WHY DO WE NEED QUANTUM THEORY?

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I. Introduction

A good starting point of this consideration can be a question "Why do we need quantum theory?". What is wrong with just using the methods of classical mechanics or electrodynamics. Although there are a number of arguments for quantum theory, many people still accept the quantum theory as an intellectual achievement having many arguments for own truth. Many of them are based on superstition of elegance of classical theory. As said Ludwig Boltzmann "Elegance should be left to shoemakers and tailors, we should keep the law of mathematics". The aim of this paper is to discuss some arguments for quantum mechanics which are mostly technical and maybe mathematical rigorous. Whereas some mathematics overstate the beginning let's are start with a little theory.

In this discussion we will use the interaction representation (also known as the Dirac picture) which is an interactive picture between the Schrödinger and the Heisenberg picture. Although it sounds ominously, it is a very effective tool in cases where the influences of disturbance simultaneously changing both the wave function and observed variable. In this case the solution is to use with the aim to express many-body solution of the Schrödinger equation. The interaction representation constructs the solution of Schrödinger equation as the solution of the free particle problem plus some unknown interaction part. In our discussion we will use a hypothetical system (not very far from reality) which contains a mixture of dissipative and other (yet unknown) subsystems with very different qualities. It has been shown that right in this configuration the interaction representation is very useful.

II. The story

As we continue in our story, assume that the system is fully described by an operator of density probability ρ, which obey the following differential equation (note **V** means the interaction part):

$$i\hbar\frac{d\hat{\varrho}}{dt} = [\hat{\mathbf{V}}, \hat{\varrho}]$$

The previous equation is ordinary differential equation, which is possible to solve with the help of traditional tools. Very useful one is to expand solution in the time series:

$$\begin{aligned}\hat{\varrho}(t+\tau) &= \hat{\varrho}^{(0)}(t) - \frac{i}{\hbar}\int_0^\tau [\hat{\mathbf{V}}(t+\tau'), \hat{\varrho}(t)]d\tau' - \\ &- \frac{1}{\hbar^2}\int_0^\tau d\tau' \int_0^{\tau'} [\hat{\mathbf{V}}(t+\tau', [\hat{\mathbf{V}}(t+\tau''), \hat{\varrho}(t)]]d\tau'' \cdots\end{aligned}$$

Now suppose that it is possible to extract operator density of probability s which describes certain parts of the system separated from the dissipative part. Mathematical image of this operation could be as follows:

$$\hat{\sigma} = \sum_{\alpha} \langle \alpha | \varrho | \alpha \rangle = \mathrm{Tr}_B \, \hat{\varrho}$$

To achieve the goals we still assume that interaction often varies periodically in time. With this in mind it is possible to develop the interaction part into Fourier series. Mathematically it could be written as follows:

$$\hat{\mathbf{V}}(t) = \sum_{r} \mathbf{V}_r exp[i(\omega_r)\mathbf{F}^{(r)}(t)]$$

If we put all together, evolution of the operator s of system could be written as other ordinary differential equation (ODE) – say so:

$$\begin{aligned}
\frac{d\sigma}{dt} &= -\frac{i}{\hbar} \sum_{r} \sum_{\alpha} F_{r;\alpha\alpha} \Xi_{\alpha} [\mathbf{V}(\omega_r), \sigma(t)] \\
&- \frac{1}{\hbar^2} \sum_{r} \sum_{\alpha\alpha'} \Xi_{\alpha} F_{-r;\alpha\alpha'} F_{r;\alpha'\alpha} [\mathbf{V}(\omega_r), \mathbf{V}(-\omega_r)\sigma(t)] 2\pi\delta(-\omega_r + \Omega_{\alpha\alpha'}) \\
&- \frac{1}{\hbar^2} \sum_{r} \sum_{\alpha\alpha'} \Xi_{\alpha} F_{r;\alpha\alpha'} F_{-r;\alpha'\alpha} [\sigma(t)\mathbf{V}(\omega_r), \mathbf{V}(-\omega_r)] 2\pi\delta(-\omega_r + \Omega_{\alpha\alpha'})
\end{aligned}$$

In this ODE is the influence of dissipation effect counted in classical approximation which is usual accepted in following form:

$$\Xi_{\alpha} = \frac{g_{\alpha} exp(-F_{\alpha}/k_B T)}{\sum_{\beta} g_{\beta} exp(-F_{\beta}/k_B T)}$$

