

# Dynamics of a lasing atom in hot plasma

N. Bar-Gill<sup>a</sup>, M. Botton, and A. Ron

Technion - Israel Institute of Technology, Department of Physics, Haifa 32000, Israel

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**Abstract.** We study theoretically the dynamics of lasing atoms in a very hot plasma capillary, which produce coherent X-ray radiation. The atoms which participate in the lasing action are treated as a dilute gas, embedded in the plasma, whose electrons play the dominant role in inducing relaxations and decoherences. The active atom interacting with the electron reservoir in thermal equilibrium is described by a general Hamiltonian. In analogy with a radiation reservoir, by eliminating the degrees of freedom of the electron reservoir, the evolution rates of the Master Equation, i.e. the transition rates for the populations and dephasing rates for coherences, are calculated. It is demonstrated, by going beyond the dipole approximation, that the contribution of the adiabatic dephasing rate is significant compared to that of the non-adiabatic rate, in contrast to the case of a radiation reservoir. We also study other dephasing mechanisms, e.g. the motion of the lasing atom's center of mass, and the role of other atomic levels.

**PACS.** 52.20.Hv Atomic, molecular, ion, and heavy-particle collisions – 32.70.Jz Line shapes, widths, and shifts

## 1 Introduction

Recently, the Z-Pinch process (e.g. [10]) has been used to create plasma conditions relevant to X-ray lasers<sup>1</sup>, via capillary discharge. A capillary discharge X-ray laser has been obtained [2,17,18,20], employing the collisional excitation pumping mechanism [7,22,24]. The theoretical modeling of this capillary discharge X-ray laser is based on a combination of a magneto-hydrodynamic numeric model (e.g., [16]) for the description of the pinch process, and Lamb's semi-classical laser theory [11] as a basic theoretical model of the laser. In this approach, Maxwell's equations are used to describe the lasing radiation, and atomic evolution equations — the gain medium of the laser. In the present paper we focus on the latter.

The gain medium equations contain evolution rates, which describe the underlying physical interactions affecting the lasing atoms. Many implementations of the laser model (e.g. [14]), including those aimed at plasma based X-ray lasers (e.g. [12]), treat the evolution rates as semi-empirical parameters. However, derivation of these rates can be found in the literature, taking into account interactions of the lasing atoms with the surrounding plasma, namely photons, electrons and other ions. The commonly used approach deals separately with the transition rates,

which are related to the changes of the level populations of the lasing atoms, and with dephasing rates, related to changes of the atomic transition dipole moments.

Transition rates are usually defined through excitation and de-excitation cross-sections. These cross-sections are usually derived using scattering techniques (e.g. [15]), employing both a classical description of the electrons, e.g., the impact parameter method [8], and a quantum mechanical description, based on partial wave theory and the Born expansion [5]. Further extensions and elaborations of this theory have been carried out (e.g. [19,21]), using oscillator strengths, and including interactions with other perturbers.

Atomic dephasing rates, which govern the time evolution of the coherences, i.e. the off diagonal elements of the system's density matrix, are defined through phase fluctuations due to various processes of the interactions between the atom and its environment. The interest in the phenomenon of dephasing arises from the fact that it affects the radiation emitted by the dephased atom, resulting in broadening and shift of the radiated lines. Collision processes, both those causing transitions among the atomic states, and those which do not, constitute dephasing processes. Broadening of spectral lines, caused by collisions with particles in the surrounding gas, is called pressure broadening. Under the impact approximation, the collisions are assumed to be uncorrelated, mostly weak, and short in comparison with the mean time between collisions (e.g. [1]). In previous studies of these effects, usually scattering formalism was employed. Both classical, through the classical path method, and quantum descriptions of

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<sup>a</sup> e-mail: bargill@tx.technion.ac.il

<sup>1</sup> A review of methods for the realization of X-ray lasers can be found in [7] and in the proceedings of the International Conference on X-ray Lasers, from the years '86, '90, '92, '94, '96, '98, '00, '02.

the perturbers were used (e.g. [9]). Further elaborations, such as inclusion of atomic center-of-mass motion (see [3]) and density matrix techniques [4,13], were also carried out. A model for both transition and dephasing effects using the density matrix formalism has been suggested as well [4].

The main shortcoming of the various methods described above lies in their use of scattering techniques. This approach results in expressions, which can usually be obtained only to first order in the interactions. Also, since dephasing rates are derived through spectrum broadening, they cannot be easily compared to transition rates. Although [4] treats both rates on the same footing, they retain the complexity of scattering methods.

In the present paper, we investigate the atomic evolution rates induced by the surrounding plasma, as a superposition of two different reservoirs, a radiation reservoir and an electron reservoir. We focus on the electron reservoir, since the treatment of a radiation reservoir is well-known (e.g. [6]). The effect of the plasma ions is not studied here, since they are slow and therefore have long interaction times, and it has been shown that they are usually negligible (the quasi-static approximation — see [1]). The radiating atoms form a dilute gas, and each lasing atom is assumed to be a small quantum system interacting with the surrounding reservoirs. This assumption is valid since only a small fraction of the plasma particles takes part in the lasing activities. Note that although we refer to the gain medium as atoms, our approach is applicable to cases where it consists of ions as well.

In our derivations we employ the impact approximation, which allows us to assume that at any moment a single interaction occurs, and that each reservoir affects the lasing atoms independently. Thus our problem is reduced to that of an atom interacting with only one reservoir at a time. Combining the effects of all interactions renders the complete model of the lasing atom's evolution. We utilize the density matrix approach, through which both transition and dephasing rates are obtained, as we formulate a *generalized Hamiltonian* for the problem of an atom interacting with a reservoir. Then we describe the electron reservoir using second quantization, which allow us to obtain an exact derivation of the evolution rates; this method is applicable to both reservoirs, thus making possible a comparison between them. Also, our formulation for the electron reservoir enables further insight and better understanding of the results obtained in previous works.

