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Scaling Laws of Biberman-Holstein Equation Green's Function and Implications for Superdiffusion Transport Algorithms

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ABSTRACT: The scaling laws of the Green's function of the Biberman-Holstein equation for the resonance atomic radiation transfer in an infinite medium are analyzed in the view of superdiffusion transport. This includes the scaling laws for the propagation front and asymptotic behavior far behind and far in advance of the propagation front. These scalings are shown to be determined by the superdiffusion mechanism. These enabled us to formulate possible implications for computational algorithms of treating the superdiffusive transport in a much broader framework.

1. INTRODUCTION

The Biberman-Holstein equation [1, 2] is a fundamental tool for describing the radiative transfer in the atomic/ionic spectral lines under condition of the complete redistribution over photon energy within spectral line width (i.e. under condition of the full loss of memory by the atomic excitation during its lifetime) in the elementary act of absorption-emission by an atom/ion in plasmas and gases (see, e.g., [3, 4], for laboratory plasmas). The complexity of treating the superdiffusive transport is characterized by the divergence of the mean squared displacement [5] and the non-reducibility of the integral equation over space variables to a diffusion-type transport equation (cf. [3-7]). Remind that the superdiffusion is defined as a transport for which the scaling law for the propagation front is as follows:

$$r_{\text{fr}}(t) \sim t^{\gamma}, \quad \gamma > 1/2. \tag{1}$$

The computational difficulties of solving an integral equation have stimulated developing the semi-analytic approaches which managed to provide rather simple models. These models originate from the approximate solution [6] of the integral equation and are known in applications as the escape probability methods (see, e.g., [8, 9]).

The Biberman-Holstein equation [1, 2] is derived from a couple of differential kinetic equations for photons and two-level atoms. Alternatively to the Biberman-Holstein equation which is widely used in laboratory plasmas, in astrophysics the above-mentioned couple of kinetic equations is often reduced to an integral, in space variables, equation for the radiation intensity, with the transport equation being of the same complexity as the Biberman-Holstein equation (cf., e.g., [10, 11]).

Because of multiple applications of the Biberman-Holstein approach, much efforts are spent on developing analytic and computational algorithms for solving it. However, the opportunities of developing and extending this experience beyond traditional frameworks are not exhausted.

Here we present a detailed analysis of the very old result for the Green's function of the non-steady-state radiative transfer in an infinite medium. The solution was derived analytically by Veklenko [5] as early as in 1959.

We use it for testing a new approach which prototype is based on the scaling laws for three main characteristics of the Green's function, namely, scaling law for

- the propagation front, defined as a relevant-to-superdiffusion average displacement,
- asymptotic behavior far beyond and far in advance of the propagation front.

These scaling laws enabled us to formulate possible implications for computational algorithms of treating the superdiffusive transport in a much broader framework.

2. GREEN'S FUNCTION OF BIBERMAN-HOLSTEIN EQUATION

The Biberman-Holstein equation for resonance radiative transfer in a uniform medium of two-level atoms/ions is obtained from a system of equations for spatial density of excited atoms, $F(\mathbf{r}, t)$, and spectral intensity of resonance radiation. This system is reduced to a single equation for $F(\mathbf{r}, t)$, which appears to be an integral equation, non-reducible to a differential diffusion-type equation:

$$\frac{\partial F(\mathbf{r},t)}{\partial t} = \frac{1}{\tau}\int_V G(|\mathbf{r}-\mathbf{r}_1|)F(\mathbf{r}_1,t)dV_1 - \left(\frac{1}{\tau}+\sigma\right)F(\mathbf{r},t) + q(\mathbf{r},t). \tag{2}$$

wheret τ is the lifetime of excited atomic state with respect to spontaneous radiative decay; σ is the rate of (collisional) quenching of excitation; q is the source of excited atoms different from population by the absorption of the resonant photon (e.g., collisional excitation). The kernel G is determined by the (normalized) emission spectral line shape, ε_ω, and the absorption coefficient k_ω. In homogeneous media, G depends on the distance r between the points of emission and absorption of the photon:

$$G(r) = -\frac{1}{4\pi r^2}\frac{dT(r)}{dr}, \quad T(r) = \int_0^\infty \varepsilon_\omega \exp\left(-k_\omega r\right) d\omega. \tag{3}$$

where $T(r)$ is the Holstein function, which gives the probability for the photon to pass the distance r without any absorption. The solution of the equation (2) in an infinite homogeneous medium with the boundary conditions $F(\mathbf{r}, t = 0) = \delta(\mathbf{r})$ (or, equivalently, $q(r, t) = \delta(r)\,\delta(t)$), i.e. the Green's function of Eq. (2), was obtained in [5] using the Fourier transformation of Eq. (2):

$$F(r,t) = \frac{-e^{-t(1/\tau+\sigma)}}{(2\pi)^2 r}\frac{\partial}{\partial r}\left\{\int_{-\infty}^{\infty} e^{-ipr}\left[\exp\left\{\frac{t}{\tau}J(p)\right\}-1\right]dp + 2\pi\delta(r)\right\}, \tag{4}$$

where

$$J(p) = \frac{1}{p}\int_0^\infty \varepsilon_\omega k_\omega \operatorname{arctg}\frac{p}{k_\omega}\,d\omega \tag{5}$$

Equation (6) gives the expression for Green's function for any spectral line shape.

It is noteworthy to recall that in the case of a monochromatic transport one has

$$J(p) = \frac{k}{p}\operatorname{arctg}\frac{p}{k}$$

and for large distance from the source one may expand $J(p)$ in series of parameter p that gives finally the well-known Green's function of the diffusion transport equation,

$$F(r,t) \approx \frac{e^{-\sigma t}}{(2\pi)^2 r}\frac{\partial}{\partial r}\int_{-\infty}^{\infty} \exp\left\{-ipr - \frac{tp^2}{3\tau k^2}\right\} dp = (4\pi Dt)^{-3/2} \exp\left(-\sigma t - \frac{r^2}{4Dt}\right), \tag{6}$$

where $D = \frac{1}{3\tau k^2}$. is the respective diffusion coefficient.

