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Quantum-Mechanical Uncertainty in NDT (Example of Scanning Tunnel Microscopy)

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Abstract
Nanodiagnostics is one of the most promising scientific directions of NDT. The greatest development of nanodiagnostic systems occurs with the use of scanning probe microscopy (SPM). In this paper we will try to estimate applicability of existing approaches to modern high-quality STM which characterized by high resolution and very small distance between probe and object (up to units Å or even less). It is shown, that standard semi-classical approximation does not work in many interesting cases. Instanton method for the calculation and estimation of tunneling processes for STM is proposed.

Keywords: Nanodiagnostics, scanning probe microscopy, tunneling, Fowler – Nordheim formula, instanton.

1. Introduction

As Academician Vladimir Kluev said "One of the main ways of developing of methods and facilities of nondestructive testing of the new generation is the use of known nanoeffects and nanosensors and nanotransformers developed on the basis of nanotechnology" [1]. Nanodiagnostics is one of the most promising scientific directions of NDT. The greatest development of nanodiagnostic systems occurs with the use of scanning probe microscopy (SPM).
The first historical example of SPM is scanning tunneling microscope (STM), which was created in 1982 by G. Binnig and H. Rohrer (Nobel Prize in Physics 1986 "for their design of the scanning tunneling microscope") /together with E. Ruska "for his fundamental work in electron optics, and for the design of the first electron microscope"/. Theoretical background of STM based on a possibility of electron emission in intense electric fields from cold metal [2]. This process can be explained by the tunnelling effect, which was explained by George Gamow [3].
Tunnelling effect is essentially quantum-mechanical phenomena. It allows justification by means of quantum-mechanical uncertainty relation (Heisenberg uncertainty relation). Because of this quantum-mechanical particle (for example electron) can penetrate through the classically forbidden area (potential barrier).
The most calculation of the effect was carried out in so-called quasiclassical approximation, which can be used for relatively small energies and large potential barriers (as for instance in [2]). But these conditions are violated often for the modern STM.
In this paper we will try to estimate applicability of existing approaches to modern high-quality STM which characterized by high resolution and very small distance between probe and object (up to units Å or even less).

2. Characteristics and Parameters of a Scanning Tunneling Microscope

The main characteristic is tunnelling current (or current of electron emission) J:

$$J \approx en\upsilon DS\,, \tag{1}$$

where e is electron charge, $n \approx 10^{28}\ m^{-3}$ – typical conduction electron density, $\upsilon \propto 10^{6} m/s$ – velocity of electrons, S is a square of tunnelling contact (up to $10^{-19} m^2$). The main quantity D, probability of tunnelling transition, is given by the following expression:

$$D(E) \approx \exp\left[-2\sqrt{\frac{2ma^2(U_0 - E)}{\hbar^2}}\right], \tag{2}$$

where $\hbar$ – Plank constant, m – electron mass, U_0 and E are height of energy barrier and electron energy correspondingly ($U_0 - E$ is so-called electron work function). And the main parameter in this context $\boldsymbol{a}$ is width of potential barrier or distance between probe and surface of conductive sample.

So, because *e, n, v* and *S* are practically given, the measurement of current *J* gives the quantity of distance between probe and surface and vice versa. This is the main physical principle of SPM work. Of course, the technical detail of mechanical scanning of surface is critically important. But the critical analysis of (2) is important first of all.

3. Probability of Tunnelling Processes in Quasi-classical Approximation and its Applicability for STM

Violation of Fowler-Nordheim formula for the autoemission current in real experiment was already discussed (see for instance [4]). We see the possible reason in incorrect using of (2) in real experimental facilities.

Let us remind several simple quantum-mechanical tasks and consider for instance standard ("student") potential (fig.1, left).