It should be emphasized that our results have a wide scope of application, although the original motivation stems from X-ray lasers research. Our Hamiltonian-based methodology for the derivation of the evolution rates is relevant to other physical problems as well. For example, this approach can be used to analyze the emissions of stellar configurations, such as solar flares, in Astrophysics.

The remainder of the paper is organized as follows: Section 2 contains the main contribution of our study, the derivation of interaction of the atomic system with an electron reservoir. The transition and dephasing rates

are obtained using the density matrix formalism, where the electrons of the plasma play the role of the reservoir. Here the second quantized electronic states of the plasma replace the second quantized photonic modes of the radiation reservoir. The resulting rates are then compared to those of the radiation bath, providing insight as to different dephasing mechanisms, and their physical origins. An hydrogen-like atom serves as a representative model and is solved in detail, allowing us to study the dependence of the rates on the parameters of the problem, and to get a feel for the time-scales in question. Section 3 addresses an additional point of interest, checking the effect of the motion of the atom's center of mass on the evolution rates, while in Section 2, the atom is assumed to be infinitely heavy. We derive a series expansion of the corrections introduced by this effect, and show that the effect is negligible. In Section 4 we explore other dephasing mechanisms, e.g., those related to the presence of many atomic levels, which are coupled to the lasing levels through the reservoir. The contributions to the dephasing phenomenon, added by this section, complete the picture of dephasing in practical physical systems.

## 2 An atom in an electron reservoir

In this section we first derive the atomic evolution rates in a general gas reservoir, in analogy with the calculations of these rates in a radiation reservoir (e.g. [6]). We describe the gas reservoir interacting with the atomic system, employing a *general* Hamiltonian formulation. Based on these general expressions, we find the evolution rates for a hydrogen-like lasing atom embedded in high temperature plasma. This provides insight into the relationship between the transition and dephasing rates, and the interaction potentials. This approach offers clarity and simplicity, based on elementary aspects of quantum mechanics. We then compare our results to those obtained for a radiation reservoir, and deduce conclusions regarding the evolution rates.

### 2.1 General gas reservoir

We consider a microscopic system, e.g., an atom, interacting with the environment particles via a general coupling potential. Following [6], the interaction Hamiltonian is generally of the form

$$H_{AB} = \sum_{\alpha} A_{\alpha} B_{\alpha}, \quad (1)$$

where  $A_{\alpha}$  are atomic operators, and  $B_{\alpha}$  are reservoir operators. The rate of *transition* from atomic state  $|n\rangle$  of energy  $\hbar\omega_n$  to the state  $|m\rangle$  of energy  $\hbar\omega_m$ , with  $\omega_{nm} = \omega_n - \omega_m$ , is expressed as

$$\Gamma_{n \rightarrow m} = \sum_{\alpha, \gamma} \langle m | A_{\alpha} | n \rangle \langle n | A_{\gamma} | m \rangle G_{\alpha\gamma}(\omega_{nm}) \quad (n \neq m), \quad (2)$$

where  $\langle m|A_\alpha|n\rangle$  is a matrix element of the atomic system. Here  $G_{\alpha\gamma}(\omega_{nm})$  is the reservoir correlation function, and it is given by:

$$G_{\alpha\gamma}(\omega) = \frac{2\pi}{\hbar} \sum_N W_N \sum_M \langle N|B_\alpha|M\rangle \langle M|B_\gamma|N\rangle \times \delta(E_N - E_M + \hbar\omega). \quad (3)$$

where  $|N\rangle$  and  $|M\rangle$  are the eigen energy states of the reservoir, of energies  $E_N$  and  $E_M$ , respectively,  $W_N$  is the probability of the  $|N\rangle$  state, and  $\langle N|B_\alpha|M\rangle$  is the matrix element of  $B_\alpha$  between these states. Notice that the correlation function depends only on the reservoir properties. The rate of *dephasing*, between the states  $|n\rangle$  and  $|m\rangle$ , which corresponds to the rate of change of the off-diagonal matrix element of the atomic density matrix,  $\sigma_{mn}$ , consists of an adiabatic component, and a non-adiabatic one. The non-adiabatic dephasing rate can be expressed in terms of the transition rates as

$$(\Gamma_{nm})_{non.ad} = \frac{1}{2} \left( \sum_{a \neq n} \Gamma_{n \rightarrow a} + \sum_{a \neq m} \Gamma_{m \rightarrow a} \right), \quad (4)$$

while the adiabatic dephasing rate is given by

$$(\Gamma_{nm})_{ad} = \frac{1}{2} \Re e \sum_{\alpha,\gamma} |\langle m|A_\alpha|m\rangle - \langle n|A_\gamma|n\rangle|^2 G_{\alpha\gamma}(0). \quad (5)$$

Note that the adiabatic dephasing term of the *coherence*  $\sigma_{mn}$  depends on the *difference* between the diagonal matrix elements of the interaction potential of states  $|n\rangle$  and  $|m\rangle$ . Intuitively, this means that the adiabatic dephasing is caused by the difference in impact of the interaction potential on the two dephased levels. As the interaction potential affects the two levels differently, fluctuations between them, and thus dephasing, occur. The transition rate and the non-adiabatic dephasing rate, on the other hand, depend on the off-diagonal matrix elements of the interaction potential of the atomic states. This difference between the evolution rates will be evident through their effect in certain cases.

