Decay on several sorts of heterogeneous centers: Special monodisperse approximation in the situation of strong unsymmetry. 2. Numerical results for the total monodisperse approximation

V.Kurasov

Victor.Kurasov@pobox.spbu.ru

1 Preliminary remarks

In [1] we have investigated the process of nucleation in the situation of the strong unsymmetry. We have analysed the system of condensation equations and suggested three different approximations.

The first approximation is the total monodisperse approximation. It has been already suggested in [2] and is a rather natural one. In this approximation the total number of the droplets on the first type centers are regarded as those formed at the initial moment of time. Then all these droplets have now one and same size which can be easily calculated. It equals to z.

Certainly this approximation is suitable in the case of the strong unsymmetry. Namely in this case it was used in [2]. But this approximation can be applied in some other cases. This approximation can be used to estimate the errors of some other approximations.

It is clear that the total monodisperse approximation is more rough than the special monodisperse approximation and the floating monodisperse approximation. Then we shall estimate the errors of the mentioned approximations by the the error of the total monodisperse approximation.

In the special monodisperse approximation we have to introduce the characteristic size Δz of the length of the spectrum due to the supersaturation fall. This value is well described in [2], [1]. Then we have to imagine that the influence of the droplets formed on the first type centers can be described as the monodisperse peak with the number of droplets determined by the special recipe.

To determine the number of droplets in the monodisperse spectrum we must calculate the number of the first type heterogeneous centers which became the centers of the droplets until $\Delta z/4$. It can be done without any influence of the second type heterogeneous centers taken into account.

The reason of concrete choice of the size $\Delta z/4$ is described in [2] in details. So, we needn't to explain it here. We have only to note that this choice is equivalent to the specific choice of time, i.e. one has to calculate the number of the droplets on the first type centers formed until the first quarter of the nucleation period. More rigorously we have to speak here about the finish of the nucleation period due to the fall of supersaturation.

In fact we can act without the special monodisperse approximation but only with the help of the floating monodisperse approximation. This approximation is similar to the already described one but has one specific feature. In the floating monodisperse approximation the influence of the droplets formed on the first type centers at the "moment" z can be presented as $z^3 N_1(z/4)$, where $N_1(z/4)$ is the number of the droplets formed on the first type centers until $z/4$. So, this approximation is formulated for all moments of time and can be used in the arbitrary moment.

Certainly when z is near Δz this approximation coincides with the special monodisperse approximation. But this approximation is more simple and universal than the previous one. We shall use below the floating monodisperse approximation instead of the special monodisperse one.

2 Calculations for the total monodisperse approximation

Now we shall turn to estimate errors of approximations. The errors of substitutions of the subintegral functions by the rectangular form are known and they are rather small. But the error of the approximation itself has to be

estimated.

The error of the number of droplets formed on the first type of heterogeneous centers can be estimated in frame of the standard iteration method and it is small. So, we need to estimate only the error in the number of the droplets formed on the second type of heterogeneous centers.

It is absolutely clear that the worst situation occurs when there is no essential exhaustion of heterogeneous centers of the second type.

It seems that the monodisperse approximation will be the worst for the pseudo homogeneous situation, i.e. when the first type centers remain practically unexhausted. But as far as we haven't any direct proof of this property we shall consider the situation with the arbitrary power of exhaustion.

As the result we can consider the system of the following form

$$G = \int_0^z \exp(-G(x))\theta_1(x)(z - x)^3 dx$$

$$\theta_1 = exp(-b \int_0^z \exp(-G(x))dx)$$

with a positive parameter b and have to estimate the error in

$$N = \int_0^\infty \exp(-lG(x))dx$$

with some parameter l.

Parameter l shows that we doesn't consider the influence of the first centers nucleation on itself but analyze the influence of the first centers nucleation on another process with another parameters. This differs our consideration from that made in [3].

