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Distribution function, reaction rates and spectral line profile

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Abstract

Quantum mechanics predicts the existence of power law "tails" in the distribution function over momentum in dense media even at the condition of thermodynamics equilibrium. Generalized expressions for the threshold process reaction rates show that reaction rates with released energy (e.g. vibrational-translational relaxation, chemical reaction, fusion rates) may be substantially increased due to quantum corrections. Spectral line profile also may have corrections at large detunings from line centre due to modification of distribution function. Cases of emission and absorption of radiation are analysed.

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1. Introduction

Studying the behaviour of absorption of resonant light in the distant "wings" of a spectral line, one can note that there is a certain connection to the behaviour of the distribution function over momentum for large magnitudes of the latter. As it was first shown in Ref. [1], due to quantum effects, the equilibrium distribution is different from the Maxwell's and contains some power asymptotics in the "tails". It is possible to

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express the asymptotic behaviour of the distribution function through the imaginary part of the retarded mass operator $\mathrm{Im}\Sigma^R(E,\vec{p}) \equiv \gamma(E,\vec{p})$ [1,2]

$$f(\vec{p}) = \int_{-\infty}^{\infty} \frac{\gamma(E,\vec{p})}{\epsilon_p^2}\, n(E)\, \frac{\mathrm{d}E}{\pi}\ . \tag{1}$$

Here, $\epsilon_p = p^2/2M$ is the kinetic energy of the particles, $n(E)$ denotes, in particular, for electrons in a dense gas, the Fermi distribution.

In Ref. [2] an approximate expression for the Lorentz gas was derived:

$$\gamma(E,\vec{p}) = \frac{\hbar n \sigma_{tot}(\vec{p})}{2}\sqrt{\frac{2E}{m_e}}\ . \tag{2}$$

Here, n is the gas density, σ_{tot} represents the total atomic (ion) scattering cross section of electrons, m_e is the electron mass. For plasma conditions one needs to take into account the shielding of Coulomb's potential in order to obtain the final value of σ_{tot}, which appears to be proportional to ϵ_p^{-2}, i.e. $\sigma_{tot} \sim 2\pi e^4 \epsilon_p^{-2}$, and from Eqs. (1) and (2) it follows (for $p \gg p_T \sim \sqrt{2Tm_e}$)

$$f(p) = \frac{2\hbar n e^4}{\epsilon_p^4}\sqrt{\frac{2}{m_e}}\int_0^{\infty} n(E)\sqrt{E}\,\mathrm{d}E\ . \tag{3}$$

In plasma, Eq. (3) means that the distribution function for electrons at large magnitudes of the momentum contains the asymptotic behaviour $f(p) \sim p^{-8}$ [1,2].

The effect of power "tails" in the distribution function can substantially modify the cross section for nonresonant fusion. Also, for the nondegenerate gas and sufficiently large positive detunings from resonance $\Delta = \omega - \omega_0 \gtrsim T/\hbar$, an effective resonance becomes possible $\epsilon_p \sim \hbar\Delta$ for large magnitudes of the momentum. This provides an asymmetric absorption profile for the detuning far to either red or blue region.

2. Reaction rates

The Lorentz gas model was used in Ref. [2] to calculate the reaction rates. In this work we generalize this approach to the case of interacting particles of comparable mass. The reaction rate for particles of "a" and "b" sorts can be found in general terms by doing the integration [2]

$$\begin{aligned} N_a N_b K_{ab} = C \int_{-\infty}^{\infty}\mathrm{d}E_a \int \mathrm{d}\vec{p}_a \int_{-\infty}^{\infty}\mathrm{d}E_b \int \mathrm{d}\vec{p} \int \mathrm{d}\vec{q} \\ \times n(E_a)(1 - n(E_a + Q_a - \omega))a_a(E_a - \epsilon_a) \\ \times n(E_b)(1 - n(E_b + \omega + Q_b))a_b(E_b - \epsilon_b) \\ \times a'_a(E_a + Q_a - \omega - \epsilon_{\vec{p}_a - \vec{q}})a'_b(E_b + \omega + Q_b - \epsilon_{\vec{p}_b + \vec{q}})|F|^2\ , \end{aligned} \tag{4}$$

where E_a, $\vec{p}_a$ are the energy and momentum, respectively, for the particle of sort "a", N_a, N_b represent concentrations for particles "a" and "b", while constant C is a normalization factor; F is the scattering amplitude of mass shell. The equilibrium population numbers for the energy are denoted as $n(E)$ [2], this model is allowed for

