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# FLOWS IN NANOSTRUCTURES: HYBRID CLASSICAL-QUANTUM MODELS

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Flow through nanotube has many interesting peculiarities.To describe these unusual properties we suggest a model of the flow based on crystallite liquid theory. Slip boundary condition is used instead of conventional no-slip condition. The condition is derived by consideration of interaction of flow particles with the nanotube wall potential in the framework of quantum mechanics. For nanotube with elastic walls another mechanism of flow plays an important role. Namely, a model of flow caused by elastic soliton wave in its wall is suggested. As for general consideration, a modification of the Navier-Stokes equations for the nanotube flow is derived from many-particle Hamiltonian in the framework of quantum statistical physics. Particularly, for a model confinement the effective viscosity of the nanotube flow is got. The obtained dependence of the viscosity on the nanotube diameter is in good correlation with the corresponding experimental results.

**Keywords:** Nanotube, flow, crystallite, soliton, quantum statistics.

## 1. Introduction

Last years, fluid and gas flows in nano-sized domains are intensively studied [1], [2]. At present, there are no general equations of nano-hydrodynamics. Usually, the molecular dynamics is used for computations [3]. As for analytical approaches, the simplest one involves introducing the slip condition at the boundary [4]. There is also a hybrid method, incorporating the continuous approach and the molecular dynamics (which is used to analyze the fluid structure and determine the rheological law) [5]. In [6], fluctuations are taken into account when deriving the hydrodynamic equations. In [7] viscous-elastic behavior of water in nano-sized gaps was experimentally studied. Great increase of effective viscosity of water in a channel of nano-width is observed. For nanochannel flow the molecular structure of the medium plays a crucial role. It is similar to Brownian motion [8] and body motion through rarefied gas [9]. More precisely, flows in nano-channels are influenced by local heterogeneity of molecular structure of the liquid if its size is compared with the channel width. A hypothesis about the existence of locally-ordered structures in liquid was put forward in [10]. During several decades scientists discuss whether there are local domains in liquid (crystallites) in which the molecular structure is similar to that for crystal [11], [12], [13]. Investigations of fluid flows in nano-sized domains show that it is strongly influenced by local ordering of nano-sized scale. Experiments [7], [14], show that the effective viscosity of water in nano-channel with hydrophilic walls is essentially greater than the corresponding macroscopic value. Calculations in the framework of molecular dynamics [14] show that there are ordered structures (like periodic) of sizes less than nanometer. Computational experiments in [15] lead to appearance of ice-like states in nanotubes of small diameters under normal conditions. Experimental and theoretical investigations of water state in carbon nanotube [16], [17] show that there is ice-like envelope with liquid water inside in the nanotube. Increasing of effective fluid viscosity via channel diameter was marked in [18] for channels of few micrometers diameters. Influence of walls isn't evident. In some experiments there are increasing of effective viscosity, but in others the opposite effect takes place. Particularly, the experiments in [19] show that the fluid flow speed through carbon nanotube (of few nanometers diameter) is essentially greater than one calculated in the framework of classical fluid theory. Possible model of such phenomenon of "superfluidity" in very narrow nanochannel is suggested in [20]. As it was mentioned earlier, the effective viscosity can be both extremely small in some cases and extremely great in other situations (in comparison with its classical value). Such non-trivial correlation between the nanotube diameter and the viscosity, possibly, is related with local ordering in the liquid. The first variant of such approach is in [21], where the molecular dynamical model of nanotube flow close to crystallite model is suggested. In the present paper the relation of the effective viscosity of a fluid in nanotube with the dynamics of locally ordered nano-sized clusters is described. The number of such clusters increases if the temperature tends to the crystallization point. The sizes of such clusters are close to the diameters of hydro-silicate nanotubes [22]. For this reason, it is of importance to study the existence of crystal clusters of this kind in a liquid inside nanotubes and the influence of clusters on the mass transport through the tube. Computations based on molecular dynamics (with the Lennard-Jones potential) show that solid nano-sized clusters can exist both in the nanotube and outside it. The clusters (crystallites) can have a size of order 1 nm, which is close to the internal diameter of silicate nanotube. Note that the computed size of crystallite depends on parameters of the interaction potential, i.e. on the chemical composition of the liquid. Moreover, in unbounded domains the clusters are also nano-sized. There is a number of experimental results confirming the existence of crystallites in a liquid [11]. It is shown experimentally in [13] that water is inhomogeneous and consists of two parts: chaotic (liquid-like) phase and patches (crystallites) having average size about 1 nm at room temperature. As for hydrodynamic aspects, the flow in our model has common features with suspension flows [23], particularly, the nanotube flow has viscosity anisotropy as some suspension flows [24].

Non-direct experimental confirmation of our hypothesis about the existence of crystallites inside nanotubes is in [25] where the flow of alcohol and water mixture through a membrane with inserted nanotubes is studied. The authors show that the concentration of alcohol decreases essentially after passing through the nanotubes. It is in correlation with the crystallite model as has been mentioned above. The concentration of crystallites in liquid increases when the temperature tends to the freezing value. The freezing temperature for water is greater than one for alcohol. That is why water crystallites dominate over alcohol crystallites. Note that water crystallite doesn't contain alcohol molecules. Hence, the concentration of alcohol decreases during the process of flow through the nanotube.

Section 5 is devoted to general consideration. We derive modified Navier-Stokes equation for nanotube flow in the framework of quantum statistical physics starting from many-particle Hamiltonian. We obtain the viscosity as a functuin of the nanotube diameter and compare the result with known experiments. The comparasion shows that there is good correlation between theoretical and experimental curves.

In the case of narrow nanotube with elastic walls (e.g., carbon nanotube) there are elastic waves, particulary, solitary waves in walls [26]. It has great influence on the flow. We suggest a solvable model of such flow. It is shown that wall soliton induces a flow, and a picture of the flow is obtained.

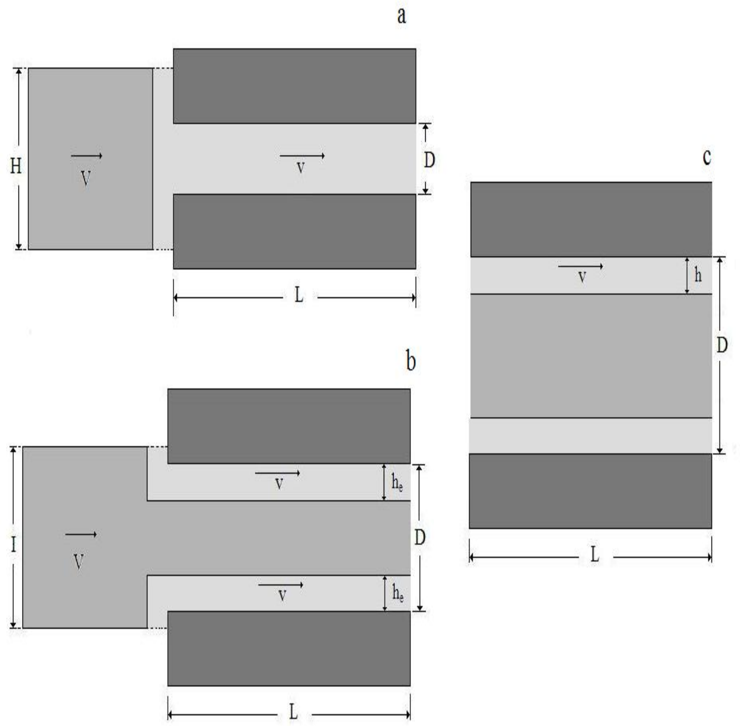

Fig. 1. Different regimes of crystallite containing flow through nanotube

## 2. Influence of crystallites on the flow through nanotube

We suggest a model based on the assumption about the existence of crystallites inside the nanotube. At first, we take into account energy transformations. Namely, we determine the power of pressure drop and equal it to the energy loss due to two reasons: viscous dissipation and melting.

