Schrödinger Equation for Nanoscience

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Abstract

The second order (in time) Schrödinger equation is proposed. The
additional term (in comparison to Schrödinger equation) describes the
interaction of particles with vacuum filled with virtual particle – antiparticle pairs (zitterbewegung).

Key words: Schrödinger equation; Nanoscience; Zitterbewegung.
Quantum mechanics has been remarkably successful in all realms of atoms molecular and solids. But even more remarkable is the fact that quantum theory still continues to fascinate researches. Interest in quantum mechanics both theoretical and experimental is probably greater now that it ever has been.

In this article we develop the modified Schrödinger equation which describes the structure of matter on the subatomic level i.e. for characteristic dimension $r_n < d < r_a$ where $r_n$ (nucleus radius) $\sim$ fm, $r_a$ (atom radius) $\sim$ nm. To that aim we use the analogy between the Schrödinger equation and diffusion equation (Fourier equation). The quantum Fourier equation which describes the heat (mass) diffusion on the atomic level has the form:

$$\frac{\partial T}{\partial t} = \frac{\hbar}{m} \nabla^2 T.$$  \hspace{1cm} (1)

When the real time $t \to it/2$ and $T \to \Psi$, Eq. (1) has the form of the free Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi.$$  \hspace{1cm} (2)

The complete Schrödinger equation has the form:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi$$  \hspace{1cm} (3)

where $V$ denotes the potential energy. When we go back to real time $t \to -2it$, $\Psi \to T$ the new parabolic quantum heat transport equation (quantum Fokker-Planck equation) is obtained:

$$\frac{\partial T}{\partial t} = \frac{\hbar}{m} \nabla^2 T - \frac{2V}{\hbar} T.$$  \hspace{1cm} (4)

Equation (4) describes the quantum heat transport for $\Delta t > \tau$. For ultra-short time processes, $\Delta t < \tau$ one obtains the generalized quantum hyperbolic heat transport equation:

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{\hbar}{m} \nabla^2 T - \frac{2V}{\hbar} T.$$  \hspace{1cm} (5)

The structure and the solutions of Eq. (5) for ultrashort thermal processes was investigated in the monograph: M. Kozlowski, J. Marciak-Kozlowska: From quarks to bulk matter, Hadronic Press, USA, 2001. The generalized
heat transport equation (5) leads to modified Schrödinger equation (MSE). After substitution \( t \rightarrow it/2, T \rightarrow \Psi \) in Eq. (5) one obtains:

\[
i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi - 2\tau \hbar \frac{\partial^2 \Psi}{\partial t^2}.
\] (6)

The additional term (in comparison to Schrödinger equation) describes the interaction of electrons with surrounding space-time filled with virtual positron-electron pairs, i.e. zitterbewegung.

One can conclude that for time period \( \Delta t < \tau \) and distance \( \Delta r < c\tau \) the description of quantum phenomena needs some revision. The numerical values for \( \Delta t \) and \( \Delta r \) can be calculated as follows. Considering that \( \tau \),

\[
\tau = \frac{\hbar}{m\alpha^2 c^2} \sim 10^{-17} \text{ s}
\] (7)

\[
c\tau = \frac{\hbar c}{m\alpha^2 c^2} \sim 1 \text{ nm},
\]

we conclude that with the help of MSE we can visit the inner atomic environment. On the other hand for \( \Delta t > 10^{-17} \text{ s}, \Delta r > \text{nm} \), in MSE the second derrivative term can be omitted and as result the SE is obtained, i.e.

\[
i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi.
\] (8)

The visit of the inner structure of the atom can be quite interesting, for the fact that atom radius remains strictly constant during the universe expansion [2].

References

[1] M. Kozlowski, J. Marciak-Kozlowska
    From Quarks to Bulk Matter
    Hadronic Press, USA, 2001

[2] W. B. Bonnor,
    Size of a hydrogen atom in the expanding universe
    Class. Quantum Grav. 16, (1999) 1313