Table 1
Reaction rates (numerical simulation) for $T = 0.05$ and 0.07 keV

	N (cm^{-3})					$\langle \sigma V \rangle_{classic}$
T (keV)	1E+20	1E+23	1E+24	1E+25	1E+26	
0.07	1.82E-33	1.59E-33	1.59E-33	9.93E-34	3.79E-33	2.34E-33
0.05	5.79E-36	5.36E-36	5.36E-36	6.87E-36	3.47E-34	1.32E-35

deviations from Boltzmann statistics. The generalized distribution function over energy and momentum can be written as follows: $f(E, p) = n(E)a(E, p)$.

For a nonideal plasma we can use the Lorentzian function

$$a(E - \epsilon_p) = \frac{\gamma(E, \epsilon_p)/\pi}{(E - \epsilon_p - \Delta(E, \epsilon_p))^2 + \gamma^2} \ . \tag{5}$$

Under conditions when plasma becomes ideal, for instance when its density becomes smaller, the parameter $\gamma(E, \epsilon_p) \to 0$, in turn, $a(E - \epsilon_p)$ approaches delta-function. Here, we use a new variable representing kinetic energy of a particle, instead of its momentum, $\epsilon_p = p^2/2m$.

The value of γ in this function is determined by the inter-particle interaction. It can be well approximated if presented in a form similar to Eq. (2).

In order to carry on the calculations for the rates of the threshold reactions a method to perform integration like the one presented above, Eq. (4), has been developed. In this model we use the distribution functions over energy $n(E)$ to substitute the probability density functions. For the same reason we use the distribution functions over momentum which are determined by the Lorentz functions, Eq. (5). Simulation of the integrals over the spatial angular variables can be performed using homogeneous probability density functions.

In the framework of the method suggested above, the cross-section of the particles can be assigned in the most general way, without whatever simplifications. For example, one can use the energy dependence of the cross-section written in the form

$$\sigma(\epsilon_p) = \frac{S(\epsilon_p)}{\epsilon_p} \, \mathrm{e}^{-2\pi\eta(\epsilon_p)} \ , \tag{6}$$

where $\eta(\epsilon_p) = Z_1 Z_2 \mathrm{e}^2 \hbar^{-1} \sqrt{m/(2\epsilon_p)}$ is the Sommerfeld factor. The simulation results are shown in Table 1. One can conclude that, at the temperature ~ 0.05–0.07keV and density $\sim 10^{26}$ cm^{-3}, the reaction rate increases with the density because of the changes occurring in generalized distribution function over momentum as the result inter-particle interaction, in the limit of nonideal plasma.

3. Detailed balance of resonance absorption and emission

In Refs. [3,4] the processes of resonance radiation transport in dense gaseous media have been studied both theoretically and experimentally. The equations describing the

radiation transport [3] were proved to have the generalized spectral radiation density $J(\omega,\vec{k})$ being a function of the frequency ω and the wave vector $\vec{k}$ which are, in turn, independent variables. The need to modify the conventional theory arises when the photon free path due to absorption in the center of resonant line k_0 becomes comparable to the radiation wavelength which is true for natrium for the density $N \gtrsim 10^{17}$ cm^{-3}.