We describe the reservoir as a gas of independent particles, which constitutes a complete state basis, where the  $i$ th particle has mass  $m$ , position  $\mathbf{r}_i$  and momentum  $\mathbf{p}_i$ . The reservoir Hamiltonian is written as

$$H_B = \sum_i^{\bar{N}} \frac{p_i^2}{2m}, \quad (6)$$

with  $\bar{N}$ , the total number of particles. The volume of the reservoir is taken to be  $V$  and the average number of particles per unit volume is  $n_0 = \bar{N}/V$ . We describe the particles in the quantization volume  $V$  in terms of plane waves with periodic boundary conditions, i.e.,

$$\frac{p^2}{2m}|\mathbf{k}\rangle = \epsilon_{\mathbf{k}}|\mathbf{k}\rangle, \quad |\mathbf{k}\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \text{and} \quad \epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}. \quad (7)$$

Thus, the energy states of the reservoir,  $|N\rangle$ , are given by

$$H_B|\{n_{\mathbf{k}}\}\rangle = E(\{n_{\mathbf{k}}\})|\{n_{\mathbf{k}}\}\rangle, \quad (8)$$

where  $|N\rangle = |\{n_{\mathbf{k}}\}\rangle$  stands for the ensemble of one-particle  $\mathbf{k}$  states, and  $n_{\mathbf{k}}$  is the number of particles in the  $\mathbf{k}$ th state.

We shall find it convenient to employ second quantization to describe the reservoir as a gas of independent particles. We introduce  $a_{\mathbf{k}}$  and  $a_{\mathbf{k}}^\dagger$  for the annihilation and creation operators for the single particle states. The Hamiltonian of the reservoir is then

$$H_B = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}}, \quad (9)$$

where  $\hat{n}_{\mathbf{k}} = a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$  is the number operator of the state  $\mathbf{k}$ , with the eigenvalues  $n_{\mathbf{k}}$ . The general Hamiltonian of interaction between the atom and the gas is assumed to be

$$H_{AB} = \sum_{i,s} \phi_{si}(\mathbf{r}_s - \mathbf{r}_i), \quad (10)$$

where  $\mathbf{r}_s$  represent the coordinates of the atomic system, e.g. the internal electrons. This is a general form of an interaction potential, which fits most physical potentials, such as the Coulomb potential, which we will employ later on. We represent the energy states  $|n\rangle$  of the atom by the orthogonal set of normalized atomic wave-functions

$$H_A \Psi_n(\{\mathbf{r}_s\}) = \epsilon_n \Psi_n(\{\mathbf{r}_s\}). \quad (11)$$

We now wish to cast our general interaction Hamiltonian, equation (10), in the form of equation (1). For a single species gas we have  $\phi_{si} = \phi_s$ , and introducing Fourier transform in space by

$$\phi_s(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \phi_s(\mathbf{q}) \quad (12)$$

we have

$$H_{AB} = \frac{1}{V} \sum_{\mathbf{q}} \sum_s \phi_s(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}_s} \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i}. \quad (13)$$

The gas density operator in space position  $\mathbf{r}$ , is expressed as

$$\hat{D}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} D_{\mathbf{q}}, \quad (14)$$

where

$$D_{\mathbf{q}} = \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i}, \quad (15)$$

or in second quantized form

$$D_{\mathbf{q}} = \sum_{\mathbf{k}} a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{k}}. \quad (16)$$

Indeed equation (1) is expressed in terms of the atomic operators

$$A_{\mathbf{q}} = \sum_s \phi_s(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}_s}, \quad (17)$$

and the reservoir operators

$$B_{\mathbf{q}} = \frac{1}{V} D_{\mathbf{q}}. \quad (18)$$

We note that Fourier space corresponds to a transition to momentum space, with  $\hbar\mathbf{q}$  being the momentum exchange of the reservoir particles with the atom.

We now move on to the derivation of the transition rates. Since we have modeled the problem employing the conventions of reference [6], we can immediately use equation (2) to write the rate as

$$\Gamma_{n \rightarrow m} = \sum_{\mathbf{q}, \mathbf{q}'} \langle m | A_{\mathbf{q}} | n \rangle \langle n | A_{\mathbf{q}'} | m \rangle G_{\mathbf{q}\mathbf{q}'}(\omega_{nm}) \quad (n \neq m). \quad (19)$$

In a thermal equilibrium reservoir, with temperature  $T$ , we write

$$G_{\mathbf{q}, \mathbf{q}'}(\omega) = \delta_{\mathbf{q}', -\mathbf{q}} G_{\mathbf{q}}(\omega), \quad (20)$$

where

$$G_{\mathbf{q}}(\omega) = \frac{2\pi}{\hbar} \sum_N \frac{e^{-\beta E_N}}{Z} \frac{1}{V^2} \sum_M \langle N | D_{\mathbf{q}} | M \rangle \langle M | D_{-\mathbf{q}} | N \rangle \times \delta(E_N - E_M + \hbar\omega), \quad (21)$$

$\beta = 1/k_B T$ ,  $k_B$  is the Boltzmann factor, and  $Z = \sum_N e^{-\beta E_N}$  is the partition function of the gas. We further observe that  $G_{\mathbf{q}}(\omega)$  is nothing but the Fourier transform in time of the density-density correlation function of the gas

$$G_{\mathbf{q}}(t) = \frac{2\pi}{\hbar} \frac{1}{V^2} \langle D_{\mathbf{q}}(t) D_{-\mathbf{q}}(0) \rangle, \quad (22)$$

where

$$\langle \dots \rangle = \text{Tr} \{ \rho_{th} \dots \} \quad (23)$$

stands for trace over  $\rho_{th}$ , the thermal equilibrium density matrix of the reservoir. It is here that the formulation in terms of the second quantized operators comes handy. With the density operator of equation (16), we write

$$\begin{aligned} \langle D_{\mathbf{q}}(t) D_{-\mathbf{q}}(0) \rangle &= \sum_{\mathbf{k}, \mathbf{k}'} \langle a_{\mathbf{k}-\mathbf{q}}^\dagger(t) a_{\mathbf{k}}(t) a_{\mathbf{k}'+\mathbf{q}}^\dagger a_{\mathbf{k}'} \rangle \\ &= \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}})t/\hbar} \langle a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{k}} a_{\mathbf{k}'+\mathbf{q}}^\dagger a_{\mathbf{k}'} \rangle \\ &= \sum_{\mathbf{k}} e^{i(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})t/\hbar} f_{\mathbf{k}-\mathbf{q}} (1 - f_{\mathbf{k}}), \end{aligned} \quad (24)$$

where

$$f_{\mathbf{k}} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} \pm 1} \quad (25)$$

is the particles' distribution function, and  $\mu$  is the chemical potential of the gas. Now, the reservoir correlation, equation (21), can be cast into

$$G_{\mathbf{q}}(\omega) = \frac{2\pi}{\hbar} \frac{1}{V^2} \sum_{\mathbf{k}} f_{\mathbf{k}} (1 - f_{\mathbf{k}+\mathbf{q}}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \hbar\omega). \quad (26)$$