We use quantum mechanical treatment to explain the type of the boundary condition on the inner surface $\Gamma$ of the nanotube

$$v_x|_\Gamma - v_s = L_s. \tag{1}$$

where $v_s$ and $L_s$ are the characteristic velocity and length (slip velocity and slip length).

The character of the flow in the nanotube depends on the correlation between the locally equilibrium size of the crystallite and the nanotube diameter. We try to find the effective viscosity $\mu_{ef}$ of the fluid in the nanotube which is defined by the following way. Consider the correlation between our nanotube (possibly, containing crystallites) and classical tube (with the Poiseille flow) of the same size and with the same pressure drop and flow rate. The viscosity of the Poiseille flow having the same parameters is called the effective viscosity of the flow in the nanotube.

Note that there is some space (of width $h$) between the crystallite and the nanotube wall. It is occupied by so-called non-autonomous phase (liquid-like) having the properties of a fluid with another viscosity $\mu_0$ [27]. Size correlations lead to a few particular cases described below (see Fig. 1). Introduce some notations. Let $D$ be the nanotube diameter, $L$ be its length, $H_e$ be the equilibrium size of the crystallite and $h_e$ be the equilibrium width of the non-autonomous phase.

For small nanotube diameter ($D < 2h_e$) there is no crystallite inside the nanotube, but it is at the entrance, and to form the flow it should transform to liquid-like non-autonomous phase. Roughly speaking, the flow is formed by “melting” of the crystallite at the ”entrance” (fig. 1a). Mass balance gives us $\pi H_e^2 V = \pi D^2 v$, where $v$ is the average (for the cross-section) velocity of the flow in the nanotube, $V$ is the crystallite velocity. Let us write down the energy balance equation. To do this let us take into account that the power of the pressure forces $N_p = \frac{\pi}{4} D^2 v \Delta P$ is equal to the sum of powers corresponding to viscous energy dissipation in the nanotube $N_\mu = a\frac{\pi}{4} D^2 L \mu_0 v\prime^2$ and to crystallite transformation to the liquid-like non-autonomous phase (at the entrance of the nanotube) $N_q = \frac{\pi}{4} H_e^2 V q$:

$$N_p = N_\mu + N_q. \tag{2}$$

Here $\Delta P$ is the pressure difference in the nanotube, $\mu_0$ is the viscosity of the non-autonomous phase inside the nanotube, $q$ is the specific heat of crystallite transformation to liquid-like non-autonomous phase (for unit volume), $a$ is some dimensionless parameter which will be chosen later, $v\prime$ is the characteristic speed of liquid deformation inside the nanotube. To estimate this speed we use the boundary condition (1). Hence, we come to the following expression

$$v' = \frac{v - v_s}{0.5D + L_s}$$

.

Using (1), one transform (1) into the form:

$$\Delta P = a\frac{\mu_0 \left(v - v_s\right)^2}{v \left(0.5D + L_s\right)^2} L + q. \tag{3}$$

Let us choose the value of the parameter $a$ in such a way that the expression (3) transforms to the corresponding expression for the classical Poiseille flow when $v >> v_s$, $D >> L_s$ and $q = 0$. It leads to the value 8 of the parameter $\alpha$. Expression 3 (valid for $v \geqslant v_s$) allows one to describe the relation between the flow velocity in the nanotube and the pressure drop (see Fig.2).

One can see that if $D < 2h_e$ then there is a flow through the nanotube only if $\Delta P \geqslant q$ (i.e. $q$ is the critical value (threshold) for the pressure drop). The described algorithm leads to the following expression for the effective viscosity:

$$\mu_{ef} = \frac{qD^2}{32vL} + \mu_0 \left[\frac{0.5D}{0.5D + L_s}\left(1 - \frac{v_s}{v}\right)\right]^2. \tag{4}$$

In relation (3) (derived from the energy balance) the power of pressure forces has the same form as in the previous case. But the losses related with viscous dissipation are localized in the layer of width $h_e$. Due to this fact one obtains the expression $N_\mu = b\pi h_e \left(D - h_e\right) L \mu_0 v'^2$, where $b$ is a dimensionless parameter which will be chosen later. The speed $v'$ of liquid deformation in the nanotube is estimated by taking into account (1). In the considered case one obtains

$$v' = \frac{v - v_s}{h_e + L_s}.$$

The power loss due to crystallite transformation (to liquid-like non-autonomous phase) has the form $N_q = \frac{\pi}{4}\left[H_e^2 - \left(D - 2h_e\right)^2\right] V q$. Here we have taken into account that there is “melting” of only that part of the crystallite, which can’t come into the nanotube. Summing up all the arguments mentioned above one gets the relation between the flow velocity in the nanotube and the pressure drop:

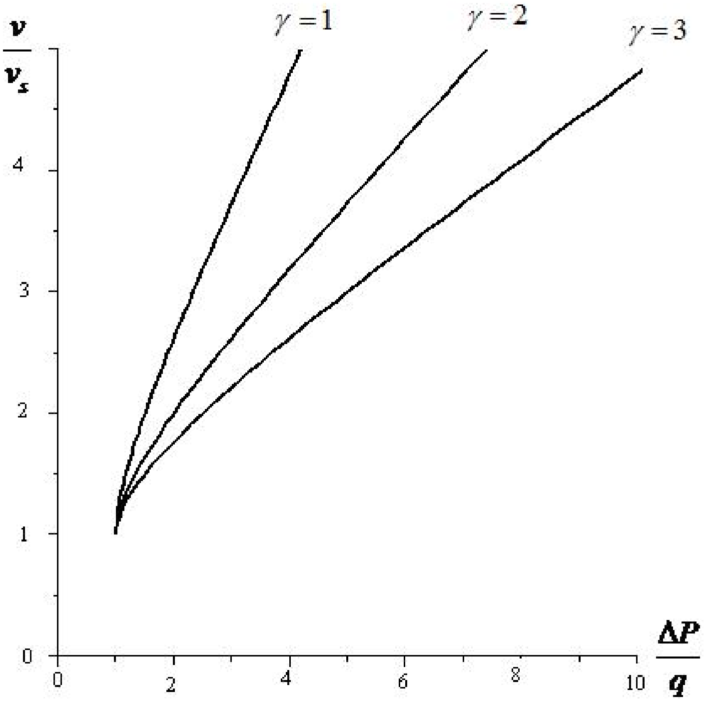

Fig. 2. Dimensionless flow velocity in the nanotube via the pressure

$$\Delta P = 4b\frac{\mu_0 \left(v - v_s\right)^2 h_e}{v \left(h_e + L_s\right)^2 D}\left(1 - \frac{h_e}{D}\right) L + q\left[1 - \left(\frac{D - 2h_e}{H_e}\right)^2\right]. \tag{5}$$

Choose the value of the parameter $b$ in such a way that ensure the coincidence of $\Delta P$ obtained from (5) and (3) for $D = 2h_e$. Taking the corresponding value of the parameter ($b = 8$), one transforms (5) to the final form. Expression (5) shows that there exists the pressure threshold ensuring the flow through the nanotube with minimal possible velocity $v = v_s$:

$$\Delta P_{\min} = q\left[1 - \left(\frac{D - 2h_e}{H_e}\right)^2\right].$$

The graph of the nanotube flow velocity via the pressure drop in this case is similar to the graph on Fig. 2.