As it follows from the theory developed therein, the residual radiation intensity from the heterogeneously heated medium in the line centre is by the orders of magnitude higher than that obtained using the conventional theory of radiation transport [5]. Another consequence, also observed experimentally [4], represents anomalous growth of the output intensity in the far red region of the spectral line which in the cited references was linked to the Boltzmann factor in the intensity of spontaneous emission from a medium in thermodynamic equilibrium.

As it was shown in Ref. [3], the frequency and angle-dependent intensity of spontaneous emission ϵ_ω (derived from integration of radiation transport equations over wave vectors k [3]) can be written in the following form:

$$\epsilon_\omega = \frac{1}{4\pi}\hbar\omega A_0 \left(\frac{\omega}{\omega_0}\right)^3 n_\omega \widetilde{N}_2(\omega)\,, \tag{7}$$

where A_0 is the probability of spontaneous emission in a vacuum, n_ω is the index of refraction in the resonance medium, $n_\omega = \mathrm{Re}\sqrt{\epsilon_\omega}$, where ϵ_ω is the dielectric permittivity (the expression of Eq. (7) was obtained in [3] neglecting spatial dispersion). $\widetilde{N}_2(\omega)$ denotes the effective spectral population of the upper state

$$\widetilde{N}_2(\omega) = \widetilde{N}_2 a(\omega)\exp[-\hbar(\omega-\omega_0)/T]\,. \tag{8}$$

In Eq. (8) T is the temperature of the equilibrium medium expressed in energy units, $a(\omega)$ is the spectral line profile ($\int a(\omega)\,\mathrm{d}\omega = 1$); $\widetilde{N}_2$ is effective population of the excited state. In equilibrium, from Eqs. (7) and (8) one can obtain the Boltzmann distribution $\widetilde{N}_2(\omega) = g_2/g_1 N_1 a(\omega)\exp(-\hbar\omega/T)$. Here, g_i is the statistical weight of the ith state ($i = 1, 2$ for a two-level atom), N_1 denotes the total population of the lower state. Note that an expression similar to Eq. (8) for a low-density medium was reported in earlier works [6] where it was obtained from the detailed balance which requires that the spectral intensity takes the Planck's form in equilibrium, i.e.,

$$J_\omega = \frac{\hbar\omega^3}{4\pi^3 c^2}\frac{1}{\mathrm{e}^{\hbar\omega/T}-1}\,, \tag{9}$$

where the "current" frequency ω is present. In the framework of the conventional theory of transport the detailed balance provides the expression of Eq. (9) with a specified transition frequency ω_0. In case of large detunings from resonance $\Delta = \omega - \omega_0$, $|\Delta| \sim T$ the expressions of Eqs. (8) and (9) become notably different from the respective expressions used in the conventional theory [5].

The most vivid deduction of expressions of type Eq. (8) was offered after the works [3,4] had been published by Richard More (private communication) who, having considered the balance of absorption and emission from a moving atom, took into account the conservation laws for energy and momentum for radiating and absorbing atoms, considering their kinetic energy being different in the ground and excited states.

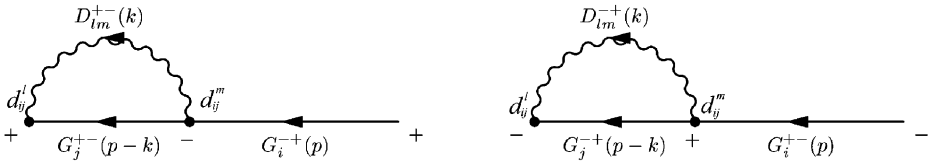

Fig. 1. Emission and absorption diagrams.

The most adequate apparatus to describe resonance radiation transport in dense media is the method of nonequilibrium Green's functions developed in Ref. [7] and used for the type of a problem under consideration in Ref. [3].