At high temperatures, when  $k_B T > \mu$ , since  $f_{\mathbf{k}} \ll 1$ , the distribution becomes Maxwellian, i.e.,

$$f_{\mathbf{k}} = C e^{-\beta \epsilon_{\mathbf{k}}}, \quad (27)$$

where  $C$  is a normalization constant, to be determined by

$$n_0 = \frac{1}{V} \sum_{\mathbf{k}} f_{\mathbf{k}}. \quad (28)$$

Since the summation over  $\mathbf{k}$  can be transformed into an integral,

$$\frac{1}{V} \sum_{\mathbf{k}} \rightarrow \frac{1}{(2\pi)^3} \int d^3k \quad (29)$$

we end up with

$$C = n_0 \hbar^3 (2\pi\beta/m)^{3/2}. \quad (30)$$

For a gas environment at high temperatures, the correlation function is

$$\begin{aligned} G_{\mathbf{q}}(\omega) &= \frac{2\pi}{\hbar} n_0 \hbar^3 (2\pi\beta/m)^{3/2} \frac{1}{V} \\ &\times \int d^3k e^{-\beta \epsilon_{\mathbf{k}}} \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \hbar\omega) \\ &= \frac{2\pi}{\hbar} \frac{(2\pi)^3}{V} \left( \frac{\beta m}{2\pi \hbar^2 q^2} \right)^{\frac{1}{2}} \\ &\times \exp \left\{ -\frac{\beta \hbar^2}{2m} \left( \frac{m\omega}{\hbar q} - \frac{q}{2} \right)^2 \right\}. \end{aligned} \quad (31)$$

We return now to the atomic matrix elements of equation (17), and write it explicitly as

$$\begin{aligned} \langle m | A_{\mathbf{q}} | n \rangle &= \prod_s \int d^3r_s \Psi_m^* (\{\mathbf{r}_s\}) \\ &\times \sum_{s'} \phi_{s'}(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}_{s'}} \Psi_n (\{\mathbf{r}_s\}). \end{aligned} \quad (32)$$

This can be calculated if the interaction potential  $\phi$ , and the eigen-functions of the atom are known. The transition rate of equation (19) is simply then

$$\Gamma_{n \rightarrow m} = \sum_{\mathbf{q}} |\langle m | A_{\mathbf{q}} | n \rangle|^2 G_{\mathbf{q}}(\omega_{nm}) \quad (n \neq m), \quad (33)$$

where the correlation function of the electron gas is given by either equation (26) or equation (31). Similarly, the adiabatic dephasing rate of equation (5), can be written as

$$(\Gamma_{mn})_{ad} = \frac{1}{2} \Re e \sum_{\mathbf{q}} |\langle m | A_{\mathbf{q}} | m \rangle - \langle n | A_{\mathbf{q}} | n \rangle|^2 G_{\mathbf{q}}(0). \quad (34)$$

Equation (33), and equation (34), are our general results for the calculations of the evolution rates.

## 2.2 Evolution rates — hydrogen-like atom in electron gas

We now use the results of the previous general study to investigate an atomic radiating system in a hot plasma, where the very hot electron gas plays a dominant role, as the reservoir. In order to actually calculate the evolution rates, the atomic wave functions must be known, and the interaction potential between the atom and the electrons has to be specified. We assume that:

1. the atomic system is hydrogen-like with a single atomic electron,
2. the interaction is Coulombic,
3. the atom is stationary (this was implicitly assumed in the previous section).

Since the atom is stationary, the position of the nucleus of the atom can be chosen to be at  $\mathbf{R} = 0$ . Therefore, the interaction Hamiltonian of equation (10) can be written as

$$H_{AB} = \sum_i e^2 \left( \frac{1}{|\mathbf{r}_i - \mathbf{r}_s|} - \frac{Z_e}{|\mathbf{r}_i|} \right), \quad (35)$$

where  $-e$  is the charge of the electron,  $Z_e$  is the nucleus charge, and  $\mathbf{r}_s$  is the radius vector of the electron, measured from the static nucleus. We now represent the interaction Hamiltonian by a sum of products of atomic operators  $A_{\mathbf{q}}$  and reservoir operators  $B_{\mathbf{q}}$  (see Eq. (1)). According to equations (13), (17) and (18), the atomic operator is:

$$A_{\mathbf{q}} = \Phi_{\mathbf{q}}(-Z_e + e^{i\mathbf{q}\cdot\mathbf{r}_s}), \quad (36)$$

where  $\Phi_{\mathbf{q}}$  is the Fourier transform of the Coulomb potential:

$$\Phi_{\mathbf{q}} = \Phi_q = \frac{4\pi e^2}{q^2}. \quad (37)$$

At this point we wish to point out that the positive background of the ions of the plasma provides a screening mechanism, and the bare Coulomb potential of equation (37) can be replaced, when a cutoff is called for, by a statically screened potential

$$\Phi_q = \frac{4\pi e^2}{q^2 + q_D^2}, \quad (38)$$

where  $q_D^2$  is the Debye screening. The reservoir operators

$$B_{\mathbf{q}} = \frac{1}{V} \sum_{\mathbf{k}} a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{k}}, \quad (39)$$

are then expressed in terms of the electron gas creation and annihilation operators. Having determined the above operators we proceed with a derivation of the transition rates, and then calculate the dephasing rates.