We shall solve this problem numerically and compare our result with some models. In the model of the total monodisperse approximation we get

$$N_A = \int_0^\infty \exp(-lG_A(x))dx$$

where G_A is

$$G_A = \frac{1}{b}(1 - \exp(-bD))x^3$$

and the constant D is given by

$$D = \int_0^\infty \exp(-x^4/4)dx = 1.28$$

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We have tried the total monodisperse approximation for b from 0.2 up to 5.2 with the step 0.2 and for l from 0.2 up to 5.2 with a step 0.2. We calculate the relative error in N. The results are drawn in fig.1 for N_A. Here r_1 is the relative error of the total monodisperse approximation in the number of droplets.

We see that even for N_A the relative error is small for all situations with moderate l. For big l the error slightly increases. This corresponds to the evident fact that when l is big the nucleation on the second sort centers is finished earlier than on the first sort centers. Here the total monodisperse approximation isn't valid.

The growth of the error for big l is rather slow but inevitably it will lead to the big value. Then this approximation will give a wrong result even in the order of the magnitude.

The calculations presented in further sections show that the maximum of errors in the floating monodisperse approximation lies near $l = 0$. So, we have to analyse the situation with small values of l. It was done in fig.2 for N_A. We see that for N_A this situation is even better than the previous situation. It is rather natural because the small values of l correspond to more strong ierarchy.

Unfortunately the situation for the floating monodisperse approximation is another. We can not find the maximum error of the results for the monodisperse approximation. We see that this error has the maximum at small b. Then we have to calculate the situation with $b = 0$. Here we have to solve the following equation

$$G = \int_0^\infty \exp(-G(x))(z - x)^3 dx$$

and to compare

$$N = \int_0^\infty \exp(-lG) dx$$

with

$$N_A = \int_0^\infty \exp(-lDz^3) dz$$

and other approximate expressions.

The results of this calculation are interesting mainly for floating monodisperse approximation and will be presented in the next sections.

References

[1] V.B.Kurasov Preprint cond-mat@xxx.lanl.gov get 0001104

[2] V.B.Kurasov, Deponed in VINITI 2594B95 from 19.09.1995, 28 p.

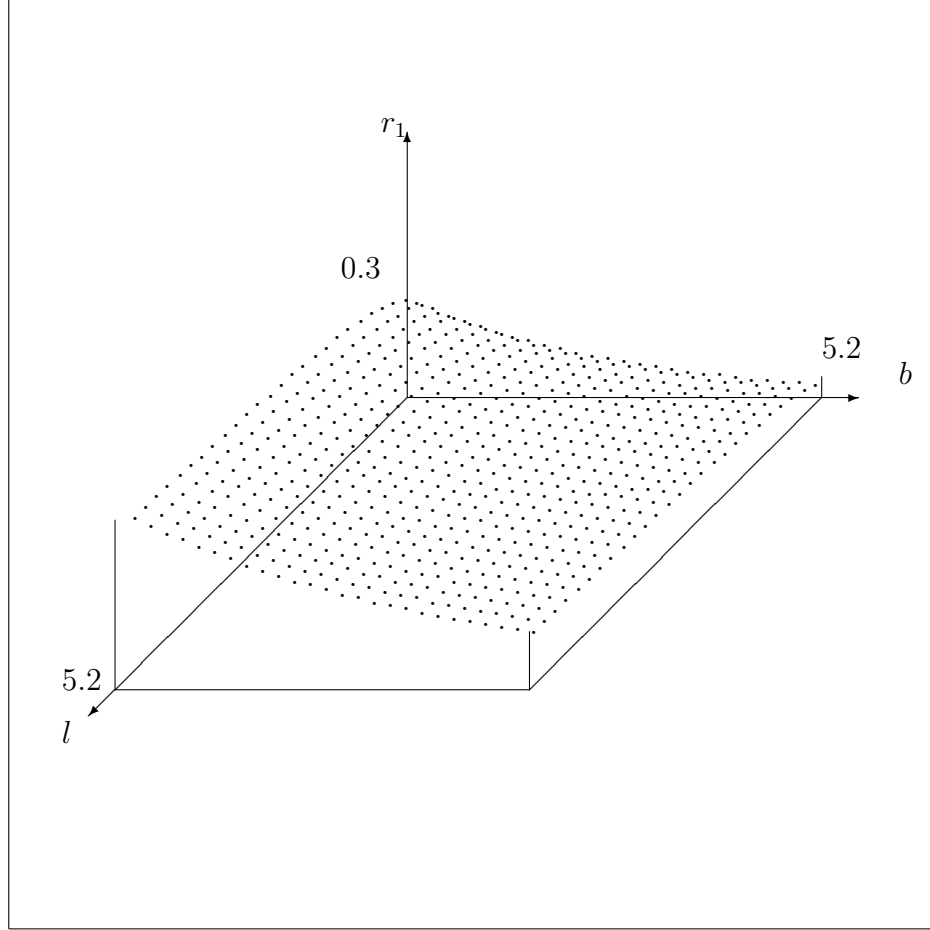[3] Kurasov V.B., Pavlov A.V., to be published in Vestnik SpbGU