Let us examine the diagram in Fig. 1 drawn using the Keldysh technique for the emission process in state i with spectral and kinetic properties described by the Green's function $G_i^{-+}(p)$ (see the notations in Ref. [8]), where $p=(\vec{p},\omega)$. Here, the solid lines represent the Green's functions for "dressed" particles, the transition to the ground state j is described by the dipole matrix element with projection $l(d_l)_{ij}$. Creation of a photon with momentum $k=(\vec{k},\omega_k)$ is reflected by the wavy line which is associated with the Green's function of a lateral photon in a resonant medium $D_{lm}^{+-}(k)$. The diagram (Fig. 1) is described by the equations (see Ref. [8])

$$\mathrm{i}M_{em} = iG_i^{-+}(p)\int iG_j^{+-}(p-k)d_{ij}^l iD_{lm}^{+-}(k)d_{ij}^m\frac{d^4k}{(2\pi)^4}\,,$$

$$\mathrm{i}M_{abs} = iG_i^{+-}(p)\int iG_j^{-+}(p-k)d_{ij}^l iD_{lm}^{-+}(k)d_{ij}^m\frac{d^4k}{(2\pi)^4}\,. \tag{10}$$

For the Green's functions found in Eq. (10), in thermodynamic equilibrium, we have

$$\mathrm{i}G_i^{-+}(p) = -\frac{1}{\mathrm{e}^{(\omega-\mu_a)/T}+1}\,a_i(\omega-\omega_i-E(\vec{p}))\,. \tag{11}$$

Here, μ_a is the chemical potential, $a_i(\omega)$ is the spectral profile of the ith state having the excitation energy ω_i and energy of translation motion $E(\vec{p})$. The population numbers of the states $n_a(\omega)$ in Eq. (11) are of Fermi type.

$$a_i = \frac{\gamma_i(\omega,\vec{p})}{\pi[(\omega-\omega_i-E(\vec{p})-\Delta_i(\omega,\vec{p}))^2+\gamma_i^2(\omega,\vec{p})]}\,. \tag{12}$$

In Eq. (12) γ_i is the width, Δ_i stands for the shift of state i due to atom–matter interaction and radiation (imaginary and real parts of the retarded operator $\Sigma_i^R(\omega,\vec{p})$)

$$\mathrm{i}D_{lm}^{+-}(k) = \left(\delta_{lm}-\frac{k_ik_j}{k^2}\right)(1+n_R(\omega_k))\,\frac{4\pi\hbar 2\omega_k^4\epsilon''_\omega(\omega_k,\vec{k})}{|\omega_k^2\epsilon_\omega(\omega_k,\vec{k})-c^2k^2|^2}\,. \tag{13}$$

Here, $\epsilon_\omega(\omega_k,\vec{k})=\epsilon'_\omega(\omega_k,\vec{k})+i\epsilon''_\omega(\omega_k,\vec{k})$ represents the complex dielectric permittivity with its real ϵ'_ω and imaginary ϵ''_ω parts; $n_R(\omega_k)=(\exp(\omega_k/T_R)-1)^{-1}$ are Bose population numbers for radiation at temperature T_R which, in general, is not the same as the temperature of the medium T.

The analysis of the detailed balance between emission and absorption proves that in a general case the spectral distribution for the atoms depends on two temperatures, i.e. temperature T and excitation temperature T_{ex}

$$n_i(\vec{p},\epsilon) = \frac{1}{\exp\{(\epsilon + E(p))/T\}\exp\{(\omega_i - \mu_a)/T_{ex}\} + 1} \,. \tag{14}$$

For the nondegenerate case ($\exp\{-\mu_a/T_{ex}\} \gg 1$) and with account for the generalization of Eq. (14), we find the emission rate

$$M_{em}^{i\to j} \sim N_i^* \exp\left\{-\frac{E(\vec{p}-\vec{k})}{T}\right\} \exp\left\{-\frac{\omega_k - \omega_0}{T}\right\}(1+n_R)\,, \tag{15}$$

where $N_i^* \sim \exp\{-(\omega_i - \mu_a)/T_{ex}\}$, is the density of excited atoms. Using the same notations we obtain the absorption rate as

$$M_{abs}^{j\to i} \sim \exp\left\{-\frac{E(\vec{p}-\vec{k})}{T}\right\} N_i^* \exp\left\{\frac{\omega_0}{T}\right\} n_R \,. \tag{16}$$

If one substitutes population numbers for the ground state N_j^*, defined similarly to Eq. (3) $N_j^* \sim \exp\{-(\omega_j - \mu_a)/T_{ex}\}$, so that (no degeneracy considered) $N_j^*/N_i^* = \exp\{\omega_0/T_{ex}\}$.