The effective viscosity of the liquid in the nanotube in this case is given by the following expression:

$$\mu_{ef} = \frac{qD^2}{32vL}\left[1 - \left(\frac{D - h_e}{H_e}\right)^2\right] + \mu_0\frac{h_e \left(D - h_e\right)}{\left(h_e + L_s\right)^2}\left(1 - \frac{v_s}{v}\right)^2. \tag{6}$$

If $H_e + 2h_e \leqslant D < 2H_e + 3h_e$ then there is not greater than one crystallite in a cross-section of the nanotube. For $H_e + 2h_e = D$, there is no transformation of the crystallite and no changing of the width of the non-autonomous phase (its sizes have the locally equilibrium values). If the diameter increases, then these conditions come to contradiction. We assume that the width of the non-autonomous phase is preserved ($h_e$) and the cross-section of the crystallite increases from $H_e$ to $\alpha H_e$($\alpha$ is some dimensionless parameter). For larger values of $D$ ($\alpha H_e + 2h_e \leqslant$

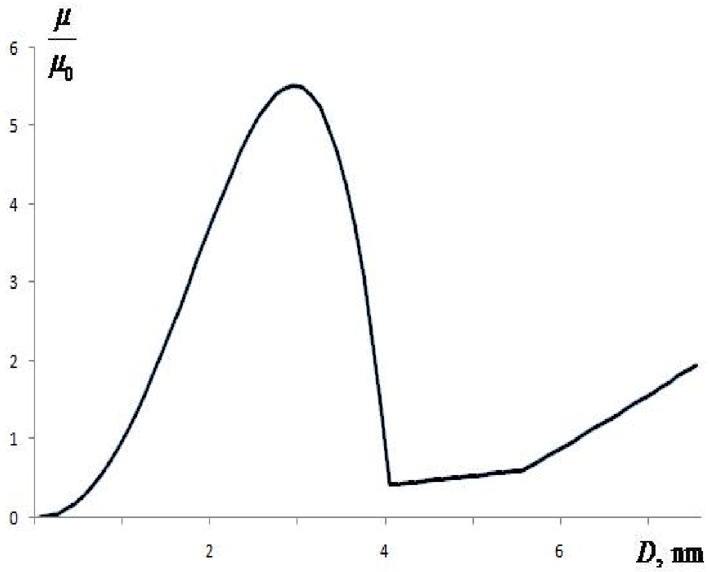

Fig. 3. The viscosity of liquid inside the nanotube via the nanotube diameter

$D < 2H + 3h_e$), the width of the crystallite is preserved ($H = \alpha H_e$) and the width of the non-autonomous phase $h$ increases: $h = 0.5\,(D - \alpha H_e)$ see Fig. 1c.

Using the procedure described above one obtains the relation between the pressure drop and the flow velocity:

$$\Delta P = 32\frac{\mu_0\,(v - v_s)^2\,h}{v\,(h + L_s)^2\,D}\left(1 - \frac{h}{D}\right)L. \tag{7}$$

The effective viscosity in this case is as follows:

$$\mu_{ef} = \mu_0\frac{h\,(D - h)}{(h + L_s)^2}\left(1 - \frac{v_s}{v}\right)^2. \tag{8}$$

Here

$$h = \begin{cases} h_e, & H_e + 2h_e < D < \alpha H_e + 2h_e, \\ 0.5\,(D - \alpha H_e)\,, & \alpha H_e + 2h_e \leqslant D < 2H_e + 3h_e. \end{cases} \tag{9}$$

Expression (7) shows that there is no pressure threshold in this case (a flow exists under any pressure drop), and minimal flow velocity is $v_s$.

The graph of effective viscosity of the liquid inside the nanotube via the tube diameter is shown on Fig. 3 for $0 < D < 2H_e + 3h_e$. Here $H = 3\,nm,\ \ h_e = 0.5\ nm,\ L = 100\,nm,\ n = 2,\ \rho_0 = \rho_c$. The character of the dependence is qualitatively correlated with the experimental results [28], [29] and [30].

## 3. Slip boundary condition and surface waves

Boundary conditions play crucial role in nanotube flow. The character of this condition is determined by the quantum interaction between liquid and walls. Classical analog of the quantum effect, which predetermined the boundary condition in our model, is the accelerated flow through nanotube due to interaction of liquid with surface mechanical waves in the nanotube wall [26].

Consider the corresponding quantum problem. Let one deal with a nanotube having a periodic set of atoms (centers) at the wall (a cylinder of radius $R$ with $OZ$ axis. These centers are at $N$ vertices of symmetric polygons. Polygons are parallel, and the distance between neighbor polygons is $h$. To describe the system we use zero range potential method [31]. Using of $\delta$-interaction allows one to simplify considerably the procedure of spectral analysis [32], [33]. Correct mathematical description of point-like interaction is given in the framework of the theory of self-adjoint extensions of symmetric operators. Formally, the Hamiltonian $H$ of the system is a perturbation of free Hamiltonian (i.e. the Laplace operator $-\Delta$) by periodic system of zero range potentials which are in the vertices (nodes) of the above mentioned polygons:

$$H = -\Delta + \sum_{n\in\mathbb{Z}_N} \sum_{s\in\mathbb{Z}} \alpha\delta(r - r_{ns}),$$

where $\alpha$ is the intensity of the perturbation, $r_{ns}$ is the radius-vector of a node having the following cylindrical coordinates: $r_{ns} = (R\cos(\theta n), R\sin(\theta n), sh), \quad s \in \mathbb{Z}, \ n \in \mathbb{Z}_N, \ \theta = 2\pi/N.$

The construction of our model is as follows. First, we restrict the Laplace operator onto the set of smooth functions vanishing at the nodes. The closure of restricted operator is symmetric and non-self-adjoint. It has self-adjoint extensions which give us the model operators [32]. To choose the particular extension it is necessary to satisfy the condition at the nodes. The continuous spectrum of the model operator contains values corresponding to modes of waveguide type concentrated near the wall of the nanotube. The corresponding wave function has the following form:

$$\psi(r) = \sum_{n,s} c_{ns} G(r_{ns}, r; E), \tag{10}$$

where the coefficients $c_{ns}, \ c_{ns} \in \mathbb{C}$, are determined by the ”boundary” conditions at the nodes, $E$ is the energy of the mode, $G(r_{ns}, r; E)$ is the Green function of the Laplace operator:

$$G(r, r'; E) = G(r - r'; E) = \frac{\exp(-\sqrt{-E}\,|r - r'|)}{4\pi\,|r - r'|}.$$

Wave function has the following asymptotics in a neighborhood of each point $r_{ns}$:

$$\psi(r) = \frac{a_{-1}}{|r - r_{ns}|} + a_0 + o(|r - r_{ns}|), \quad r \to r_{ns}.$$

The “boundary” condition at the node $r_{ns}$ gives us the following correlation: $a_0 = \alpha a_{-1}$. This condition means that for each center $r_{ns}$:

$$\lim_{|r - r_{ns}|\to 0} \frac{1}{|r - r_{ns}|\,\psi} \frac{\partial}{\partial\,|r - r_{ns}|} (|r - r_{ns}|\,\psi) = \alpha.$$

Using well-known asymptotic expansion for $G(r_{ns}, r; E)$ in a neighborhood of each point $r_{ns}$, one obtains the following system for $c_{ns}$:

$$(-\alpha - \sqrt{-E}) c_{ns} + 4\pi \textstyle\sum_{n', s'(n', s') \neq (n, s)} c_{n's'} G(r_{ns} - r_{n's'}; E),$$
$$s = 0, \pm 1, \pm 2, ..., \ n \in \mathbb{Z}_N.$$

To use Bloch’s theory let us introduce a function

$$\widehat{c}(j, q) = \sum_{n,s} c_{ns} e^{-iqs} e^{-i\theta jn}, \ \ j \in \mathbb{Z}_N, \ \ q \in [0, 2\pi],$$