The non-locality (superdiffusion) of the radiative transfer described by the Biberman-Holstein demands special definition of the mean time, $\bar{t}(r)$, needed for a photon to pass the distance r from a point instant source, $q(\mathbf{r}, t) = \delta(\mathbf{r} - \mathbf{r}_0)\delta(t - t_0)$. The usually used concept of the average distance passed by a photon for the given time is inapplicable in the case of superdiffusion, because the function $F(\mathbf{r}, t)$ decreases too slowly and this leads to the divergence of the integral, which defines the mean squared devation, $\overline{r^2}$. The definition of $\bar{t}(r)$ which is relevant to the case of superdiffusion, is introduced in [5] and has the following form:

$$\bar{t} = \int_0^{\infty}\int_0^{r} 4\pi r_1^2 F(r_1, t)\, dr_1 dt. \tag{7}$$

The analytic analysis of Eq. (4) and (7) is given in [5] for two spectral line shapes, namely, Lorentz line shape

$$k_\omega = \frac{k_0}{1 + \left[2(\omega - \omega_0)/\Delta\omega_c\right]^2};\ \varepsilon_\omega = \frac{2}{\pi\Delta\omega_c}\frac{1}{1 + \left[2(\omega - \omega_c)/\Delta\omega_c\right]^2}, \tag{8}$$

and Doppler line shape,

$$k_\omega = k_0 \exp\left\{-\left[\frac{2(\omega - \omega_0)}{\Delta\omega_D}\sqrt{\ln 2}\right]^2\right\};\ \varepsilon_\omega = \frac{2}{\Delta\omega_D}\sqrt{\frac{\ln 2}{\pi}} \exp\left\{-\left[\frac{2(\omega - \omega_0)}{\Delta\omega_D}\sqrt{\ln 2}\right]^2\right\}. \tag{9}$$

In particular, it was shown that for the Lorentz line shape (8) one has the motion, which corresponds to an acceleration ($r \propto t^2$, i.e. $\gamma = 2$),

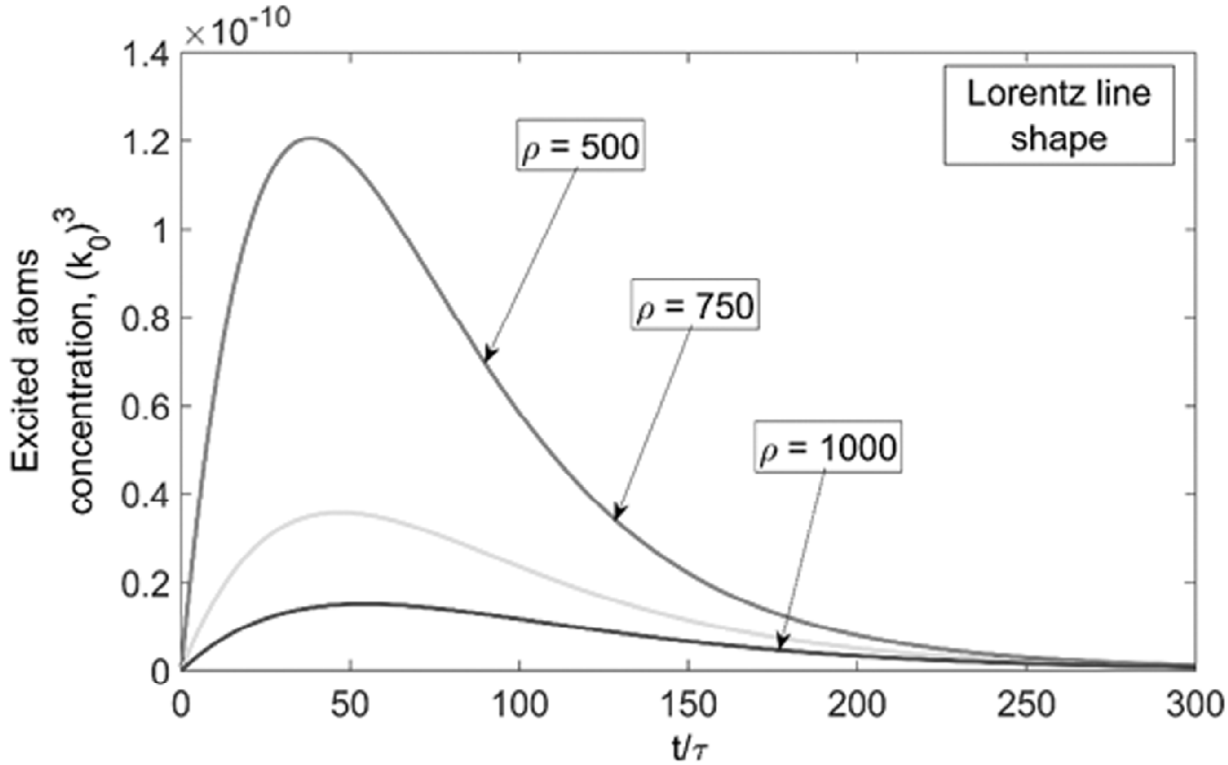
$$\bar{t} = 3\tau\sqrt{k_0 r/\pi} = 1{,}7\tau\sqrt{k_0 r}, \quad t >> \tau,\ k_0 r >> 1, \tag{10}$$

while for the Doppler line shape the respective motion is nearly like a free one ($r \propto t\, ln(t/\tau)$, i.e. $\gamma \approx 1$):