4. On asymmetry of resonance absorption factor

Disregarding the corrections describing stimulated emission ($\widetilde{N}_i \ll N_j$), in this limit one can find the absorption factor to be

$$k(\omega) = \frac{2\pi\hbar\omega}{c}\frac{d^2}{3}\int \frac{\mathrm{d}E\,\mathrm{d}\vec{p}}{(2\pi)^4} G_i^{+-}(p+k) G_j^{-+}(\vec{p}) \,. \tag{17}$$

Using Eqs. (11) and (12), from Eq. (17) we obtain

$$k(\omega) = \hbar\frac{\lambda^2}{4} A_0 \int \frac{\mathrm{d}E\,\mathrm{d}\vec{p}}{(2\pi)^3} n(E)(1 - n(E+\hbar\omega)) \times a_j(E - \epsilon_p - E_j) a_i(E - \epsilon_{\vec{p}+\vec{k}} - E_i + \hbar\omega) \,. \tag{18}$$

In order to estimate the width characterizing the spectral profiles of states i and j we shall use the estimations of type Eq. (2):

$$\gamma_j(E,\vec{p}) = \frac{\hbar n \sigma_T(p)}{2}\sqrt{\frac{2E}{M}} \,. \tag{19}$$

Here, σ_T is the gas kinetic cross-section for the atomic scattering, for instance, with heavy buffer gas of density n, M is the mass of a resonant atom. We have:

$$\gamma_i(E+\hbar\omega, \vec{p}+\hbar\vec{k}) = \gamma_j(E+\hbar\omega, \vec{p}+\hbar\vec{k}) + \frac{\hbar N_p \pi d_{ij}^2}{\hbar|\vec{v} + \hbar\vec{k}/M|}\sqrt{\frac{2(E+\hbar\omega)}{M}} \,. \tag{20}$$

In Eq. (20) the second term describes additional broadening of state i due to resonant excitation exchange.

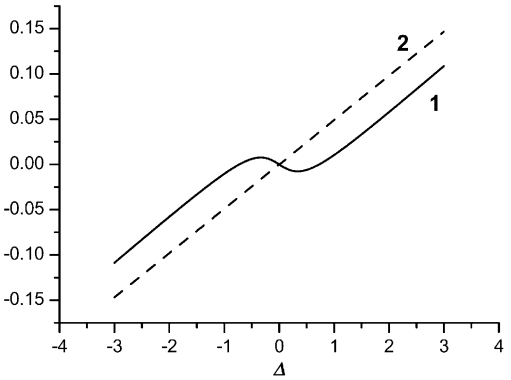

Fig. 2. Asymmetry of resonance absorption factor in units of $2(k(\omega_0 - \Delta) - k(\omega_0 + \Delta))/(k(\omega_0 - \Delta) + k(\omega_0 + \Delta))$ as a function of detuning Δ for $\omega_0/T = 20$, $\mu/T = -20$, $\gamma_1/T = 3,26 \times 10^{-5}$, $\gamma_2/T = 1,81 \times 10^{-3}$, and for the densities: (1) $n = 10^{21}$ cm^{-3}, (2) $n = 10^{19}$ cm^{-3}.

The total asymmetric character of the absorption factor is shown in Fig. 2. The asymmetry is explained by the effective resonance at large values of the momentum $\epsilon_p = \hbar(\omega - \omega_0)$. Besides, some subsidiary asymmetry is introduced by the fact that the effective width of state i is a function of frequency ω (see Eq. (20)).

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