### 2.2.1 Transition rates

To find the transition rate, as given by equation (33), we first turn to the atomic contribution, namely to the off-diagonal matrix element  $\langle m|A_{\mathbf{q}}|n\rangle$ . In the present case

equation (32) is simplified, with equation (36), into

$$\langle m|A_{\mathbf{q}}|n\rangle = \Phi_q \int d^3r \Psi_m^*(\mathbf{r})(-Z_e + e^{i\mathbf{q}\cdot\mathbf{r}})\Psi_n(\mathbf{r}), \quad (40)$$

where  $\mathbf{r}$  replaces  $\mathbf{r}_s$  for brevity. Since the states  $|n\rangle$  and  $|m\rangle$  are orthogonal, the first term in the integral, i.e., the nucleus contribution, vanishes. At this point we have to decide on the atomic wave functions, which we choose to be those of the ground state  $|m\rangle = |g\rangle = (1, 0, 0)$  and the first excited state  $|n\rangle = |e\rangle = (2, 1, 0)$  of the hydrogen-like atom, i.e.,

$$\begin{aligned} \Psi_g(\mathbf{r}) &= \frac{1}{\sqrt{4\pi}} 2 \left( \frac{Z_e}{a_0} \right)^{\frac{3}{2}} e^{-Z_e r/a_0} \\ \Psi_e(\mathbf{r}) &= \sqrt{\frac{1}{4\pi}} \left( \frac{Z_e}{2a_0} \right)^{\frac{3}{2}} \frac{Z_e}{a_0} \mathbf{r} \cdot \mathbf{u} e^{-Z_e r/2a_0}. \end{aligned} \quad (41)$$

Here  $a_0 = \hbar^2/me^2$  is the Bohr radius, and  $\mathbf{u}$  is an arbitrary unit vector related to the quantization axis of the hydrogen atom. Substituting these wave function into equation (40) we have

$$\begin{aligned} \langle e|A_{\mathbf{q}}|g\rangle &= \Phi_q \frac{1}{4\sqrt{2}\pi} \left( \frac{Z_e}{a_0} \right)^4 \\ &\quad \times \int d^3r e^{-3Z_e r/2a_0} \mathbf{r} \cdot \mathbf{u} e^{i\mathbf{q}\cdot\mathbf{r}}, \end{aligned} \quad (42)$$

or explicitly

$$\langle e|A_{\mathbf{q}}|g\rangle = i6\sqrt{2} \left( \frac{2}{3} \right)^6 \left( \frac{a_0}{Z_e} \right) \Phi_q \frac{\mathbf{q} \cdot \mathbf{u}}{\left[ 1 + (2a_0 q/3Z_e)^2 \right]^3}. \quad (43)$$

Substituting equation (43) for the matrix element, and equation (31) for the reservoir correlation function in equation (33) for the transition rate, we find

$$\begin{aligned} \Gamma_{e \rightarrow g} &= \frac{2^{18} \sqrt{2\pi}}{3^{11}} n_0 \sqrt{m\beta} \frac{e^4}{\hbar^2} \left( \frac{a_0}{Z_e} \right)^2 \\ &\quad \times \int_0^\infty dq \frac{1}{q} \left[ 1 + \left( \frac{2a_0 q}{3Z_e} \right)^2 \right]^{-6} \\ &\quad \times \exp \left\{ -\frac{\beta \hbar^2}{2m} \left( \frac{m\omega}{\hbar q} - \frac{q}{2} \right)^2 \right\}, \end{aligned} \quad (44)$$

where  $\omega = \omega_{eg}$ . Equation (44) is our general result for the exact transition rate of a hydrogen-like atom from level  $(2, 1, 0)$  to level  $(1, 0, 0)$  due to Coulomb interaction with an electron reservoir. The single integral over  $q$  can be evaluated numerically; e.g., for a plasma with electron gas at temperature  $k_B T = 150$  [eV] and density  $n_0 = 10^{18}$  [cm $^{-3}$ ], the transition rate is  $\Gamma_{e \rightarrow g} = 7.9 \times 10^8$  [s $^{-1}$ ].

To gain some more insight, we attempt an analytic expression for the transition rate when the dipole approximation is valid. Since we are interested in a regime relevant to the Z-Pinch process, we assume the electrons in

the plasma to be “fast”, namely having very small momentum exchange with the atom’s electron, i.e., we consider the limit where  $q(a_0/Z_e) \ll 1$ . This is the dipole approximation limit, when the inverse wave vector,  $2\pi/q$ , which is involved in the interaction process is much larger than the atomic radius  $a_0/Z_e$ . Notice that this small dipole limit is not the same as that which occurs when an atom is embedded in a radiation reservoir, where  $2\pi/q$  is rather the radiation wave length. We expand the denominator of equation (44), and write

$$\left[1 + \left(\frac{2a_0q}{3Z_e}\right)^2\right]^{-6} = 1 - 6\left(\frac{2a_0q}{3Z_e}\right)^2 + O\left(\left(\frac{a_0q}{Z_e}\right)^4\right). \quad (45)$$

The first term in this expansion yields the dipole approximation. Substituting this term into equation (44) gives the result:

$$\Gamma_{e \rightarrow g} \simeq 3.71 n_0 \sqrt{m\beta} \frac{e^4}{\hbar^2} \left(\frac{a_0}{Z_e}\right)^2 e^{\beta\hbar\omega/2} K_0\left(\frac{\beta\hbar\omega}{2}\right), \quad (46)$$

where  $K_0(x)$  is the modified Bessel function of order 0. A numerical verification shows that the dipole approximation differs from the exact solution (for the parameters given above) by 6%. If the next term of the expansion is used, the result agrees with the exact calculation to within an error of 1%. Our result, equation (46) of the dipole approximation, agrees with results found in the literature (e.g., [21]).