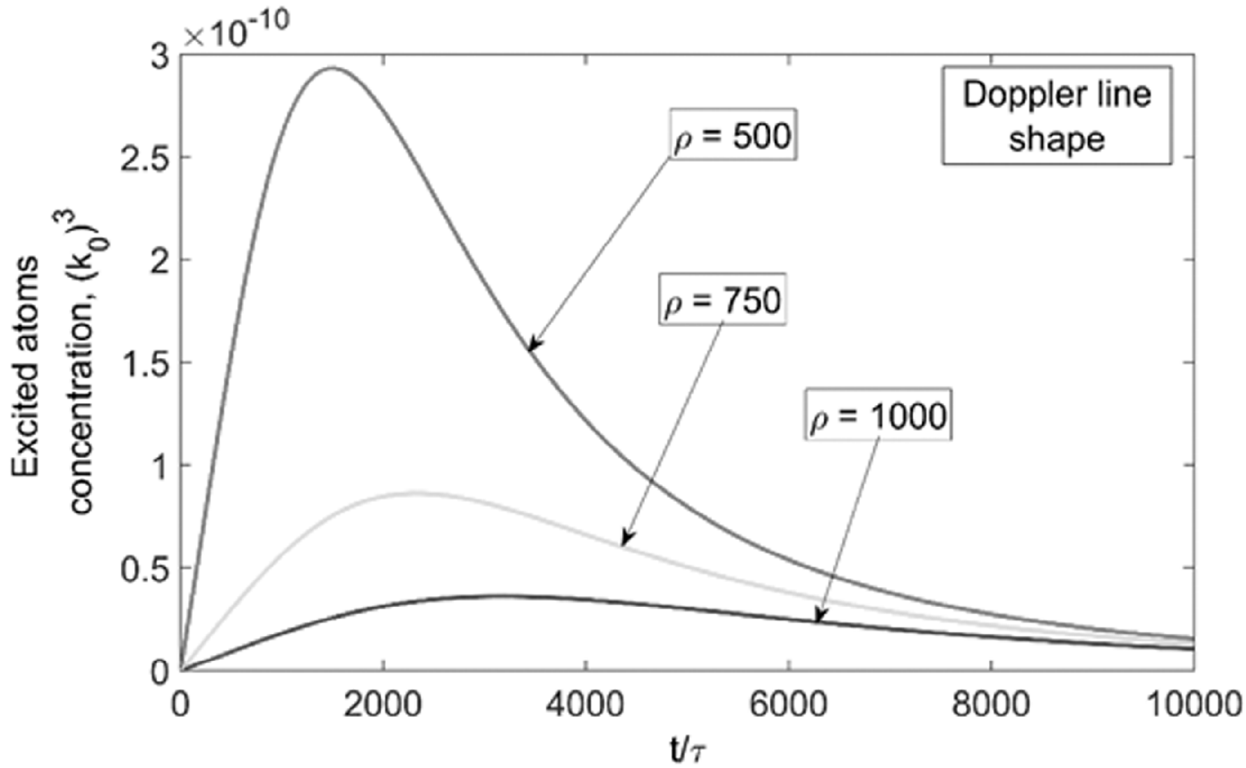
$$\bar{t} = 1.4\tau k_0 r\sqrt{\ln k_0 r}, \quad t >> \tau,\ k_0 r >> 1. \tag{11}$$

The results of numerical calculations of Green's function (4) are shown in Figure 1.

It follows from Figure 1 that in a certain point of the space, the evolution of the excitation takes the form of the arriving excitation, with a rather distinct front, and of a rather fast decay after the arrival of the front. That fact that the Green's function has a clearly pronounced maximum enables one to assume the existence of an effective front of the propagation of excitation. Therefore, in order to describe in a universal way the behavior of the Green's function, one has to find the scaling laws for two asymptotics, namely, those far behind and far in advance of the propagation front, and to identify how the average time of Eq. (7) is related to the local maximum of the Green's function in the certain point of the space and whether it is possible to define reasonably the propagation front. We start our analysis with clarifying the latter issue.



(a)



(b)

Figure 1: Numerical calculations of the exact Green's function [5] for various distances from the source for (a) Lorentz line shape and (b) Doppler line shape; t stands for time, τ is the lifetime of excited atomic state with respect to spontaneous radiative decay; $\rho \equiv k_0 r$, and k_0 is the absorption coefficient for the frequency ω_0, corresponding to the center of the spectral line

3. SCALING LAW FOR THE PROPAGATION FRONT

As seen from Eqs. (10) and (11), the mean time for these spectral line shapes strongly deviates from the diffusion law of Eq. (6), $r \propto (Dt)^{1/2}$. The unification of Eqs. (10) and (11), which extends this law to an arbitrary long-tailed line shape, i.e. compatible with superdiffusion, was suggested in [7]:

$$\overline{t}\,(\rho) = C\tau/[T_{as}(\rho)],\ t >> \tau, \tag{12}$$

where $\rho \equiv k_0 r$, and $T_{as}(\rho)$ is the asymptotics of the Holstein functional T at $\rho >> 1$, and C is the constant close to unity. The dependence of the propagation front essentially of the asymptoics of the Holstein function means that the main contribution to this law comes from the long-free-path photons, that, in turn, mean that this law is essentially superdiffusive one.

We suggest Eq. (12) with $C = 1$ to be the equation which defines the propagation front, $\rho_{fr}(t)$.

Our numerical analysis of the Green's function [5] for various line shapes shows that the scaling law defined by Eq. (12) gives good approximation for the time moment when $F(r, t)$ attains its maximum value at the distance r from the source. The results of such a comparison are shown in Figure 2.

It is seen that the scaling law of Eq. (12) gives good approximation of the local maximum of the exact Green's function as a function of time.