Fig.1

The relative error of N_A drawn as the function of l and b. Parameter l goes from 0.2 up to 5.2 with a step 0.2. Parameter b goes from 0.2 up to 5.2 with a step 0.2.

One can see the essential negative slope when b increases and the slight positive slope when l increases.
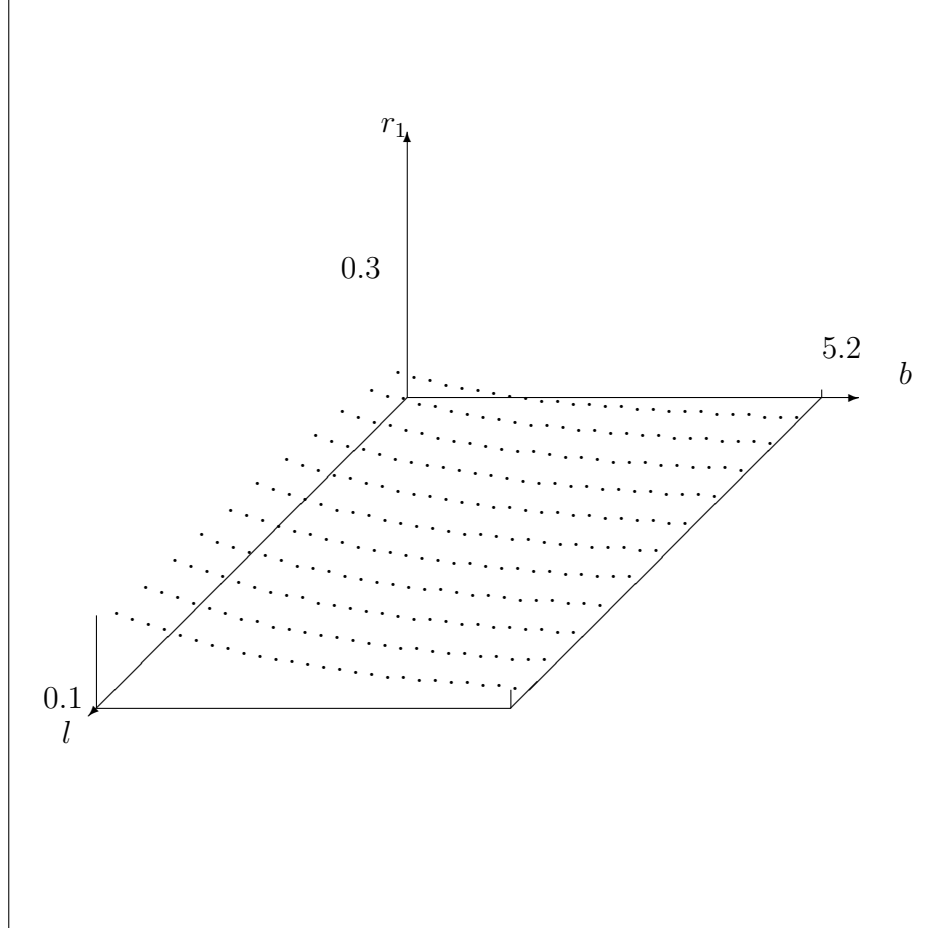
Fig.2

The relative error of N_A drawn as the function of l and b. Parameter l goes from 0.01 up to 0.11 with a step 0.01. Parameter b goes from 0.2 up to 5.2 with a step 0.2.

One can see the essential negative slope when b increases and the slight positive slope when l increases. The qualitative character is absolutely the same as in fig. 1.