Reduction of 3D Hartree-like equations in thin threads. (Roman Nekrasov, Institute for Problems in Mechanics RAS)

One important equation of biophysics is considered:

$$i\Psi_t = \widehat{\mathcal{H}}_{\Psi}\Psi, \qquad \widehat{\mathcal{H}}_{\Psi} = -\frac{1}{2}\mathbf{\Delta} + v_{\text{int}}(x, \mathbf{y}/\mu) + \kappa \iiint G(\mathbf{r}, \mathbf{r}')|\Psi(\mathbf{r}')|^2 d\mathbf{r}',$$
 (1)

where $\Psi = \Psi(\mathbf{r}, t)$ is an unknown function of space and time, Δ – Laplace operator; $x, \mathbf{y} = (y_1, y_2)$ – some curvlinear coordinates; μ – small parameter; $v_{\text{int}}(x, \mathbf{y}/\mu)$ – confinement potential; $G(\mathbf{r}, \mathbf{r}')$ – some smooth kernel of nonlinear term.

This Hartree-like equation describes distribution of vibratory perturbations in a long protein molecule, for example. In such molecules transversal sizes are much smaller than longitudinal ones. It gives the small parameter μ in the problem. From physical point of view, it is clear, that in first approximation, the presence of different scales (longitudinal and transversal) in the problem allows one to replace the 3-dimensional equation with a 1-dimensional one along the x-axis.

An asymptotic reduction of (1) is produced. It includes not only long-wave longitudinal functions as solutions of reduced equations, but semiclassically concentrated solutions also (it means that longitudinal wave's length h is non fixed, and we may have different reductions for different small parameters $h = h(\mu)$). Semiclassically concentrated solutions, in stable cases, describe ballistic transport of some perturbations like Davydov's solitons in the case of local (nearest-neighbor) interaction between sites of a molecule. The stability depends on a parameter of non-linearity κ , the dependence has zone structure for some Sturm-Liouville problem.