4. SCALING LAWS FOR ASYMPTOTICS

For a short time, $\tau << t << t_{fr}(\rho)$ (or, equivalently, far in advance of propagation front arrival at the distance ρ, $\rho >> \rho_{fr}(t) >> 1$), the asymptotics of the Green's function for Doppler and Lorentz line shapes were obtained in [5] and have the following form for Doppler line shape,

$$f\left(r,t\right) \approx \frac{2}{\left(4\pi\right)^{3/2}} \frac{t}{\tau} \frac{e^{-\sigma t}}{\sqrt{\ln k_0 r}} \frac{1}{k_0 r^4},\ t >> \overline{t} = 1,\ 4\tau k_0 r \sqrt{\ln k_0 r}. \tag{13}$$

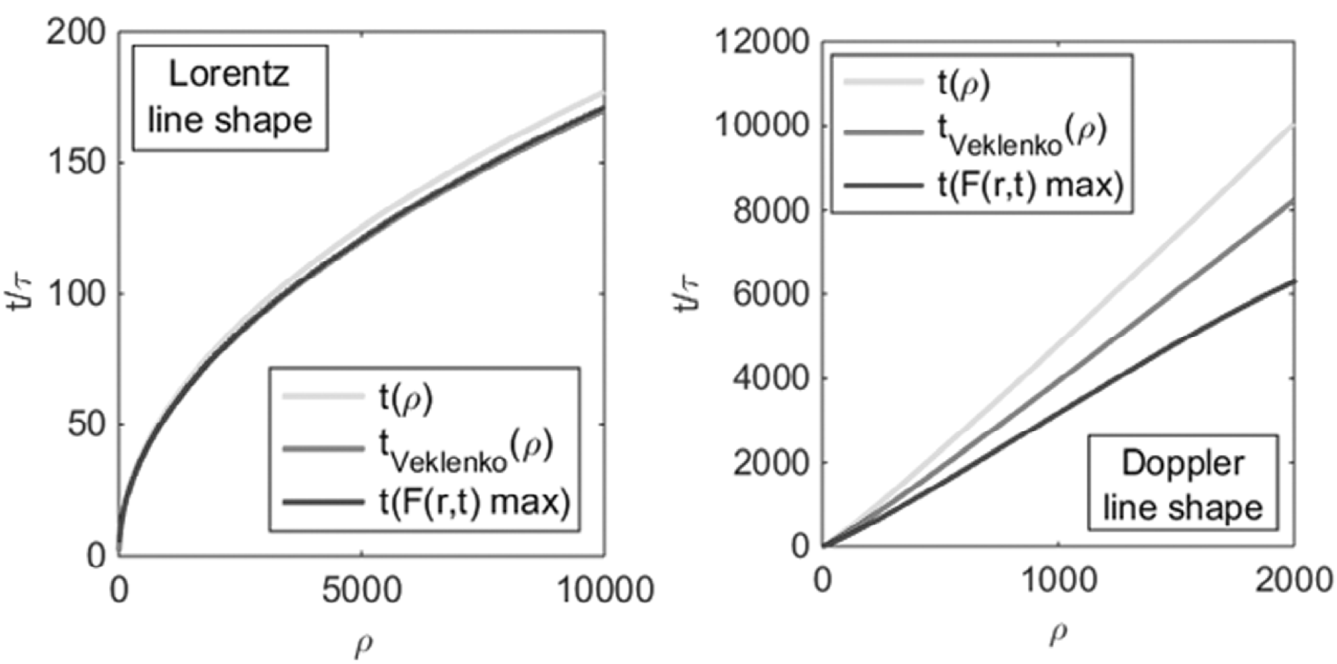


Figure 2: Time moment when $F(r, t)$ attains its maximum value at the distance r from the source (blue curve), as a function of $\rho \equiv k_0 r$, and its comparison with Eq. (4) for $C = 1$ (green curve) and C taken from exact value of the average time in Eqs. (10) and (11) (red): $(C_{as})^{-1} = 0.96$ for Lorentz line shape and $(C_{as})^{-1} = 0.82$ for Doppler line shape.

and Lorentz line shape,

$$f(r,t) \approx \frac{1}{(4\pi)^{3/2}} \frac{t}{\tau} \frac{e^{-\sigma t}}{\sqrt{k_0 r}} \frac{1}{r^3}, \; t >> \overline{t} = 3\tau\sqrt{k_0 r/\pi} = 1, \; 7\tau\sqrt{k_0 r}. \tag{14}$$

These asymptotics may be written in a universal form:

$$F \approx t\, G(\rho) \tag{15}$$

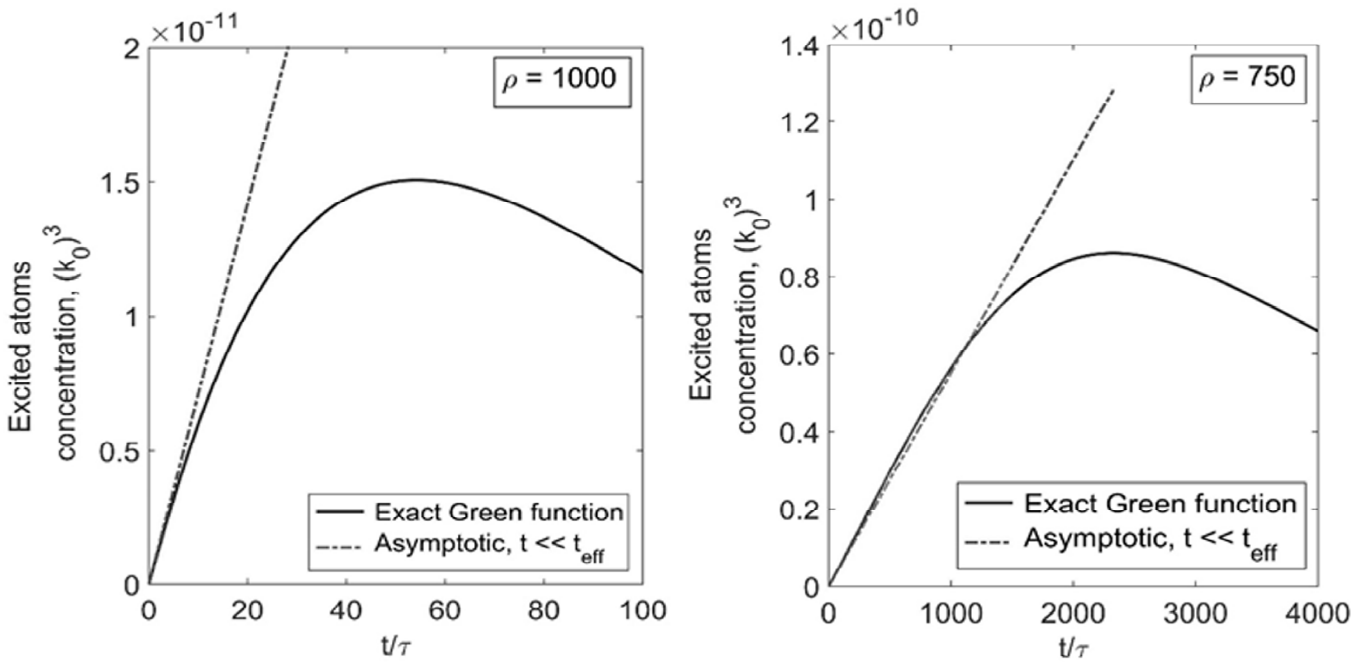
which corresponds to the direct excitation of distant atoms by the photons from the source (which is the slightly diffused but still approximately a point) in the far wings of the spectral line shape. Thus, Eq. (15) has essentially superdiffusive nature.

The Green's function far behind the propagation front, $\rho << \rho_{fr}(t)$, or equivalently $t >> t_{fr} >> \tau$, may be estimated assuming the local uniformity of the excitation distribution due to the fast exchange of atoms with photons in the core of the spectral line shape. The respective quasi-plateau solution in the 3D case takes the form:

$$F(t >> t_{\text{eff}}) = \frac{1}{\frac{4}{3}\pi \left(r^*(t)\right)^3} \eta\left(r^*(t) - r\right). \tag{16}$$

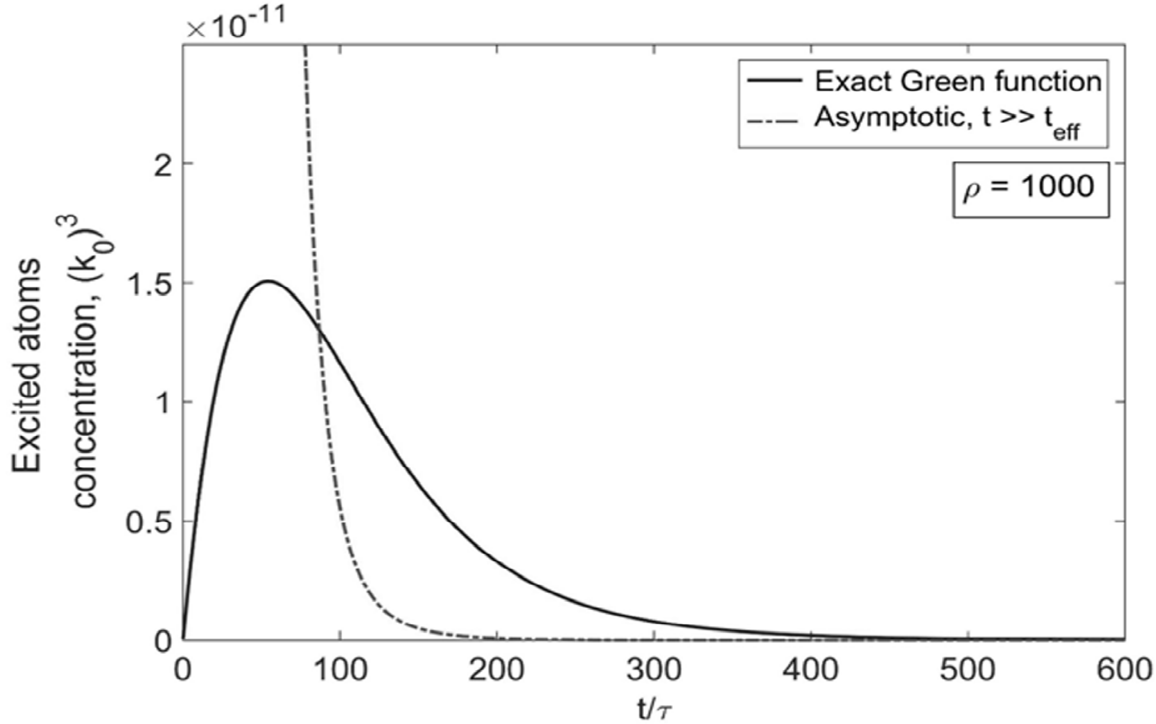
It is natural to expect that $r^*(t) \propto r_{fr}(t)$, whereas the exact relation between them is available from comparison of Eq. (16) with numerical calculations of the exact Green's function [5]. Such a comparison is shown in Figures 4 and 5.