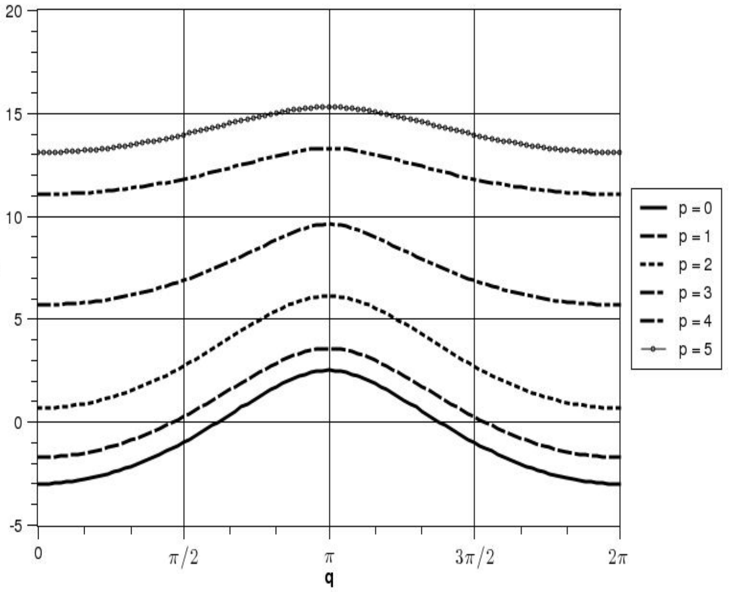

Fig. 4. Waveguide energy bands

Due to the formula for the Fourier coefficients one has

$$c_{ns} = \sum_{j \in \mathbb{Z}_N} \frac{e^{i\theta jn}}{2\pi} \int_0^{2\pi} \widehat{c}(j,q) e^{iqs} dq.$$

Then, the dispersion equation takes the form

$$(-\alpha - \sqrt{-E} - \widehat{G}(j,q;E))\widehat{c}(j,q) = 0, \ \ \forall j,q,$$

$$\widehat{G}(j,q;E) =$$
$$= \sum\nolimits_{n,s:(n,s)\neq(0,0)} \frac{\exp(-iqs - i\theta jn)\exp(-\sqrt{-E}\sqrt{2R^2(1-\cos(\theta n)) + h^2 s^2})}{\sqrt{2R^2(1-\cos(\theta n)) + h^2 s^2}}$$

If for any fixed values $j = j_0, \ q = q_0$ one has $\widehat{c}(j,q) \in L^2$, and the following relation takes place

$$\alpha = -\sqrt{-E} - \widehat{G}(j,q;E), \tag{11}$$

then the wave function is given by (10) with the coefficients (12):

$$c_{ns} = \frac{1}{2\pi} e^{iqs + i\theta jn} \tag{12}$$

Here we used that

$$\widehat{c}(j,q) = \delta_{jj_0} \delta(q - q_0)$$

Particularly, we calculate roots $z = -E$ of the dispersion equation (11) for the following values of the parameters: $\alpha = 1, N = 10, K = 2000,$ $K$ is the number of series terms taken into account. The graph of waveguide bands (i.e. the dependence of energy on the quasi-momentum $q$) is shown on Fig. 4 for $p \leqslant 5$., $p$ is the number of the band. For other values of $p$ one has the analogous pictures. The dependence of band width ($2 \leqslant p \leqslant 4$) on the number $N$ of polygon vertices ($6 \leqslant N \leqslant 15$) is shown on Fig. 5 for fixed parameters $\alpha = 1, K = 2000$.

To explain fast flow in nanochannels, which is observed in experiments some authors (see, e.g., [4], [34]) formally replace the no-slip condition by the slip one. The parameter $v_s$, slip speed, is chosen empirically. We have shown above that there exist waveguide modes

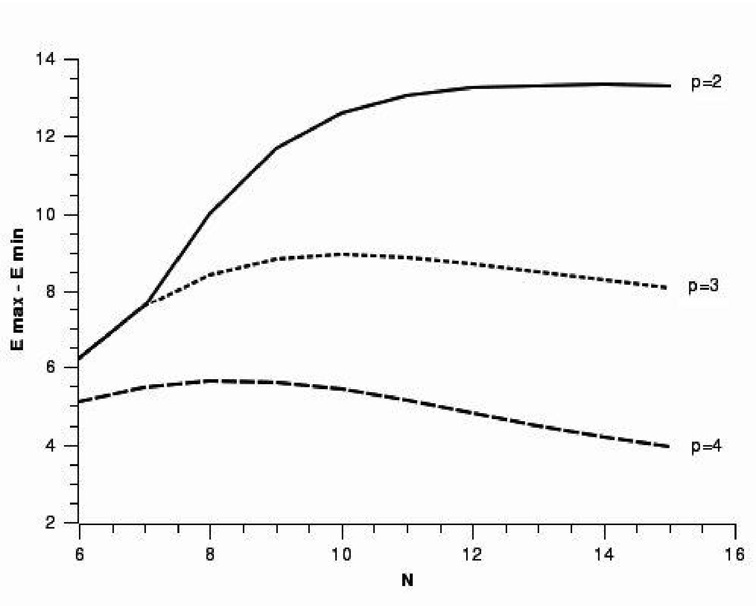

Fig. 5. Dependence of the band width on the number of vertexes of N-polygon

concentrated near the channel wall and have found its parameters. The existence of these surface waves leads to the slip condition. One can determine the slip speed by the following way. Consider the quantum scattering of a particle by the wall potential to determine the momentum transmitted to the wall. We use a way analogous to that in [35].

Let $H_0$ be the unperturbed Hamiltonian, $H_1$ be the perturbation (wall potential $V$) ,$\psi_a$ be the solution of the scattering problem by the wall potential $V$ corresponding to the particle with fixed momentum $p_a$. The momentum operator $\widehat{p}$ commutes with $H_0$, $\Phi_a$ is the eigenfunction of $\widehat{p}$ ($\widehat{p}\Phi_a = p_a\Phi_a$). Solution $\psi_a$ corresponds to $\Phi_a$, i.e. satisfies the equation:

$$\psi_a = \Phi_a + (E - H_0 + i0)^{-1} H_1 \psi_a, \qquad (13)$$

$$(E - H_0)\psi_a = H_1 \psi_a.$$

Let us determine the mean value of the operator $(i\hbar)^{-1}[\widehat{p}, H] = (i\hbar)^{-1}[\widehat{p}, H_1]$:

$$(\psi_a, (i\hbar)^{-1}[\widehat{p}, H_1]\psi_a) = (\psi_a, (i\hbar)^{-1}\widehat{p}H_1\psi_a) - (\psi_a, (i\hbar)^{-1}H_1\widehat{p}\psi_a).$$

Taking into account the completeness of the system $\{\Phi_b\}$, one has

$$H_1\psi_a = \sum_b (\Phi_b, H_1\psi_a)\Phi_b, \quad \psi_a = \sum_b (\Phi_b, \psi_a)\Phi_b.$$

Hence,

$$\begin{aligned}&(\psi_a, (i\hbar)^{-1}[\widehat{p}, H_1]\psi_a) = \\ &-(i\hbar)^{-1}(\psi_a, \textstyle\sum_b(\Phi_b, H_1\psi_a)p_b\Phi_b) + (i\hbar)^{-1}(\psi_a, \textstyle\sum_b(\Phi_b, \psi_a)p_b H_1\Phi_b) = \\ &-(i\hbar)^{-1}\sum_b p_b((\Phi_b, H_1\psi_a)(\psi_a, \Phi_b) - (\Phi_b, \psi_a)(\psi_a, H_1\Phi_b)).\end{aligned}$$

Consequently,

$$(\psi_a, (i\hbar)^{-1}[\widehat{p}, H_1]\psi_a) = 2\hbar^{-1}\sum_b p_b Im((\Phi_b, H_1\psi_a)(\psi_a, \Phi_b)) \qquad (14)$$

Taking into account (13), one gets

$$\begin{array}{l}(\psi_a, \Phi_b) = (\Phi_a + (E_a - H_0 + i0)^{-1} H_1 \psi_a, \Phi_b) = \\ \delta_{ab} + (E_a - E_b - i0)^{-1} (H_1 \psi_a, \Phi_b)\end{array} \tag{15}$$