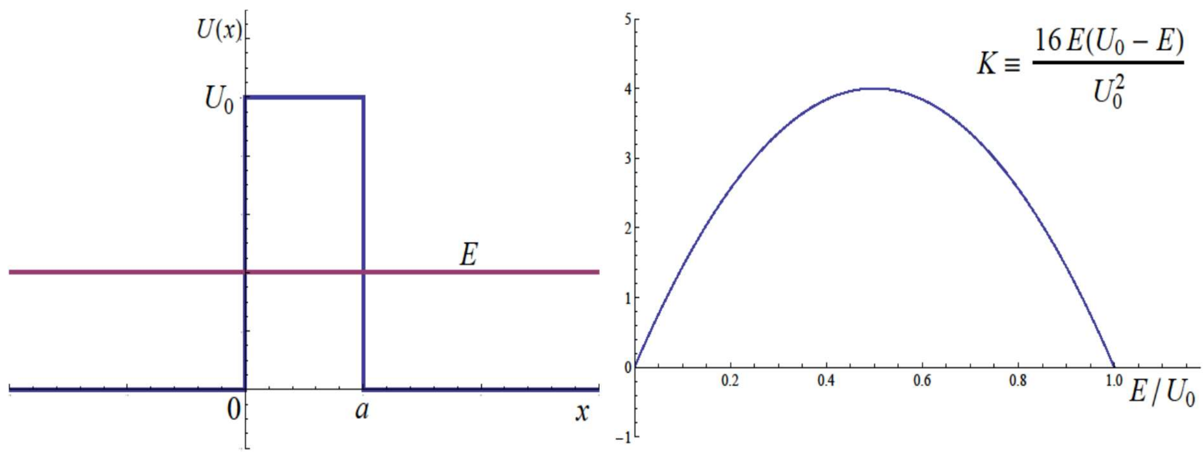


Fig.1. Rectangular potential barrier, energy of the particle $E < U_0$ (left). The dependence of pre-exponential factor on energy ratio (right).

The decision in quasi-classical approximation is given by well-known formula:

$$D(E) \approx \frac{16E(U_0 - E)}{U_0^2} \exp\left[-2\sqrt{\frac{2ma^2(U_0 - E)}{\hbar^2}}\right] \ll 1, \quad \frac{ma^2(U_0 - E)}{\hbar^2} \gg 1. \tag{3}$$

This expression is very similar to (2) with the exception of pre-exponential factor. Here we pay attention, it is not equal to unit even approximately (see fig.1, right) and can be carefully taken into account.
Expression (3) can be applicable for “large“ potential barrier and “low” electron energies. By the way, these conditions are not applicable in general case in modern STM schemes.
The exact solution for probability of barrier penetration is well-known:

$$D(E) = \frac{4\,E\,(U_0 - E)}{4\,E\,(U_0 - E) + U_0 \mathrm{sh}^2\sqrt{2\,m\,(U_0 - E)a^2/\hbar^2}}, \qquad E < U_0; \tag{4}$$

But, as we know, this expression is used very rarely for solved considered tasks.

We can see (see below some differences between semi-classical (3) and exact (4) for different cases, fig.2), that taken into account of pure quantum (in sense not semi-classical expressions) effects can be critical for 0.1 nm (atomic size) and essential for 0.3 nm. One can consider more realistic (not rectangular) potential for the process of cold electron emission in electric fields. In our opinion it does not matter (see fig.3).

4. Conclusion

It is very important that it is essentially quantum effect, which can be possible due to quantum-mechanical uncertainty relations (Heisenberg uncertainty relations):

$$\Delta p \Delta x \geq \hbar/2 \tag{5}$$

$$\Delta E \Delta t \geq \hbar \tag{6}$$

where uncertainties are given by formulas

$$\Delta p = \sqrt{< p^2 > - < p >^2} \, . \tag{7}$$

Thus, we think, that the effect of quantum-mechanical uncertainty in NDT will be studied more carefully.

Of course, Fowler–Nordheim formula is more approximate to the real potentials and has been refined many times, but quantum aspects didn’t take into account carefully every time.

There is very strong method for the calculation and estimation of tunneling processes. This is so-called instanton method. It based on analysis of the classical calculation in imaginary time(see for example [5]). Some results can be found in [6].