As seen from Figures 4 and 5, comparison of Eq. (16) with numerical calculations of the exact Green's function [5] proves the asymptotics (16) to give a good scaling for the time dependence for various line shapes

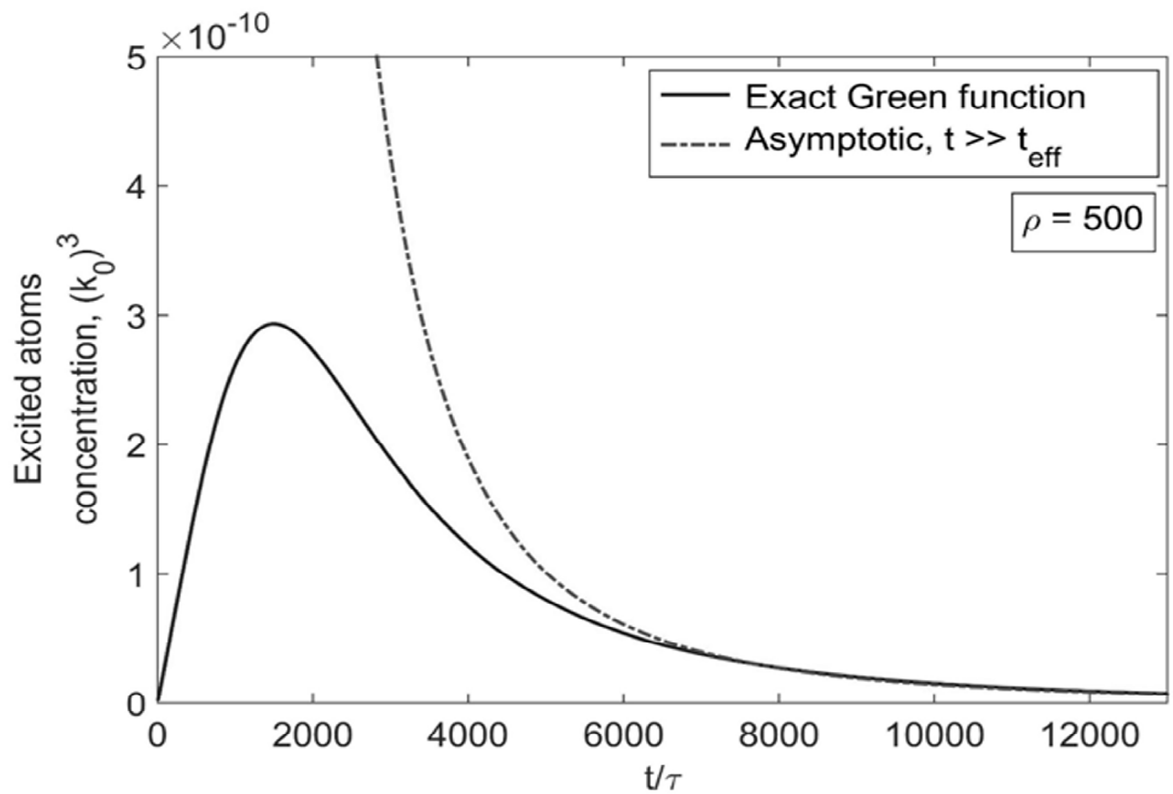


(a) **(b)**

Figure 3: Comparison of the exact Green's function *F*(*r*, *t*) with its asymptotics for short times; (a) Lorentz line shape, (b) Doppler line shape; *t* stands for time, τ is the lifetime of excited atomic state with respect to spontaneous radiative decay; $\rho \equiv k_0 r$, k_0 is the absorption coefficient for the frequency ω_0, corresponding to the center of the spectral line



(a)



(b)

Figure 4: Comparison of the exact Green's function $F(r, t)$ with its model asymptotic for large times, where $r^*(t) = r_{fr}(t)$; (a) Lorentz line shape, (b) Doppler line shape