Using the well known formula

$$(x - i0)^{-1} = x^{-1} + i\pi\delta(x), \quad \Im\,(x - i0)^{-1} = \pi\delta(x),$$

one obtains from ( 14), (15):

$$\begin{array}{l}(\psi_a, (i\hbar)^{-1}[\widehat{p}, H_1]\psi_a) = \\ 2\hbar^{-1}\Im \sum_b p_b (\Phi_b, H_1\psi_a)(\delta_{ab} + \pi\delta(E_a - E_b)(H_1\psi_a, \Phi_b)),\end{array}$$

$$\begin{array}{l}(\psi_a, (i\hbar)^{-1}[\widehat{p}, H_1]\psi_a) = \\ 2\hbar^{-1} p_a \Im\,(\Phi_a, H_1\psi_a) + 2\pi\hbar^{-1} \sum_b p_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b).\end{array} \tag{16}$$

If one takes the identical operator instead of $\widehat{p}$, then (15) transforms to the form

$$0 = 2\hbar^{-1}\Im\,(\Phi_a, H_1\psi_a) + 2\pi\hbar^{-1} \sum_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b). \tag{17}$$

One gets the expression for $\Im\,(\Phi_a, H_1\psi_a)$ from (17) and inserts it into (16). Then,

$$\begin{array}{l}(\psi_a, (i\hbar)^{-1}[\widehat{p}, H_1]\psi_a) = \\ 2\pi\hbar^{-1} \sum_b (p_b - p_a) \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b).\end{array} \tag{18}$$

Note that the right hand side of (18) is the mean momentum transmitted during the scattering of $\psi_a$ per 1 second. Summation over all states $\psi_a$ gives us the full mean transmitted momentum. We are interested in the longitudinal transmitted momentum $\delta p$:

$$\delta p = (\psi_a, (i\hbar)^{-1}[\widehat{p_\tau}, H_1]\psi_a).$$

Using (18), one obtains

$$\delta p = 2\pi\hbar^{-1} \sum_b (p_b - p_a) \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b),$$

or

$$\begin{array}{l}\delta p = 2\pi\hbar^{-1} \sum_b p_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b) - \\ -2\pi\hbar^{-1} p_a \sum_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b)\end{array},$$

$$\delta p = 2\pi\hbar^{-1} \sum_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b) \left( \frac{\sum_b p_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b)}{\sum_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b)} - p_a \right)$$

Hence, the expression takes the form

$$\delta p = \gamma\,(p_s - p)\,, \tag{19}$$

where

$$\gamma = 2\pi\hbar^{-1} \sum_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b), \tag{20}$$

$$p_s = \frac{\sum_b p_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b)}{\sum_b \left|(\Phi_b, H_1\psi_a)\right|^2 \delta(E_a - E_b)} \tag{21}$$

In our case $H_1 = V$.

**Remark**. One can get for the mean momentum transmitted during the scattering of $\psi_a$ per 1 second the expression analogous to that in [35] : $\delta p = (\psi_a, (-\frac{\partial V}{\partial \tau})\psi_a)$, where $\frac{\partial V}{\partial \tau}$ is the derivative of the wall potential in the longitudinal direction (and $\psi_a$ is considered as a distribution).

Variation of flow velocity per 1 second due to the interaction with wall can be estimated as $\delta v = -\frac{\delta p}{m}$, where $m$ is the molecule mass for the liquid. Hence, one can get the following formula for the normal derivative of the velocity of the flow at the wall:

$$\frac{\partial v}{\partial n} = -\frac{\tau}{a}\frac{\delta p}{m} = \frac{\tau\gamma}{a}\left(\frac{p}{m} - \frac{p_s}{m}\right).$$

Consequently,

$$\frac{\partial v}{\partial n} = \frac{1}{L_s}(v - v_s),$$

$$v = \frac{p}{m}, v_s = \frac{p_s}{m}, L_s = \frac{a}{\tau\gamma},$$

where $\tau$ is the mean time of molecule transition between two equilibrium states (”Frenkel transition”) [36], $a$ is the distance between these equilibrium positions.

## 4. Statistical derivation of modified hydrodynamic equations for nanotube flows

At present there is no general theory of the nanoflows. A natural question appears: what is the form of the hydrodynamic equations for the nanotube flow? To answer the question it is necessary to consider the background of the equation. The problem of the Navier-Stokes equation derivation is discussed during a long time. Initially, it was derived from a continuum formulation of conservation of mass and momentum. One can ask the deeper question of how to obtain these equations directly from microscopic models, in particular from many body Hamiltonian systems. Then one can ask for the microscopic origin of the viscosity, the nonlinearity, and the time irreversibility. At the present time there is no rigorous derivation of fluid dynamics from Hamiltonian mechanics. In [37] the Euler equations are derived from the Hamiltonian systems under some weak ergodicity assumptions. Some authors [38], [39] derive the Navier-Stokes equation from the Boltzmann equation, but the Boltzmann equation isn’t really a microscopic model. An alternative way is to substitute at the microscopic level various simplified and regularized versions for the Hamiltonian systems. One class of simplified models is the lattice gas, in which the particles are confined to a lattice [37]. One can mention also other models [40], [41], [42], [43]. We follow the dynamical Bogolyubov approach and the Zwanzig projection operator method [44], to derive the modified Navier-Stokes equation for the flow through nanotube. The main peculiarity is that we have a quantization (quantum statistics) in the nanotube cross-section and the classical statistics for the longitudinal direction.

First, we introduce few basic definitions. The statistical operator (density function) $\widehat{\rho}(t)$ describes macro-state of a system which can be in a great number of micro-states (with some probabilities). This macro-state in called a non-equilibrium state, as it evaluates in time in accordance with the Liouville equation. The Zwanzig projection operator method is based on the consideration of the reduced (quasi-equilibrium) statistical operator. Quasi-equilibrium state is described by quasi-equilibrium statistical operator$\widehat{\rho_l}(t)$ which ensures the maximum of the system entropy under the normalization condition and some additional conditions. Namely, if the average value $\left\langle \widehat{A} \right\rangle^t$ of some observable $\widehat{A} = \left\{ \widehat{A_\gamma} \right\}$ then these conditions takes the form

$$\int d\Gamma\ \widehat{\rho} = 1, \qquad \int d\Gamma\ \widehat{A_\gamma}\widehat{\rho} = \left\langle \widehat{A_\gamma} \right\rangle^t. \tag{22}$$

The entropy principle has the form

$$\delta\left\{-\int d\Gamma\ \widehat{\rho}\ln\widehat{\rho}-(\Phi(t)-1)\int d\Gamma\,\widehat{\rho}-\sum_{\gamma}F_{\gamma}(t)\int d\Gamma\ \widehat{A_{\gamma}\rho}\right\}=0,$$

where $\Phi(t)-1,\ \ F_{\gamma}(t)$ are the Lagrange multiplies. It gives us the following expression for $\widehat{\rho_l}(t)$:

$$\widehat{\rho_l}(t)=\exp\left\{-\Phi(t)-\sum_{\gamma}F_{\gamma}(t)\widehat{A_{\gamma}}\right\}, \tag{23}$$

where the Lagrange multipliers are determined by (22).

We consider locally homogeneous system, i.e. a system with weak spatial heterogeneity, for which one has $kr_c \ll 1$, where $k$ is the wave number, $r_c$ is the correlation radius. For these systems the length corresponding to essential variation of average local characteristics is essentially greater than $r_c$. The starting point for the derivation of the hydrodynamic equations is the conservation laws which have (for some value $a$) the following general form

$$\frac{\partial a}{\partial t}=-\sum_{\beta}\frac{\partial j_{\beta}}{\partial r_{\beta}}\ , \tag{24}$$

where $j_{\beta}(t)=\left\langle\widehat{j_{\beta}}\right\rangle^{t}$ is the corresponding average flux density. Greek index $\beta$ run over three values marking spatial coordinates. Let one represents the full statistical operator in the form $\widehat{\rho}(t)=\widehat{\rho_l}(t)+\Delta\widehat{\rho}(t)$. Introduce the statistical part of the flux density: $j_{\beta}^{(s)}=\left\langle\widehat{j_{\beta}}\right\rangle_{l}^{t}$. Let us pass to local moving coordinate system at each point $(r,t)$. In this system the concentration and the densities of energy and momentum are as follows: $n'=nh'=e,\ p'_{\beta}=0,$, where $e$ is the average density of the internal energy. Hence, for the corresponding fluxes one has

$$j_{0\beta}^{(s)'}=0,\ j_{\alpha\beta}^{(s)'}=\delta_{\alpha\beta}P,\ \ j_{1\beta}^{(s)'}=0.$$

