O-36

On exact solution of the Kardar-Parisi-Zhang equation with determinate spatially-inhomogeneous source

A.E. Rassadin[1], T.S. Sazanova[2], A.V. Stepanov[1,3], L.A. Fomin[1,4]

[1]Nizhny Novgorod Mathematical Society, 603950, Nizhny Novgorod, Russia
e-mail: brat_ras@list.ru

[2]Nizhny Novgorod State Technical University after R.E. Alekseev, 603950, Nizhny Novgorod, Russia

[3]Chuvash State Agricultural Academy, 428000, Cheboksary, Russia

[4]Institute of Microelectronics Technology and High Purity Materials RAS, 142432, Chernogolovka, Russia

At present studying of peculiarities for nano- and microstructures is of great importance because information about these features can be used in the design and prediction of physical and physicochemical properties of nano- and micromaterials. Nowadays one of the most popular models for epitaxial growth of surface of solid state is the so-called Kardar-Parisi-Zhang (KPZ) model suggested in article [1]. In the report presented we consider the next kind of this model:

$$\frac{\partial H}{\partial t} = c + \frac{c}{2}\cdot\left(\frac{\partial H}{\partial x}\right)^2 + \nu\cdot\frac{\partial^2 H}{\partial x^2} + Q(x),\ H(x,0) = h_0(x),\ Q(x)\geq 0,\ x\in R, \qquad (1)$$

where $H(x,t)$ is the height of growing surface with a cylindrical generatrix, c is the rate of its growth along the local normal to it, ν is the coefficient of surface diffusion and $h_0(x)$ is initial shape of the surface. For instance model (1) is highly adequate for simulation of technological process for manufacturing of X-ray multilayer diffraction gratings and mirrors [2]. But there is a sharp distinction between our model (1) and the ordinary KPZ models namely in our case extra spatially-inhomogeneous source of particles deposition $Q(x)$ is thought to be determinate in contrast to stochastic one in papers [1, 2].

Introducing new unknown function $\varphi(x,t)$ as:

$$H(x,t) = c\cdot t + \frac{2\cdot\nu}{c}\cdot\ln\varphi(x,t), \qquad (2)$$

one can reduce nonlinear equation (1) to the Cauchy problem for the linear parabolic equation:

$$\frac{\partial\varphi}{\partial t} = \nu\cdot\frac{\partial^2\varphi}{\partial x^2} + \frac{c\cdot Q(x)}{2\cdot\nu}\cdot\varphi,\quad \varphi(x,0) = \exp\left[\frac{c\cdot h_0(x)}{2\cdot\nu}\right]. \qquad (3)$$

Exact solution of equation (3) can be expressed as:

$$\varphi(x,t) = \int_{-\infty}^{+\infty} G(x,\xi;t)\cdot\varphi(\xi,0)\cdot d\xi, \qquad (4)$$

where its Green function $G(x,\xi;t)$ is equal to:

$$G(x,\xi;t) = \sum_{n=0}^{N-1}\exp(-E_n\cdot t)\cdot\psi_n(x)\cdot\psi_n^*(\xi) + \int_0^{+\infty}\exp(-E\cdot t)\cdot\psi(x,E)\cdot\psi^*(\xi,E)\cdot dE. \qquad (5)$$

Formula (5) contains functions $\psi_n(x)$ ($n=\overline{0,N-1}$) and $\psi(x,E)$ which are solutions of the next stationary Schrödinger equation:

$$-\nu\cdot\frac{d^2\psi}{dx^2} + U(x)\cdot\psi = E\cdot\psi, \qquad (6)$$

where role of potential energy is played by function $U(x)\equiv -\frac{c}{2\cdot\nu}\cdot Q(x)$.

Due to nonnegativity of source $Q(x)$ there are both discrete spectrum of negative eigenvalues E_n ($n=\overline{0,N-1}$) and continuous spectrum of positive eigenvalues E . N eigenfunctions of discrete spectrum $\psi_n(x)$ and eigenfunctions $\psi(x,E)$ of continuous spectrum ought to be normalized in accordance with standard rules of quantum mechanics [3, 4]:

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\cdot\psi_m(x)\cdot dx = \delta_{nm}\ ,\quad \int_{-\infty}^{+\infty} \psi^*(x,E)\cdot\psi(x,E')\cdot dx = \delta(E-E')\,. \tag{7}$$

The Green function having been found from expressions (5)-(7), we can return to investigation of the height $H(x,t)$ by means of formulae (4) and (2).

In this report above described method has been applied to the next source:

$$Q(x) = \begin{cases} Q_0, & |x| \le a \\ 0, & |x| > a \end{cases}. \tag{8}$$

This source corresponds to the well-known quantum mechanical problem about rectangular potential well [3]. Physically function (8) can be obtained from homogeneous stream of external particles with help of rectangular aperture.

Furthermore under time tending to infinity for arbitrary initial shapes $h_0(x)$ difference $H(x,t) - c\cdot t$ is sure to tend to some stationary limit $\mathrm{H}(x)$ obeying to the following equation:

$$\frac{c}{2}\cdot\left(\frac{d\mathrm{H}}{dx}\right)^2 + \nu\cdot\frac{d^2\mathrm{H}}{dx^2} + Q(x) = 0\,. \tag{9}$$

It is easy to see that for function $u(x) = -\dfrac{d\mathrm{H}(x)}{dx}$ equation (9) reduces to the well-known Riccati equation.

In the report for a number of model examples of initial shapes of the surface under investigation for source (8) we consider details of these passages to this limit shape $\mathrm{H}(x)$. Also we describe the case when width $2\cdot a$ of rectangular well (8) tends to zero under constant value of the product $Q_0\cdot a \equiv q_0$ and therefore profile of source (8) tends to delta-function: $Q(x) = 2\cdot q_0\cdot\delta(x)$ This situation is reduced to the well-known quantum mechanical problem about delta-functional well [4] and physically can be realized by means of the channeling of slow atomic particles along carbon nanotube [5].

The theory developed in this report may be verified by means of atomic force microscopy.

At last the above described method is of great importance for the situation when extra source $Q(x)$ is considered to be a control. In this case equation (1) ought to be added by requirement of minimization of some functional. For example as this functional one can choose:

$$\int_{-\infty}^{+\infty} [H(x,T) - H_*(x)]^2 dx \to \min\,. \tag{10}$$

Conditions (1) and (10) form the problem of optimal control by distributed parameter system [6] namely starting from initial shape $h_0(x)$ by means of control $Q(x)$ it is required to achieve minimal functional difference (10) between height $H(x,T)$ and fixed shape $H_*(x)$ at moment of time $t = T$. In other words it is the problem of nano engineering.

This work was supported by RFBR, grant N 18-08-01356-a.

1. M. Kardar, G. Parisi, Y.C. Zhang, *Phys. Rev. Lett.* **56**, 889 (1986).
2. L.I. Goray, M.N. Lubov, *Journal of Surface Investigation: X-Ray, Synchrotron and Neutron Techniques.* **8**, 444 (2014).
3. S. Flügge, *Practical Quantum Mechanics I* (Springer-Verlag), 62 (1971).
4. V.M. Galitsky, B.M. Karnakov, V.I. Kogan, *Problems on Quantum Mechanics* (Nauka), 237 (1992).
5. A.V. Stepanov, *Journal of Surface Investigation: X-Ray, Synchrotron and Neutron Techniques.* **9**, 789 (2015).
6. A.I. Korotkii, D.O. Mikhailova, *Proceedings of the Steklov Institute of Mathematics (Supplementary issues).* **280**, 98 (2013).