### 2.2.2 Dephasing rate

Following the same procedure as in the calculation of the transition rate, we now calculate the dephasing rate. This is done again in our particular model, for the levels  $|g\rangle = (1, 0, 0)$  and  $|e\rangle = (2, 1, 0)$  of a hydrogen-like atom. Our derivation uses equation (34) as a starting point. Note that by dephasing rate we mean only the adiabatic part, since the non-adiabatic component, equation (4), can be readily calculated from the transition rate, obtained in the previous section.

In this case only diagonal matrix elements of the atomic operator  $A_{\mathbf{q}}$  play a role. For the ground state, using equation (36), we write

$$\langle g|A_{\mathbf{q}}|g\rangle = \Phi_q \int d^3r \Psi_g^*(\mathbf{r})(-Z_e + e^{i\mathbf{q}\cdot\mathbf{r}})\Psi_g(\mathbf{r}), \quad (47)$$

and with the first wave-function of equation (41) we obtain two terms,

$$\langle g|A_{\mathbf{q}}|g\rangle_1 = -Z_e\Phi_q, \quad (48)$$

and

$$\langle g|A_{\mathbf{q}}|g\rangle_2 = \Phi_q \left[1 + \left(\frac{a_0q}{2Z_e}\right)^2\right]^{-2}. \quad (49)$$

Next, for the excited state

$$\langle e|A_{\mathbf{q}}|e\rangle = \Phi_q \int d^3r \Psi_e^*(\mathbf{r})(-Z_e + e^{i\mathbf{q}\cdot\mathbf{r}})\Psi_e(\mathbf{r}), \quad (50)$$

again we obtain two terms, the first one

$$\langle e|A_{\mathbf{q}}|e\rangle_1 = -Z_e\Phi_q \quad (51)$$

is the same as equation (48), while the second one

$$\langle e|A_{\mathbf{q}}|e\rangle_2 = \Phi_q \frac{1}{4\pi} \left(\frac{Z_e}{2a_0}\right)^3 \left(\frac{Z_e}{a_0}\right)^2 \times \int d^3r (\mathbf{r} \cdot \mathbf{u})^2 e^{-Z_e r/a_0} e^{i\mathbf{q}\cdot\mathbf{r}}, \quad (52)$$

yields

$$\langle e|A_{\mathbf{q}}|e\rangle_2 = \frac{\Phi_q}{\left[1 + \left(\frac{a_0q}{Z_e}\right)^2\right]^3} \left[1 - 6 \cos^2 \chi \frac{\left(\frac{a_0q}{Z_e}\right)^2}{1 + \left(\frac{a_0q}{Z_e}\right)^2}\right] \quad (53)$$

where  $\cos \chi = \mathbf{q} \cdot \mathbf{u}/q$ .

We return now to equation (34) and first observe that the contribution of the nucleus vanishes, since equation (48) is canceled by equation (51). Next, from equation (31) we get

$$G_{\mathbf{q}}(0) = \frac{2\pi}{\hbar} \frac{(2\pi)^3}{V} \left(\frac{\beta m}{2\pi\hbar^2 q^2}\right)^{\frac{1}{2}} e^{-\beta\hbar^2 q^2/8m}, \quad (54)$$

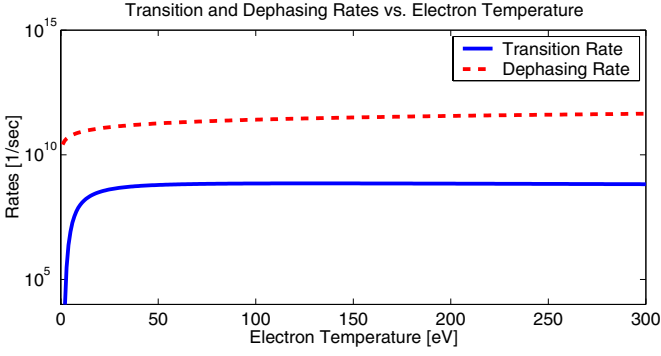
and the dephasing rate is

$$(\Gamma_{eg})_{ad} = \frac{\pi}{\hbar} n_0 \left(\frac{\beta m}{2\pi\hbar^2}\right)^{\frac{1}{2}} \int d^3q \Phi_q^2 \frac{1}{q} e^{-\beta\hbar^2 q^2/8m} \times \left\{ \frac{\left[1 - 6 \cos^2 \chi \frac{\left(\frac{a_0q}{Z_e}\right)^2}{1 + \left(\frac{a_0q}{Z_e}\right)^2}\right]}{\left[1 + \left(\frac{a_0q}{Z_e}\right)^2\right]^3} - \frac{1}{\left[1 + \left(\frac{a_0q}{Z_e}\right)^2\right]^2} \right\}. \quad (55)$$

Equation (55) is our general result for the exact dephasing rate of a hydrogen-like atom from level (2, 1, 0) to level (1, 0, 0) due to Coulomb interaction with an electron reservoir. The integration over the spherical angle can be easily carried out, and we are left with a single integral over  $q$ , which can be evaluated numerically. E.g., for plasma with an electron gas at temperature  $k_B T = 150$  [eV] and density  $n_0 = 10^{18}$  [cm<sup>-3</sup>], the dephasing rate is  $(\Gamma_{eg})_{ad} = 8.4 \times 10^{10}$  [s<sup>-1</sup>]. Note that this rate is 2 orders of magnitude larger than the transition rate, calculated for the same parameters. In contrast we observe that in the case of an interaction with a radiation reservoir (e.g. [6]), the adiabatic dephasing vanishes, and thus the dephasing and the transition rates are of the same order of magnitude. The electron reservoir induces rather significant dephasing.