Here $P$ is the pressure. The full flux has the form:

$$j_{0\beta}^{(s)'}=I_{0\beta},\ j_{\alpha\beta}^{(s)'}=\delta_{\alpha\beta}P+I_{\alpha\beta},\ \ j_{1\beta}^{(s)'}=0.$$

Here $I_{\alpha\beta}, I_{0\beta}$ are the contributions to the average values given by non-equilibrium addition $\Delta\widehat{\rho}(t)$ to the statistical operator. The corresponding contribution to the flux of particles number is zero. We take into account that

$$p_{\beta}=\tau v_{\beta},\ \ h=e+\sum_{\alpha}\tau v_{\alpha}^{2}/2,\ \ j_{1\beta}=nv_{\beta},$$

where $\tau(r)=m\,n(r)$is the average mass density, $m$ is particle mass, $n$ is the concentration. Transformation to immovable coordinate system is given by the following formulas:

$$\widehat{j_{\alpha\beta}}=mv_{\alpha}v_{\beta}\widehat{n}'+v_{\alpha}\widehat{p_{\beta}}'+v_{\beta}\widehat{p_{\alpha}}'+\widehat{j_{\alpha\beta}}',$$

$$\widehat{j_{0\beta}}=v_{\beta}\left(\widehat{h}'+\textstyle\sum_{\alpha}(\tau v_{\alpha}^{2}\widehat{n'}/2+v_{\alpha}\widehat{p'_{\alpha}})\right)+$$
$$\textstyle\sum_{\alpha}(v_{\alpha}^{2}\widehat{p'_{\beta}}/2+v_{\alpha}\widehat{j'_{\alpha\beta}})+\widehat{j_{0\beta}}'.$$

Hence,

$$j_{\alpha\beta}=\tau v_{\alpha}v_{\beta}+\delta_{\alpha\beta}P+I_{\alpha\beta}, \tag{25}$$

$$j_{0\beta} = v_\beta(e + \sum_\alpha \tau v_\alpha^2/2) + v_\beta P + \sum_\alpha v_\alpha I_{\alpha\beta} + I_{0\beta}. \tag{26}$$

Equation 24 takes the following form for mass, momentum and energy, correspondingly:

$$\frac{\partial \tau}{\partial t} = -\sum_\beta \frac{\partial(\tau v_\beta)}{\partial r_\beta}, \ \frac{\partial(\tau v_\alpha)}{\partial t} = -\sum_\beta \frac{\partial(j_{\alpha\beta})}{\partial r_\beta}, \tag{27}$$

$$\frac{\partial}{\partial t}\left(e + \sum_\alpha \tau v_\alpha^2/2\right) = -\sum_\beta \frac{\partial(j_{0\beta})}{\partial r_\beta}. \tag{28}$$

Introducing so-called material derivatives [45], [46]

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \sum_\beta v_\beta \frac{\partial}{\partial r_\beta}$$

and taking into account (25), (26), one transform (27), (28) to the following form:

$$\tau \frac{Dv_\alpha}{Dt} = -\sum_\beta \frac{\partial}{\partial r_\beta}(\delta_{\alpha\beta} P + I_{\alpha\beta}), \tag{29}$$

$$\tau \frac{D}{Dt}\left(\frac{e}{\tau} + \frac{1}{2}\sum_\alpha v_\alpha^2\right) = -\sum_\beta \frac{\partial}{\partial r_\beta}(v_\beta P + \sum_\alpha v_\alpha I_{\alpha\beta} + I_{0\beta}). \tag{30}$$

Equation (29) is well-known Navier-Stokes equation (it corresponds to the momentum conservation law). The form of the equation in these notations is the same for nanotube flow as for conventional hydrodynamics. The difference is in the values of the including terms. The most interesting is the term $I_{\alpha\beta}$. It is related with the internal friction, i.e. with the viscosity. Namely, $I_{\alpha\beta}$ is the contribution to the average value of the momentum flux of the non-equilibrium addition $\Delta\widehat{\rho}(t)$ to the statistical operator in local moving (with flow velocity) coordinate system. In conventional hydrodynamics one has the classical statistical operator. As for the nanotube flow, there is a quantization in orthogonal cross-section of the tube (i.e. quantum statistics) and classical moving in the longitudinal direction (classical statistics). Correspondingly, the values of $I_{\alpha\beta}$ are absolutely different, particularly, we have anisotropy and viscosity matrix instead of scalar value of the viscosity in conventional equation. The viscosity matrix depends on assumptions concerning to the quantum statistical operator in the nanotube cross-section. Rigorous derivation of this matrix is difficult problem. As for estimations, one can make averaging over the nanotube cross-section and transit to one-dimensional hydrodynamic model. Then the 1D viscosity will be proportional to the average energy density for the cross-section which can be calculated by conventional way (estimation of the statistical sum). Naturally, it depends on the eigenvalues distribution, i.e. on the model used for the cross-section quantum ensemble. The simplest case is when we assume that the nanotube confinement is a parabolic potential (with a parameter proportional to $R^{-2}$, $R$ is the nanotube radius) and one has the ensemble of non-interacting fermions. Then the energy levels are equidistant and proportional to $R^{-2}$. It leads to the dependence of the viscosity on the radius of nanotube cross-section. Namely, it is proportional to

$$\left(\sum_{n=0}^{\infty} e^{-aR^{-2}n}\right)^{-1} \sum_{n=0}^{\infty} akTR^{-4}ne^{-aR^{-2}n}.$$

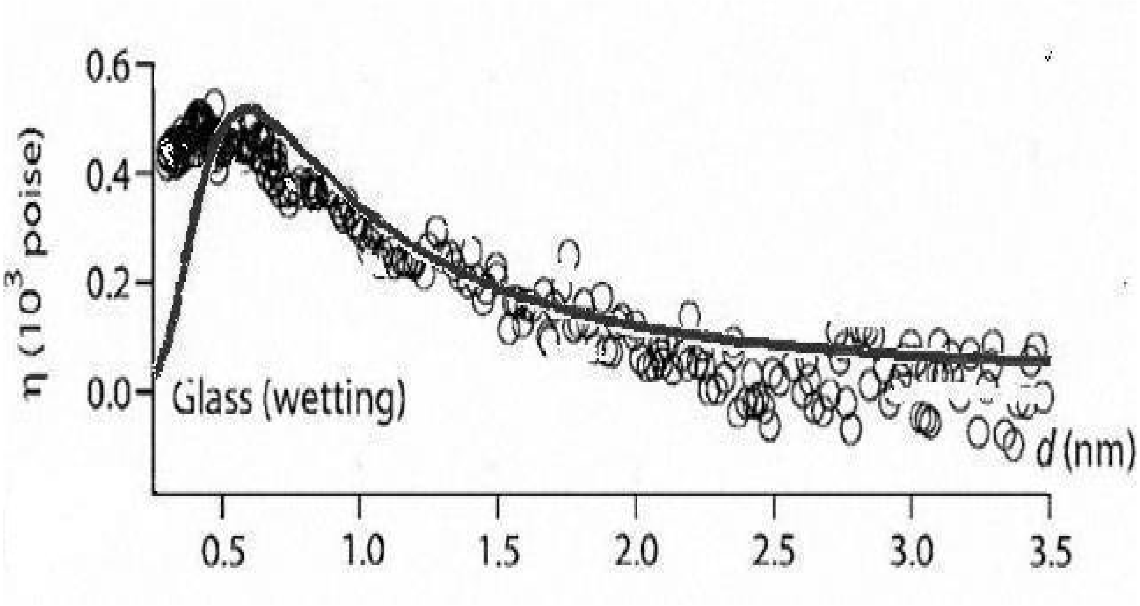

Fig. 6. Dependence of the viscosity $\eta$ on the nanochannel diameter $d$

Here $k$ is the Boltzmann constant, $T$ is the temperature. The parameter of the parabolic potential is $akT(\hbar R^2)^{-1}$. Consequently, in this case the viscosity $\eta$ is as follows