It is very important to note, that dissipative part should be thermostatic. Otherwise need to change some considerations. After much effort (believe us, it's really difficult) and portion of happiness (happiness is always need in such calculations) we could get the results. Since during the calculation, we used the most diverse tricks result may be surprising. Really, the result shows on normal relaxation time, as we know from classical physics [1]. Just look:

$$\begin{aligned}
\frac{1}{\mathcal{T}_{nm}} &= \sum_{r=1}^{\infty} \sum_{j} \Big\{ (V_{r;nj} V^*_{r;jn} + V^*_{r;mj} V_{r;jm})] A_1^{(r)} \\
&+ (V^*_{r;nj} V_{r;jn} + V^*_{r;mj} V_{r;jm})] A_2^{(r)} exp(\hbar\omega_r / k_B T)] \Big\}
\end{aligned}$$

After a very difficult calculation and an enormous effort we come to what we can get through the physics of the 19th century. What is going on in this big Jigsaw? Is all this effort worth it? Is it really true, that all what we need was discovered one hundred and fifty years ago? Actually, it may surprise us only when the result is considered in the context of 19th century. Moreover, this result is widely accepted, even in the case of quantum systems. The

picture will change, until we begin with quantum effects - for example with those we lost when adjusting equations. Missing quantum effects we include with the help of second quantization which is a powerful procedure used in quantum field theory for describing the many-particle systems by quantizing the field with the aim to describe the number of electrons. We will do it by changing classical interaction with quantum operators:

$$\begin{aligned} \mathbf{V}_r &\rightarrow \hat{a}_{\mathbf{r}} \\ \mathbf{V}_r^* &\rightarrow \hat{a}_{\mathbf{r}}^+ \end{aligned}$$

The system suddenly starts behaving differently than we can imagine in classical physics. Quite simply, some electrons occupy the energy levels infinity long period of time and the concept of relaxation time become meaningless. In some cases, the electron would leave its energetical level through the mechanism, which is known as quantum tunneling, of course, if the conditions are suitable.
Mechanism of quantum tunneling tried many authors to explain on some macroscopic model. As an example could be addressed a model of metallic tube with the gradually increasing potential. Electron is trying to get through the growing potential as water through the water pipeline. It's all drawn in the Figure bellow:

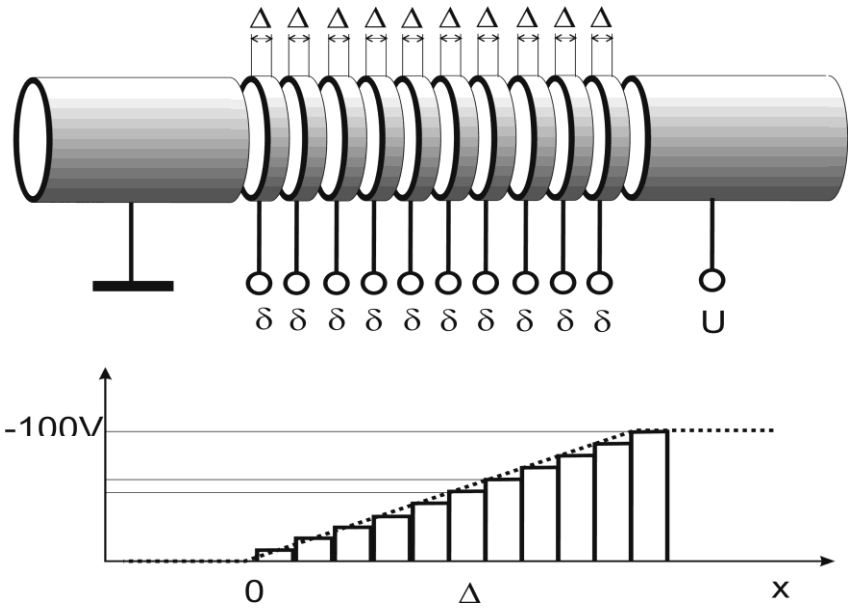

Fig. 1: *Mechanical model of linear growing barrier (Top panel). Linear growing potential as a sequence of rectangular gradually increasing barriers (Bottom panel).*