We now attempt to calculate equation (55) analytically, using a power series expansion in the presumably small parameter  $(a_0/Z_e)q$ , as was done previously for the transition rate. The dominant contribution comes from the second order term in  $(a_0/Z_e)q$ , and yields

$$(\Gamma_{eg})_{ad} = 2.33 \times 10^5 n_0 \sqrt{m\beta} \left(\frac{e^4 a_0^2}{\hbar^2 Z_e^2}\right) \left(\frac{m a_0^2}{\beta \hbar^2 Z_e^2}\right), \quad (56)$$



**Fig. 1.** Transition and dephasing rates (in logarithmic scale) vs. electron temperature. The rates are given by equations (46) and (56), describing the leading term. The figure shows that the rates are nearly constant for temperatures ranging from 0 to 300 [eV]. The dephasing rate is two orders of magnitude larger than the transition rate.

i.e. it is second order in the dipole approximation. Again we find that this dephasing rate is about two orders of magnitude larger than the dipole approximation result, equation (46), for the transition rate. Comparing equation (56) to equation (46), we see that in both cases the dependence on  $n_0$  is linear. The dependence on  $T$  is less obvious, although a numerical check shows that for a wide range of temperatures the rates change little; they are determined mainly by the atomic parameters. This is demonstrated in Figure 1. It can be deduced that for our problem of a capillary discharge X-ray laser, the adiabatic dephasing rate due to the electron reservoir is much larger than the transition rate, for the entire relevant temperature range. This is true for a variety of physical problems operating in similar regimes as well.

### 3 Dependence of evolution rates on atomic center of mass motion

In this section we study the evolution rates, taking into account the motion of the center of mass of the radiating atom, which was previously assumed to be infinitely heavy<sup>2</sup>. We incorporate the center of mass momentum as an additional variable of the density matrix, and recalculate the rates by eliminating this extra degree of freedom. An element of the extended atomic density matrix will be written as  $\sigma_{m\mathbf{P}',n\mathbf{P}}$ , between the atomic state  $m$  with momentum  $\mathbf{P}'$  and the atomic state  $n$  with momentum  $\mathbf{P}$ . The motion of the nucleus of mass  $M$ , is described by the Hamiltonian  $H = P^2/2M$ , and the eigenfunctions

$$\phi_{\mathbf{P}}(\mathbf{R}) = \frac{1}{\sqrt{V}} e^{i\mathbf{P}\cdot\mathbf{R}/\hbar}, \quad (57)$$

<sup>2</sup> Our treatment does not deal with the direct effect of the center-of-mass motion on the radiation. This effect, called the Doppler effect, is significant, and should be included in a complete description of the emission spectrum. The Doppler effect is discussed in [23], for example.

where  $\mathbf{R}$  is the position of the center of mass. Since the nucleus is indeed heavy compared to the particles of the reservoir, i.e. the electrons, we find that the effect of its movement can be written as small corrections to the results of the previous sections.

We start by calculating the transition rates for an ion in an electron reservoir. The Hamiltonian for the problem, including the center of mass motion of the ion, is:

$$H = \underbrace{\frac{P^2}{2M} + \frac{p_s^2}{2m} - \frac{Z_e e^2}{|\mathbf{r}_s - \mathbf{R}|}}_{H_A} + \underbrace{\sum_i \frac{p_i^2}{2m}}_{H_B} + \underbrace{\sum_i \left[ \frac{e^2}{|\mathbf{r}_s - \mathbf{r}_i|} - \frac{Z_e e^2}{|\mathbf{r}_i - \mathbf{R}|} \right]}_{H_{AB}} \quad (58)$$

where again the  $s$  subscript denotes a bound electron, and the  $i$  subscript — a reservoir electron. Introducing the Fourier transform in space, we rewrite the interaction part of the Hamiltonian as:

$$H_{AB} = \frac{1}{V} \sum_q \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i} \Phi_q [e^{i\mathbf{q}\cdot\mathbf{r}_s} - Z_e e^{i\mathbf{q}\cdot\mathbf{R}}] \quad (59)$$

where  $\Phi_q$  is the Fourier transform of the interaction potential (Eq. (37)). Following the notation of the previous section (Eq. (4)), we express the transition rate as

$$\Gamma_{m\mathbf{P}' \rightarrow n\mathbf{P}} = \sum_q G_q(\omega, \mathbf{P}, \mathbf{P}') |\langle n, \mathbf{P} | A_q | m, \mathbf{P}' \rangle|^2, \quad (60)$$

where  $\omega$  is given by the energy difference between the levels  $m$  and  $n$ , i.e.  $\hbar\omega \equiv \hbar\omega_m - \hbar\omega_n$ . The reservoir correlation function of equation (31) is then

$$G_q(\omega, \mathbf{P}, \mathbf{P}') = \frac{2\pi}{\hbar V} \frac{C}{(2\pi)^3} \int d^3\mathbf{k} e^{-\beta\varepsilon_k} \times \delta\left(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \hbar\omega + \frac{P^2}{2M} - \frac{P'^2}{2M}\right), \quad (61)$$

where the normalization constant  $C$  is given by equation (30). The atomic operator  $A_q$  now depends on the radius vector of the atomic nucleus  $R$  through the term  $e^{i\mathbf{q}\cdot\mathbf{R}}$ , in contrast to equation (36). This affects only the center of mass degrees of freedom, namely

$$\langle n, \mathbf{P} | A_q | m, \mathbf{P}' \rangle = \langle n | A_q | m \rangle_0 \int d^3\mathbf{R} \Psi_{\mathbf{P}}^* e^{i\mathbf{q}\cdot\mathbf{R}} \Psi_{\mathbf{P}'}, \quad (62)$$

where  $\langle n | A_q | m \rangle_0$  is the atomic matrix element for a stationary atom. Remember that the contribution of the nucleus term of the atomic operator vanishes in the derivation of the evolution rates. The integration of equation (62) yields

$$\langle n, \mathbf{P} | A_q | m, \mathbf{P}' \rangle = \langle n | A_q | m \rangle_0 \delta_{\mathbf{P}', \mathbf{P} - \hbar\mathbf{q}}. \quad (63)$$