$$\eta = b\, d^{-4}(e^{ad^{-2}} - 1)^{-1}$$

($b, a$ are some constants, $d = 2R$). This viscosity via nanotube radius dependence is in correlation with the experimental results [14]. The comparison is shown on Fig. 6.
The values of the parameters are as follows: $a = 0.57\ nm^2,\ \ b = 250\, poise \cdot nm^4$. Experimental results from [14] are marked as small circles. One can see the correlation between the theoretical curve and the experimental results. Particularly, there is a local maximum of the viscosity for some value of nanotube radius. There are no experimental data for $d < 0.25\, nm$ and one has no possibility to compare thoroughly the increase rate for theoretical and experimental curves near zero. Our model gives $\lim_{d\to 0} \eta = 0$. The viscosity $\eta$ practically vanishes for $d = 0.25\, nm$. It corresponds to one-atom cross-section of the nanotube. Hence, for one-atom chain inside the nanotube we obtain zero viscosity, i.e. "superfluidity". The analogous phenomenon is in Maslov's model [20] for very narrow nanotube.

## 5. Soliton induced flow in nanotube

For the case of narrow channel (below the flow threshold) another effect can play an important role. It should be stressed that boundary condition, wall structure and profile play crucial role. Namely, it is necessary to take into account vibration and waves in molecular chains forming the nanotube wall. There are experimental evidences of such wall vibration [26]. The most interesting is solitary wave. There are different models describing such solutions (see, e.g., [47]). We shall consider so-called "Davidov soliton", stable solution of this type in long molecular chain. The analogous waves are also in nanotubes [48].

### 5.1. Preliminary estimations

Consider the soliton influence on the flow. Soliton moves in nanotube wall and looks like a moving local extension (or constriction) of the tube. Let the area of the cross-section of the tube be $S = S\,(x - Vt)$, where $x$ is the longitudinal coordinate, $V$ is the soliton velocity. The continuity equation has the form

$$\frac{\partial S}{\partial t} + \frac{\partial (Su)}{\partial x} = 0, \tag{31}$$

where $u$ is the velocity of the flow. Integration of 31 gives one the relation between the flow velocity and the cross-section area:

$$u = V + (v - V)\,\frac{S_0}{S}, \tag{32}$$

where $v$ and $S_0$ are the flow velocity and the area of the cross-section outside the domain occupied by the soliton. Taking the pressure forces power equals to the power related with the viscous dissipation, one obtains:

$$vS_0\Delta P = \mu \int_0^L \left(\frac{u - v_s}{R + L_s}\right)^2 \pi R^2 dx. \tag{33}$$

Let $\bar{v}$ be the flow in the same nanotube without soliton, i.e.

$$\bar{v}S_0\Delta P = \mu \left(\frac{\bar{v} - v_s}{R + L_s}\right)^2 \pi R^2 L. \tag{34}$$

Assuming that the perturbation of the area due to soliton is small, one obtains the corrected expression for the flow velocity

$$v = \bar{v} + 2\left(1 - \frac{< S >}{S_0}\right) \frac{V - \bar{v}}{1 + v_s/\bar{v}}, \tag{35}$$

where $< S >$ is the average area of the nanotube cross-section. Expression 35 shows that solution causes the increasing of the flow velocity in two cases: a) $V > \overline{v}$, $\langle S\rangle > S_0$ (fast soliton corresponds to the extension of the nanotube); b) $V < \overline{v}$, $\langle S\rangle < S_0$ (slow soliton corresponds to the constriction of the nanotube). In other cases the soliton causes the decreasing of the flow velocity.

### 5.2. Solitons

To describe this solution one can consider an exciton of effective mass $m$ interacting with displacement $u(x,t)$ of molecules having masses $M$ from the equilibrium positions at points $x = na$. The corresponding Hamiltonian is [49]

$$H = \frac{1}{a}\int \left(\frac{\hbar^2}{2m}\left|\psi_x\right|^2 + \frac{1}{2}Mu_t^2 + MV_0^2 U(\rho) - \vartheta\rho\left|\psi\right|^2\right)dx,$$

where $\rho$ is the relative decreasing of the equilibrium distance $a$ between neighbor molecules, $\rho = -u_x$, $V_0$ is the longitudinal sound speed in the linear approximation of the chain, $\vartheta$ is the energy which characterizes the interaction of the exciton and the displacement, $U(\rho)$ is the dimensionless potential of intermolecular interaction having minimum at $\rho = 0$, $\psi$ is normalized exciton wave function. The Hamiltonian leads to the following system of equations:

$$i\hbar\psi_t + \frac{\hbar^2}{2m}\psi_{xx} + \vartheta\rho\psi = 0,$$

$$u_{tt} - V_0^2 U_{\rho\rho} u_{xx} = \frac{\vartheta}{M}(|\psi|^2)_x.$$

The system has a stable solution having the form of solitary wave of the profile $\Phi$ depending on $U$. Particularly, for cubic nonlinearity, $U(\rho) = \frac{1}{2}\rho^2 + \frac{\gamma}{3}\rho^3$:

$$\Phi(\xi) = \frac{1}{2}\left(\frac{3\sigma}{4}\right)^{1/3}\left(\frac{\tau}{\gamma}\right)^{1/3} sch^2\left(\frac{1}{2}\left(\frac{\tau\sigma^2}{6\gamma}\right)^{1/3}\xi\right).$$

The speed $V$ of this soliton is as follows:

$$V = V_0\frac{1 + \frac{\tau M}{\gamma m}\left(1 - \frac{3}{5}(\gamma\sigma)^{1/3}(\tau/6)^{2/3}\right)}{1 + \frac{\tau M}{\gamma m}},$$

$$\sigma = \frac{2\vartheta m a^2}{\hbar^2},\quad \tau = \frac{\vartheta}{M V_0^2}.$$

Geometrically, this solution seems as a local extension (or constriction) of the tube, which moves with velocity $V$. This motion causes the motion of the liquid in the neighborhood of this extension (restriction). We shall consider the flow in nanolayer between two planes. The estimation of the Reynolds number shows that for many cases the Stokes approximation is appropriate.

### 5.3. Stokeslet model of creeping flow

To describe the flow we use a model in which the local perturbation (occupied small spatial region) is replaced by a point-like one [50], [51]. The mathematical background of the model is the theory of self-adjoint extensions of symmetric operators [33]. Consider two-dimensional straight channel (strip). The result for cylindrical channel is absolutely analogous. The Stokes flow for this case is described by the stream function $\psi$ satisfying the biharmonic equation. As for the boundary conditions, it is more convenient to study moving boundary and fixed singularity, i.e. we assume that the normal derivative of the stream function isn't zero (it is equal to the wall velocity).

