long, is certainly still incomplete.
NI. THE SCHRÖDINGER EQUATION

Consider that an extended particle (or the probability to find a point particle, respectively), is represented by a
normalizable spatial density distribution \( \rho(t, \vec{x}) \)
\[
\int \rho(t, \vec{x}) \, d^3x = 1. \tag{1}
\]
We regard the density as a positive definite quantity: \( \rho \geq 0 \). In order to fulfill this requirement, we express the
density by the square modulus of (a sum of) auxiliary functions \( \psi_i(t, \vec{x}) \) such that
\[
\rho(t, \vec{x}) = \sum_i \psi_i^2(t, \vec{x}). \tag{2}
\]
For simplicity - and without loss of generality - we may use complex numbers and chose the following positive
semidefinite expression
\[
\rho(t, \vec{x}) = \psi(t, \vec{x})^* \psi(t, \vec{x}). \tag{3}
\]
The auxiliary function \( \psi(t, \vec{x}) \) is then due to Eq. [1] square integrable. It is therefore a member of some Hilbert space
and the Fourier transform \( \tilde{\psi}(\omega, \vec{k}) \) is known to exist:
\[
\psi(t, \vec{x}) \propto \int \tilde{\psi}(\omega, \vec{k}) \exp[-i(\omega t - \vec{k} \cdot \vec{x})] \, d^3k \, d\omega. \tag{4}
\]
But the Fourier transformation alone, without any further
constraint, does not yield a physical model of anything. All known physical waves are characterized by a relation between frequency and wavelength, i.e. by a dispersion relation. It can be demonstrated that the
necessary existence of a dispersion relation is a consequence of a causality requirement [56–58]. The dispersion relation
then allows to obtain an expression for the velocity of the “wave packet”, namely the so-called group velocity [57–61]:
\[
\vec{v}_{gr} = \vec{\nabla}_k \omega(\vec{k}) = \left( \frac{\partial \omega}{\partial k_x}, \frac{\partial \omega}{\partial k_y}, \frac{\partial \omega}{\partial k_z} \right)^T, \tag{5}
\]
where \( \omega(\vec{k}) \) is the mentioned dispersion relation. Eq. [5] has precisely the form of the velocity equation of classical
Hamiltonian mechanics, which relates the velocity to the gradient of the energy (i.e. the Hamiltonian function) in
momentum space:
\[
\vec{v} = \vec{\nabla}_p \mathcal{H}(\vec{p}) \tag{6}
\]
Hence, if the wave packet is supposed to provide a description of a classical particle, the (average) velocity of
the wave packet must agree with the Hamiltonian expression [2]:
\[
\vec{v} \omega(\vec{k}) = \vec{\nabla}_p \mathcal{H}(\vec{p}). \tag{7}
\]
A solution that complies with Eq. [7] where energy and momentum have the usual units, requires the introduction
of a proportionality constant with the unit of action, let’s call it \( \hbar \). It is, in the context of our derivation, not a
substantial physical unit and does not imply any quantization of energy. Conversion factors can not be derived theoretically [64]:
\[
\hbar \omega(\vec{k}) = \mathcal{H}(\vec{p}) + q \phi(\vec{x}). \tag{8}
\]
with some arbitrary constant \( q \). Note that this is not a physical hypothesis, but a formulation of the linear
restriction that the wave ensemble has to comply with, if it is supposed to consistently represent a classical particle in some way. The “integration constants” \( \phi \) and \( \vec{A} \) are well known in classical mechanics and can assumed to be zero for a free particle.

The total normalization must of course be preserved and this requires that the wave motion is adiabatic. Max
Born referred to the classical adiabatic invariance of the phase space volume \( \Phi = \text{const} \) and to the fact that energy (change) and frequency (change) are, in such processes, proportional to each other \( \delta \mathcal{E} = \Phi \delta \omega \) [66]. Furthermore it is long known that the real and imaginary components of the wave function are subject to Hamiltonian motion [67–68].