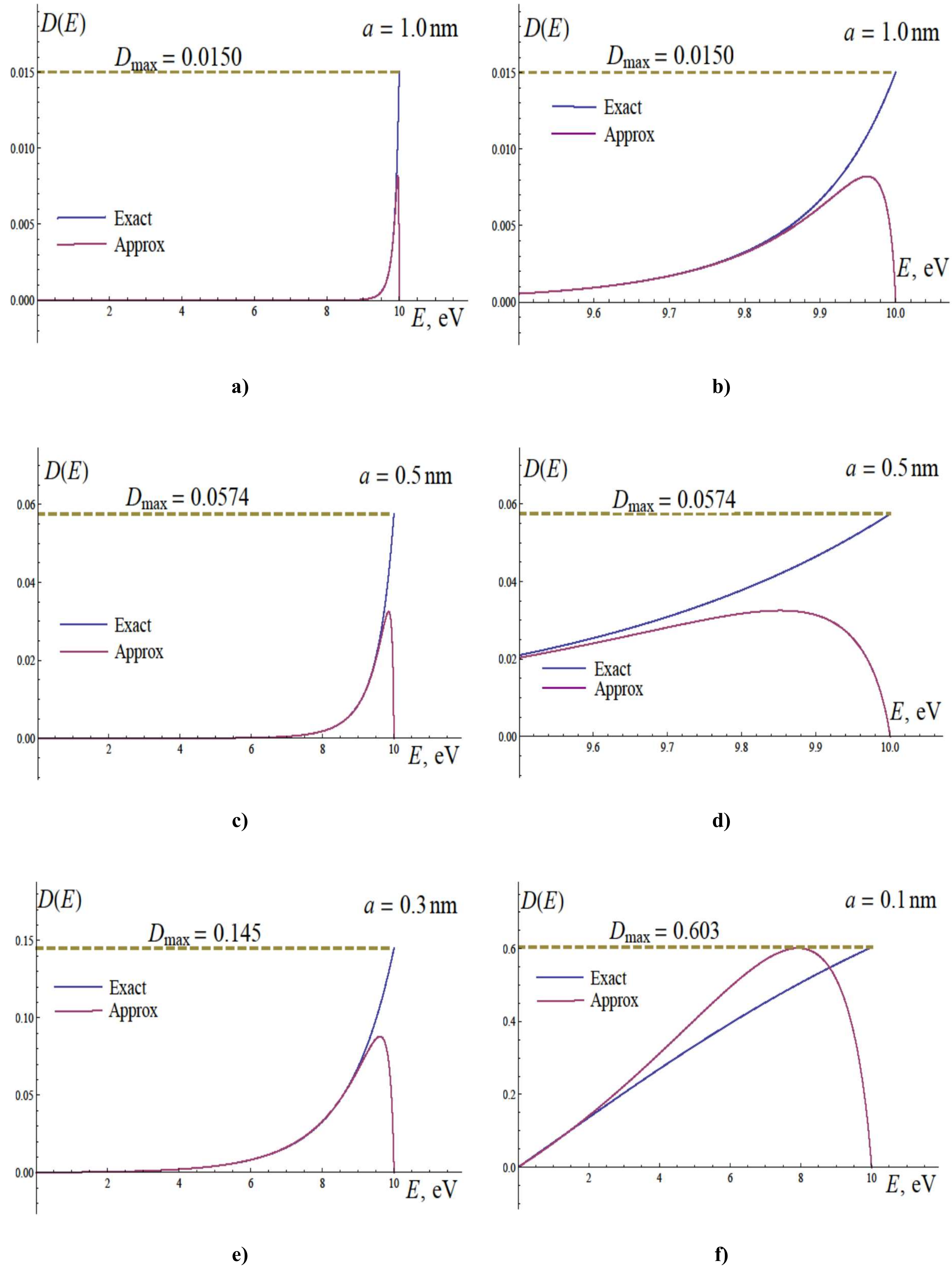
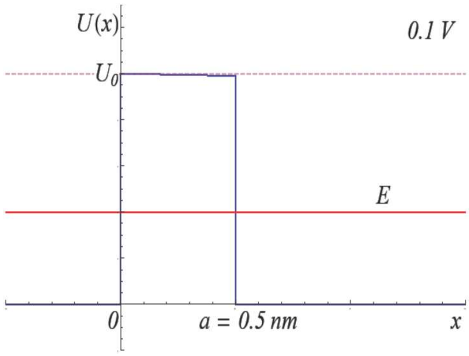


Fig.2. The dependence of coefficient of barrier penetration *D(E)* on different parameters (exact solution and semi-classical approximation).



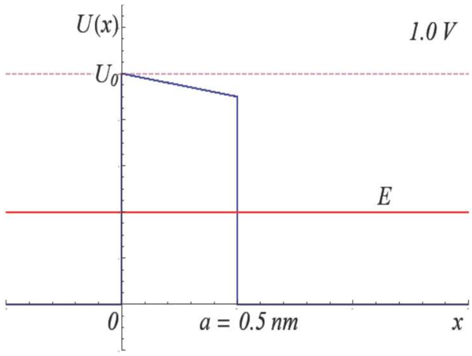


Fig.3. Realistic potential for voltage 0.1 (left) and 1.0 (right) V.

Our estimations and discussions in no way diminish role of the developers and creators of scanning probe microscopy, but only underscore their crucial role in the development of nanotechnology.

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