Let us describe briefly the model of point-like perturbation for the Stokes flow. The starting point is the operator $\Delta_0^2$ which is the closure of the restriction of $\Delta^2$ onto the set of smooth functions vanishing in a neighborhood of zero. The domain of the operator is

$$D(\Delta_0^2) = \left\{u,\ u \in L_2(\Omega),\, \Delta^2 u \in L_2(\Omega),\, u(0) = u'_{x_i}(0) = u''_{x_i x_j}(0) = 0,\, i,j = 1,2\right\}.$$

Model operator $\Delta_e^2$ is obtained as a self-adjoint extension of symmetric operator $\Delta_0^2$. Due to the correlation $\Delta_0^2 \subset \Delta_e^2 \subset \Delta_0^{2*}$one can search an extension as a restriction of the adjoint operator. The domain of the operator $\Delta_0^{2*}$ consists from the elements of the following form:

$$\begin{gathered} u(x) = \textstyle\sum_{i,j=1}^2 c_{ij}^u g_{x_i x_j}(x) + \sum_{i=1}^2 c_i^u g_{x_i}(x) + c_0 g(x) + \\ \xi(x)(a_0 + \textstyle\sum_{i=1}^2 a_i^u x_i + \sum_{i,j=1}^2 a_{ij}^u \beta_{ij} x_i x_j) + u_0(x). \end{gathered}$$

Here $u_0 \in D(\Delta_0)$, $\beta_{ij} = 1,\, i \neq j,\ \beta_{ii} = 2^{-1}$,$g is the Stokslet$ $\xi(x)-$ smooth cutting function: $\xi(x) = 1,\, |x| \leqslant 1,\ \xi(x) = 0,\, |x| \geqslant 2$. To construct the model operator one should establish some correlation between these coefficients in the asymptotic expansion, for example,

$$U_0 = AU_1,\, U_1 = (c_0^u, c_1^u, c_2^u, c_{11}^u, c_{12}^u, c_{22}^u),\ U_0 = (a_0^u, a_1^u, a_2^u, a_{11}^u, a_{12}^u, a_{22}^u),\, A = A^*$$

.

As for detailed description of all classes of extensions, see [52].

### 5.4. Soliton induced flow in nanolayer

We consider the Stokes flow in a layer induced by rotlet line, i.e. the flow with translation symmetry along this line. This flow is two-dimensional and it is necessary to deal with point-like perturbation (rotlet) in $\mathbb{R}^2$. The stream function for the model operator constructed above gives us the model for the Stokes flow with rotlet in two-dimensional strip. In our case there are two perturbations in opposite points of the channel walls (soliton position). Let the channel walls be $\{(x,y): \ x=0\}$, $\{(x,y): \ x=2\}$. Due to the linearity of the problem it is possible to consider the equivalent task – moving boundary and point perturbations at fixed positions (instead of moving perturbations and unmoving boundary). The solution has the form of a sum of solutions corresponding to each perturbation (at points $(0,0),\ (2,0)$):

$$\psi(x,y)=\psi(x,y,0,0)+\psi(x,y,2,0),$$
$$\psi(x,y,0,0)=\Psi(x,y,0,0)+\int_{-\infty}^{\infty}(\Psi(x,y,0,\eta)+\Psi(x,y,2,\eta))v(\eta)d\eta.$$

Here $\Psi(x,y,0,0)$ is the solution corresponding to the rotlet at the point $(0,0)$.The solution is obtained in explicit form:

$$\begin{aligned}&\psi(x,y,0,0)=\tfrac{x\cdot c}{2}+Re[\textstyle\sum_{n=1}^{\infty}(A\cdot[x\cdot\sin(\frac{1}{2}\lambda_n\cdot x)-\ tan(\frac{1}{2}\lambda_n)\cdot\cos(\frac{1}{2}\lambda_n\cdot x)]\cdot\exp(-\frac{1}{2}\lambda_n\cdot|y|)+\\&+B\cdot[x\cdot\cos(\tfrac{1}{2}\mu_n\cdot x)-\cot(\tfrac{1}{2}\mu_n)\cdot\sin(\tfrac{1}{2}\mu_n\cdot x)]\cdot\exp(-\tfrac{1}{2}\mu_n\cdot|y|)+\\&+\textstyle\int_{-\infty}^{\infty}\sum_{n=1}^{\infty}(a\cdot[x\cdot\sin(\frac{1}{2}\lambda_n\cdot x)-\tan(\frac{1}{2}\lambda_n)\cdot\cos(\frac{1}{2}\lambda_n\cdot x)]\cdot\exp(-\frac{1}{2}\lambda_n\cdot|y-\eta|)+\\&+b\cdot[x\cdot\cos(\tfrac{1}{2}\mu_n\cdot x)-\cot(\tfrac{1}{2}\mu_n)\cdot\sin(\tfrac{1}{2}\mu_n\cdot x)]\cdot\exp(-\tfrac{1}{2}\lambda_n\cdot|y-\eta|))d\eta\cdot(v-\tfrac{c}{2})].\end{aligned}$$

Here $\lambda_n,\ \mu_n$ are complex roots of equations

$$\sin\lambda_n+\lambda_n=0,\sin\mu_n-\mu_n=0,$$

$A$, $B$, $a$, $b$ are some constants (model parameters, $c$, $v$ are flow parameters, namely, $c$ is the flux through the cross-section of the channel, $v$ is the rotlet velocity (in our case it is the wall velocity). The pictures of the streamlines are different for different values of the flow parameters. Particularly, for $c=10,\ v=10$ there is a cell occupying the whole cross-section of the channel where one has an eddy (Fig. 7). For the flow parameters greater than $c=50,\ v=50$ the cell is divided into two parts by the flow in the center of the channel (Fig. 8).

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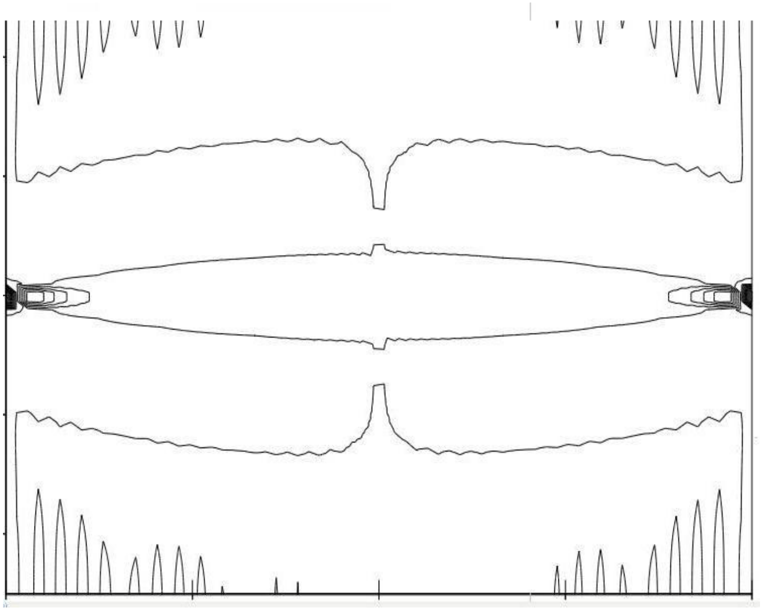

Fig. 7. Soliton induced flow in nanolayer (cellular structure)

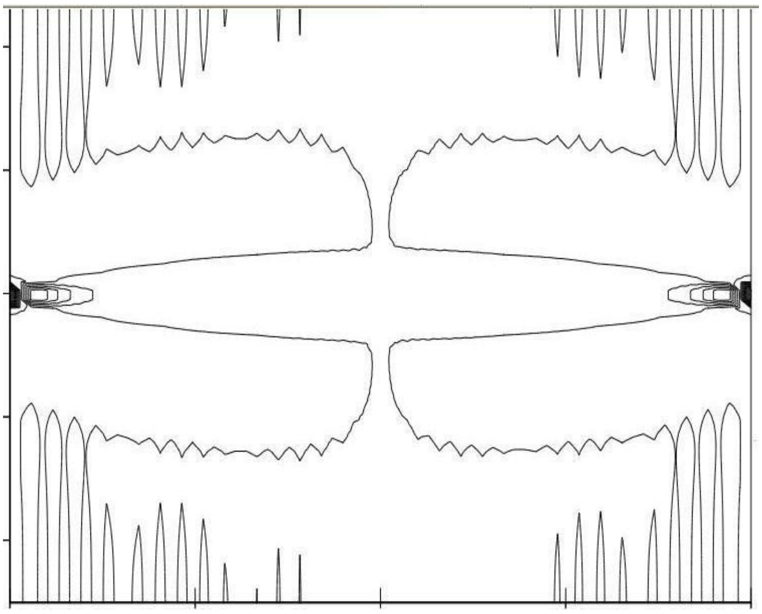

Fig. 8. Soliton induced flow in nanolayer (absence of cellular structure)

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