In cases where the potential increases slowly and rings are wide enough, we can use some classical approximation which is known since the 19th century. We employ a well known WKB approximation, originally developed in optics. After some algebra we get very familiar expression that many knew from books, but few understood it. There you have it:

$$T = e^{-2\int_0^d \{\sqrt{\frac{2m}{\hbar^2}(V(x)-E)}\}dx}$$

The expression gives coefficient of transparency *T* which describes the clearness of the system. It looks really nice. Everything is alright, not try this procedure to microscopic objects of nanometers size. In the case of nano-objects we need really use Schrödinger equation which should be solved in three areas; before the barrier, through the barrier, and behind the barrier.

$$\begin{aligned} \frac{d^2\Psi(x)}{dx^2} + k_0^2\Psi(x) &= 0 \qquad x < 0 \\ \frac{d^2\Psi(x)}{dx^2} - (q_0^2 - k_0^2 + q_0^2\frac{x}{a})\Psi(x) &= 0 \qquad 0 \le x < d \\ \frac{d^2\Psi(x)}{dx^2} + k_0^2\Psi(x) &= 0 \qquad x \ge d \end{aligned}$$

The system of equations can be solved, even assuming compliance with all quantum rules. It takes great patience, but the result is worth it. The coefficient of transparency *T*, now looks very different, but is mathematical correct even in a wide range of sizes.

$$\begin{aligned} T \equiv |\vartheta|^2 = & \frac{\varrho}{\{[Bi(\mu)Ai'(-\varrho) - Ai(\mu)Bi(-\varrho)]^2 + \varrho[Bi(\mu)Ai(-\varrho) - Ai(\mu)Bi(-\varrho)]^2\}} \\ \times & \frac{1}{\{[Bi'(\mu)Ai'(-\varrho) - Ai'(\mu)Bi(-\varrho)]^2 + \varrho[Bi'(\mu)Ai(-\varrho) - Ai'(\mu)Bi(-\varrho)]^2\}} \end{aligned}$$

In this expression Ai(x) and Bi(x) mean Airy functions, which are solutions of Airy ODE. Prime means differentiation.

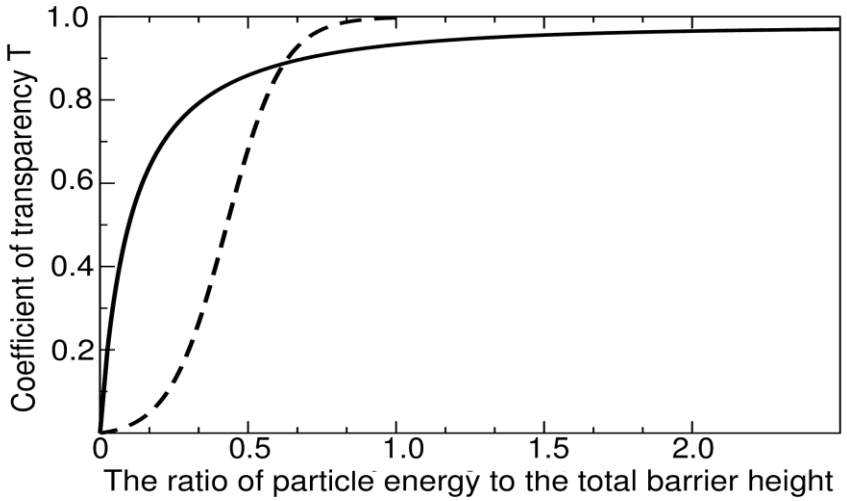

Fig. 2: *Dependence of transparency of triangular barrier depending on the particle energy passing through the barrier in ratio to the barrier height. WKB approximation - dashed line, exact solution - solid line.*

It is of course a very thin barrier, the production of which, however, is now entirely possible. At first sight one can see that the differences between exact (quantum) approach and WKB (which is in fact classical solution) can be very large.

III. Conclusion

So why do we need a quantum theory? Because correctly describes the world of nano dimensions. This is true, but not just because we love it and not only from this perspective we need to know (and teach our students) quantum theory. Is the right way to understand the world and the the right road to the technological and personal growth. As Niels Bohr said: “Anyone who is not shocked by quantum theory has not understood it“.

Acknowledgement

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Reference

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