2 Several authors of standard textbooks on QM, for instance Messiah [3], Schiff [62] and as well as Weinberg [65] use this equation, not to derive Schrödinger’s equation, but merely to make it “plausible”.

Instead of showing that Schrödinger’s equation implies Hamiltonian notions, we consider the reverse argument: if one presumes the validity of energy conservation and hence of classical Hamiltonian notions in wave dynamics, then Eq. 4 is automatically valid. The de-Broglie relations then immediately follow:

\[ \mathcal{E} = h \omega \]
\[ \vec{p} = h \vec{k} . \]  

(9)

Inserting this into the Fourier transform gives:

\[ \psi(t, \vec{r}) \propto \int \hat{\psi}(\mathcal{E}, \vec{k}) \exp \left\{ -i (\mathcal{E} t - \vec{p} \cdot \vec{x})/\hbar \right\} d^3p d\mathcal{E} . \]  

(10)

Then the energy is equal to the time derivative, and the momentum to the spatial gradient. That is, the canonical “quantization” rules directly follow:

\[ \mathcal{E} \psi(t, \vec{r}) = i \hbar \frac{\partial}{\partial t} \psi(t, \vec{r}) \]
\[ \vec{p} \psi(t, \vec{r}) = -i \hbar \vec{\nabla} \psi(t, \vec{r}) . \]  

(11)

Using these relations one can express the classical (kinetic) energy of a free particle \( \mathcal{E} = \frac{\vec{p}^2}{2m} \), which results in Schrödinger’s equation for a free particle:

\[ i \hbar \frac{\partial}{\partial t} \psi(t, \vec{x}) = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(t, \vec{r}) . \]  

(12)

Adding a potential energy (density) \( \rho(t, \vec{x}) \phi(\vec{x}) \) readily yields Schrödinger’s equation in potential \( \phi(\vec{x}) \):

\[ i \hbar \frac{\partial}{\partial t} \psi(t, \vec{x}) = \left( -\frac{\hbar^2}{2m} \vec{\nabla}^2 + \phi(\vec{x}) \right) \psi(t, \vec{r}) . \]  

(13)

This derivation of Schrödinger’s equation is short and rigorously follows from the assumption that the presence of a material particle must have a mathematical representation by a finite normalizable positive semidefinite density. This could be described as the logical classical alternative to the representation of a particle as mathematical point without extension. It provides a new perspective on the relationship between classical mechanics and quantum theory and shows that, contrary to usual assertions, these theories are not mathematically disjunct.

Our derivation neither presumed nor suggested a specific interpretation of the “wave function”. It only provides a different perspective on the mathematical form of Schrödinger’s equation and demonstrates that there are indeed classical arguments which lead to an action constant of universal physical significance.

### III. SUMMARY AND CONCLUSIONS

As Rohrlich’s analysis reveals, the alleged intuitiveness and logic of the notion of the point particle fails, on closer inspection, to provide a physically and logically consistent classical picture. If we dispense this notion, Schrödinger’s equation can be derived and might be regarded as a kind of regularization, which allows to circumvent the problematic infinities of the point-particle-idealization. Nonetheless it is ahistorical to depict the point-particle-idealization as “classical”, since most textbook authors of the pre-quantum era stayed, like Maxwell, agnostic about the true nature of the “smallest parts” [54].

The given presentation uses the “Born rule”, which states that \( \psi^* \psi \) is a (probability) density, as a mathematical method rather than as a part of it’s interpretation.

However, as well-known (though often ignored), Schrödinger’s equation is not the most fundamental equation of quantum theory. It has to be derived from the Dirac equation. Only the Lorentz covariant Dirac equation provides full compatibility with electromagnetic theory. It was shown elsewhere how the Dirac equation can, in momentum space, be derived from Hamiltonian methods [69–71]. The derivation automatically yields the Lorentz transformations, the Lorentz force law [72–74] and Maxwell’s equations [69] in a single coherent framework.

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