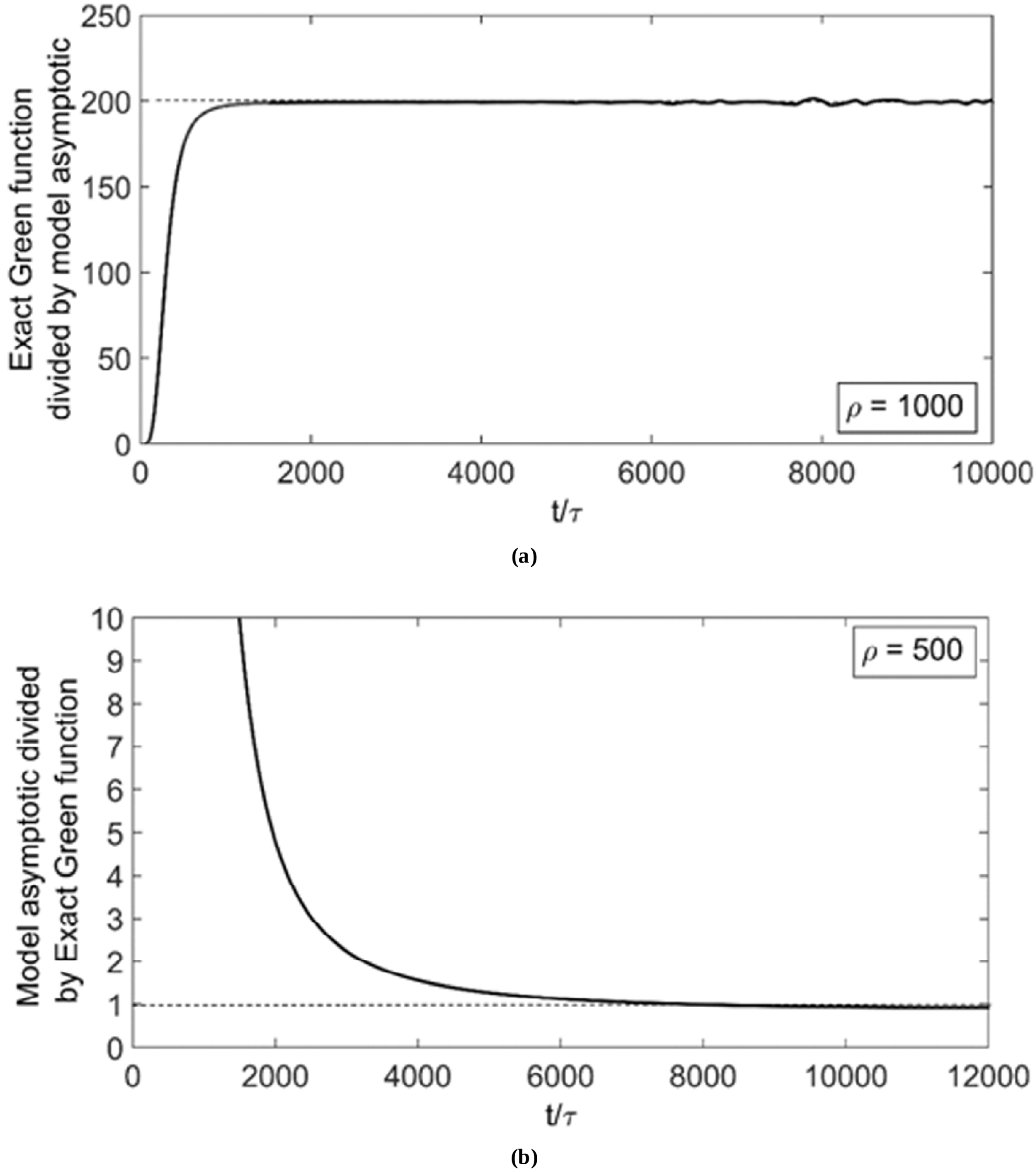


Figure 5: (a) The exact Green's function *F*(*r*, *t*) divided by its model asymptotics of Eq. (16) for large times in the case of Lorentz line shape, (b) model asymptotics for large times, Eq. (16), divided by exact Green's function *F*(*r*, *t*) in the case of Doppler line shape

$$F(r,t) \approx \frac{200}{\frac{4}{3}\pi\left(r_{\text{fr}}(t)\right)^3}\eta\left(r_{\text{fr}}(t)-r\right) \tag{17}$$

However, the absolute values of Eq. (16) and the asymptotics of the exact Green's function may differ by a constant which amounts to a factor of unity for Doppler line shape and ~200 for Lorentz line shape.

It is possible to estimate analytically a constant by which Eq. (16) differs from Eq. (17), the asymptotics of the exact Green's function. For example, consider the Lorentz line shape. For this purpose we investigate Eq. (4)

at small p. Expanding the imaginary exponent into a series and using an approximate form [5] of $J(p)$ function at small p,

$$J(p) \approx 1 - \frac{1}{3}\sqrt{\frac{2p}{k_0}}, \quad p \geq 0, \tag{18}$$

one has

$$F(\rho, T) \approx -\frac{k_0^3}{(2\pi)^2} \int_{-\infty}^{\infty} \left(-P^2 + \frac{P^4 \rho^2}{6} \right) \exp\left[-\frac{T}{3}\sqrt{2|P|} \right] dP, \tag{19}$$

where $\rho = k_0 r$, $P = p/k_0$, $T = t/\tau$.

The comparison of Eq. (19) with model asymptotic solution (16) at large times is shown in Figure 6.

Introducing a new variable $Q = T\sqrt{2P/3}$ in Eq. (19) and neglecting all terms except the first one in parentheses in the integrand, we express the resulting equation in terms of the quasi-plateau (17), where for $r_{fr}(t)$ we use the function inverse to the average time needed for a photon to pass the given distance. In the case of Lorentz line shape, it is [5] $\overline{T} = 1.69\sqrt{\rho}\,(T = t/\tau,\ \rho = k_0 r)$, so $\rho_{fr}(T) = (T/1.69)^2$, and we finally obtain

$$F(R, T) \approx 191 \cdot \frac{1}{\frac{4}{3}\pi \left(r_{fr}(T) \right)^3}, \quad r_{fr}(T) = \frac{1}{k_0}\left(\frac{T}{1.69} \right)^2. \tag{20}$$

Thus, one can see that the constant by which Eq. (16) differs from the asymptotics of the exact Green's function, Eq. (17), appears to be close to 200 (cf. Figure 5 (a)).The large value of the constant may be explained by the longer

