Position: operator or coordinate?

Erik Deumens*

April 10, 2023

Abstract

Clarifying the role of position in nonrelativistic quantum mechanics to be "conceptually" in line with relativity. The second quantization formulation introduce by Fock in 1932 provides an elegant and powerful way to resolve the tension between position as an operator-observable and time as a coordinate-parameter.

This note # 7 in a series of notes to untangle quantum mechanics for general audience and experts alike.

URL https://people.clas.ufl.edu/deumens/files/pap-position.pdf

It is generally accepted in the discussions pertaining to the foundations of quantum mechanics, that the framework of non-relativistic quantum mechanics is appropriate [**?**]. In principle, one would want to discuss relativistic effects in the context of quantum field theory, but the formalism is much more complex and tends to hinder the discussions more than help them. There is, however, a foundational issue that is not discussed much in the literature, namely the conceptual discrepancy between position and time, as they are defined in nonrelativistic quantum mechanics.

It is perfectly acceptable to discuss conceptual issues in cases where all speeds of objects are small compared to the speed of light so that relativistic effects are small and negligible. The numerical limit from large velocities does not include a change in foundational concepts, even if dramatically new effects, like time dilation, are involved at large velocities.

But it is not acceptable to consider this limit when there are conceptual changes in foundational concepts. That is the case in nonrelativistic quantum mechanics where position is treated as an observable, which is represented mathematically by a Hermitian operator, and where time is treated as a coordinate or parameter, which is represented as a real-valued number. That means that the relativistic description of a Lorentz transformation between different inertial frames is conceptually at odds with the way space, the position operator, and the time coordinate value are handled.

*Quantum Theory Project, University of Florida, ORCID 0000-0002-7398-3090

To discuss relativistic issues in nonrelativistic quantum mechanics, one must use a formulation where both space and time are treated on the same conceptual footing. This was accomplished in 1932 by Vladmir Fock [3] with the introduction of the number representation of wavefunction, also known as "second quaantizatin." This formulation has proven to be very powerful for writing the computer software the solves the Schrödinger equation for molecular systems [4] and materials [2, 1], as well as for work in quantum field theory [5]. In the second-quantization formulation every system is described as a field and the position and time are coordinates of where whatever is described by the wave function is created or desctoyed by creation and annihilation operators $\boldsymbol{a}^{\dagger}(\vec{r}, t), \boldsymbol{a}(\vec{r}, t)$, labeled by the spacetime coordinates $(\vec{r}, t)$.

Even though the numerical details of the calculations performed are not relativistic and they will not give correct values when systems are moving at speeds close to the speed of light, the formulation is conceptually correct and valid across nonrelativistic quantum mechanics and quantum field theory.

In the second-quantization formulation, nonrelativistic systems are not described by wavefunctions that depend on position, but they are specified by creation and annihilation field operators. Wavefunctions can be computed for the strengths of thoses fields, which can have multiple components. There can be components of electric and magnetic field strength vectors, of vector potentials, or spinor (qubit) components at a particular point $\vec{r}$ in space at a moment t in time.

References

[1] Anisimov, V., Izyuov, Y.: Electronic Structure of Strongly Correlated Materials, *Springer Series in Solid State Physics*, vol. 163. Springer, Heidelberg Dordrecht London New York (2010). DOI 10.1007/978-3-641-04826-5

[2] Ashcroft, N.W., Mermin, N.D.: Solid State Physics. Brooks/Cole, Cengage Learning, Belmont, California (1976)

[3] Fock, V.: Konfigurationsraum und zweite Quantelung. Zeitschrift für Physik **75**, 622–647 (1932)

[4] Helgaker, T., Jørgensen, P., Olsen, J.: Molecular Electronic Structure Theory. John Wiley & Sons Ltd, Chichester, England (2000)

[5] Schwartz, M.D.: Quantum Field Theory and the Standard Model. Cambridge University Press, New York (2014)