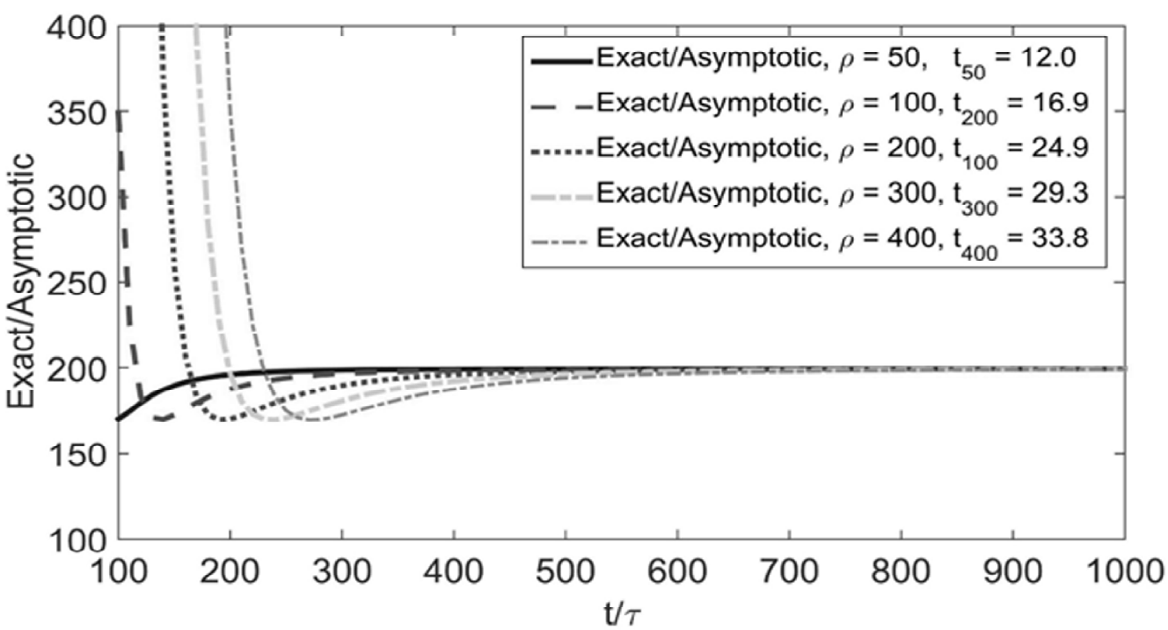


Figure 6: The Green function $F(r, t)$ from Eq. (19) divided by its model asymptotics for large times, Eq. (16), for different distances $\rho \equiv k_0 r$ from the source. Time T_{fr} is the average time needed for a photon to pass the given distance ρ. As it was already in Figure 4a, the ratio tends to a constant ≈ 200

precursor to the excitation front of Eq. (8) in the case of the longer PDF tail that, in turn, stems from a wider wings of the Lorentz line shape.

Thus, Eq. (17) for the asymptotics far behind the propagation front has essentially superdiffusive nature, similarly to that of equations for the propagation front and for asymptotics far in advance of the propagation front.

5. IMPLICATIONS FOR SUPERDIFFUSION TRANSPORT ALGORITHMS

The revealed scaling laws for superdiffusion transport of resonance radiation in plasmas and gases suggest the following implications for the algorithms of treating the superdiffusion transport far beyond the above physics problem.

All the scaling laws of Secs. 3 and 4 are closely related to the dominant contribution of the long-free-path travels of the carriers of the excitation of the medium. Such a phenomenon is well known in mathematics and various applied problems as the Lévy flights (see, e.g., [12-14]). The respective step-length probability distribution function (PDF) has, at large distances, a power-law decay, rather than exponential one. It is the long-tailed PDF that is responsible for the domination of the Lévy flights in many transport problems. The complexity of treating simultaneously the diffusion-like evolution of excitation, which is transported in the central part of the spectral line shape, with the essentially superdiffusion transport, which comes from the transport in the wings of the line shape, has been recognized and already used in the quasi-steady-state problems (see Sec. 1). However, in the non-steady-state problems of resonance radiation transport, and many other problems beyond this physics, the capabilities of the scaling laws inherent to the Lévy flights-based transport are not exhausted. For instance, to simplify the treatment of such problems the truncated PDF are used, which are substantiated by the reasonable arguments. However, as seen from the resonance radiation transport, the truncation is not necessary and even may be incorrect. Despite the model of complete redistribution (CRD) of photons over frequency within the spectral line shape, assumed in the Biberman-Holstein equation, may be violated in the far wings of the line shape, the range of detuning from the rest-frame transition frequency, where the CRD is applicable, is pretty broad, and an artificial truncation of the wings may be an oversimplification of the problem, dictated by the difficulty of treating the superdiffusion.

The main implications of considerations of Secs. 2-4 may be formulated in terms of identifying the role of Lévy flights and using the scaling laws in the computational algorithms. The general algorithm of solving the superdiffusion transport problem may include the following steps.

- Identification of scaling laws for the propagation front by comparing the scaling law of Eq. (12) with exact solutions of the transport equation in some particular cases.
- Identification of scaling laws for far in advance and far behind the propagation front by comparing the scaling law of Eqs. (15) and (16) with exact solutions of the transport problem in some particular cases.
- Identification of the class of functions, which may interpolate between the asymptotics far in advance and far behind the propagation front, and obey the law of propagation front. For instance, for the Biberman-Holstein equation one could suggest the following interpolation, where the parameters of interpolation, including the constant, should be considered as the free parameters to be found by comparing with the available set of exact solutions:

$$F(r,t) \approx t\,G\left(\sqrt{r^2 + B\rho_{\rm fr}^2(t)}\right) \tag{21}$$

- Elaboration of the algorithm of mathematical identification of the free parameters of the above (or similar) interpolation, using a set of a number of exact numerical solutions of the problem.

The latter algorithm should be implemented in a distributed computational environment. To this end, it has to include the following procedures and obey the following conditions:

- all integration in equations must be implemented via open source procedure in ANSI C programming language, e.g. GSL (GNU Scientific Library), https://www.gnu.org/software/gsl;

- for the purpose of above integration procedure, all the discrete series of input data (either experimental or phantom theoretical) should be processed by the smoothing routines, e.g. by GSL cubic spline;
- the problem of free parameters' identification should be stated as a mathematical programming (optimization) problem and formulated in terms of the AMPL modeling language (ampl.com).

All the components listed above may be implemented as web-services and deployed in the distributed computing environment by means of the Everest programming toolkit [15], http://everest.distcomp.org. Special "distributed enhancement" of the standard AMPL-translator, namely the AMPLX toolkit, http://gitlab.com/ssmir/amplx, is used to integrate all these web-services together within the computing scenario also available as a composite web-service. This service may be used by researchers to perform multivariant calculations. The computing infrastructure of the Center for Distributed Computing, dcs.isa.ru, of Institute for Information Transmission Problems (Kharkevich Institute), iitp.ru, is used for these purposes.

6. CONCLUSIONS

The revealed scaling laws of the Green's function of the Biberman-Holstein equation for the resonance atomic radiation transfer in an infinite medium suggest the possibility of using them in the computational algorithms of superdiffusion transport in the transport problems far beyond the physics of radiative transfer. The latter hint is suggested by the role of the long-free-path carriers which are identified in many mathematical and applied problems as the Lévy flights. These scaling laws includes those for the propagation front and for asymptotic behavior far behind and far in advance of the propagation front. These enabled us to formulate the possible computational algorithm of treating the superdiffusive transport in a much broader framework.

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