Let us focus first on the calculation of the transition rate. For simplicity, we take the atomic operator  $A_q$  to first

order only, and encapsulate it as  $A_q = \Phi_q q x_{mn} \delta_{\mathbf{P}-\hbar\mathbf{q}, \mathbf{P}'}$ . using equations (60–63) we write

$$\Gamma_{m\mathbf{P}' \rightarrow n\mathbf{P}} = \frac{2\pi}{\hbar} \frac{C}{(2\pi)^6} \int d^3\mathbf{q} \Phi_q^2 \delta_{\mathbf{P}-\hbar\mathbf{q}, \mathbf{P}'}^2 q^2 x_{mn}^2 \int d^3\mathbf{k} e^{-\beta\varepsilon_k} \times \delta\left(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_k - \hbar\omega + \frac{P^2}{2M} - \frac{P'^2}{2M}\right). \quad (64)$$

We use  $\delta_{\mathbf{P}-\hbar\mathbf{q}, \mathbf{P}'}$  to eliminate the final state  $\mathbf{P}$  and write

$$\Gamma_{m\mathbf{P}' \rightarrow n} = \frac{2\pi}{\hbar} \frac{C}{(2\pi)^6} \int d^3\mathbf{q} \Phi_q^2 q^2 x_{mn}^2 I, \quad (65)$$

where

$$I = 2\pi \int_0^\infty dk k^2 e^{-\beta\varepsilon_k} \frac{m}{\hbar^2 k q} \int_{-\frac{\hbar^2 k q}{m}}^{\frac{\hbar^2 k q}{m}} dE \times \delta\left(E + \frac{\hbar^2 q^2}{2m} - \hbar\omega + \frac{\hbar q P' y}{M} + \frac{\hbar^2 q^2}{2M}\right) \quad (66)$$

with  $x = \cos(\mathbf{k} \cdot \mathbf{q}/|k||q|)$ , and  $y = \cos(\mathbf{q} \cdot \mathbf{P}'/|q||P'|)$ . To proceed we observe that the momentum terms, with  $1/M$ , in the delta function are small compared to the original frequency-dependent terms, and expand the  $\delta$ -function up to second order as

$$\begin{aligned} & \delta\left(E + \frac{\hbar^2 q^2}{2m} - \hbar\omega + \frac{\hbar q P' y}{M} + \frac{\hbar^2 q^2}{2M}\right) \\ & \simeq \delta\left(E + \frac{\hbar^2 q^2}{2m} - \hbar\omega\right) \\ & - \left(\frac{\hbar q P' y}{M} + \frac{\hbar^2 q^2}{2M}\right) \delta'\left(E + \frac{\hbar^2 q^2}{2m} - \hbar\omega\right) \\ & + \frac{1}{2} \left(\frac{\hbar q P' y}{M} + \frac{\hbar^2 q^2}{2M}\right)^2 \delta''\left(E + \frac{\hbar^2 q^2}{2m} - \hbar\omega\right). \quad (67) \end{aligned}$$

We readily see that the zeroth order term yields the original transition rate, without center of mass motion. After some algebra, we find the correction due to the first order term to be

$$\Gamma_{m \rightarrow n}^{(1)} = \Gamma_0 \left(\frac{m}{M} \beta \hbar \omega\right) \left[ \frac{K_1\left(\frac{\beta \hbar \omega}{2}\right)}{K_0\left(\frac{\beta \hbar \omega}{2}\right)} - 1 \right], \quad (68)$$

where  $K_i(z)$  is the  $i$ th order of the modified Bessel function. The first order correction is therefore small, of the order of  $(m/M) \beta \hbar \omega$ . However, since the dependence on  $\mathbf{P}'$  vanished in the first order, we calculate the second order correction as well, and find

$$\begin{aligned} \Gamma_{m \rightarrow n}^{(2)} & \simeq \Gamma_0 \frac{m}{M} \beta \hbar \omega \\ & \times \left[ K_0\left(\frac{\beta \hbar \omega}{2}\right) + 2 \left(\frac{1}{\beta \hbar \omega}\right) K_0\left(\frac{\beta \hbar \omega}{2}\right) \right]. \quad (69) \end{aligned}$$

We conclude that the contribution to the transition rate of the motion of the center of mass, due to the interaction

with the electron reservoir, is dominantly of order  $m/M$ . This factor, which is  $1/(10^3 A)$  for an atom with atomic number  $A$ , is indeed very small. In a similar manner we treat the dephasing rate, and reach the same conclusion. We can therefore conclude that the corrections due to the center of mass motion are negligible for all evolution rates.

## 4 Dephasing rate in a multi-level atom

In the previous sections, transition and dephasing rates were calculated for the interaction of an atomic system with an electron reservoir. So far we have concentrated on the lasing pair of levels of the atomic system, and on the adiabatic dephasing rate of their coherence. In this section we will extend our investigation and consider how the presence of other levels of the atomic system affects the evolution rates of this lasing pair. Our definitions of the different rates must be revised due to the presence of other levels. Resorting to the nomenclature of laser theory, we will focus on the two lasing levels, deriving their dephasing rate, referred to as  $1/T_2$ , and the decay rate of their population difference, referred to as  $1/T_1$ . The ratio between these two rates is important in laser theory, affecting the gain and the characteristics of the laser.

The dephasing rate between the two lasing levels is increased due to the transitions to the non-lasing states, as indicated by equation (4). This is important since in certain cases this effect can be of the same order of, or even larger than, that of the adiabatic dephasing. A simple example of this is the Ne-like capillary discharge X-ray laser. This laser can be described as a three-level atom, the two upper levels being the lasing levels. In this case the lower lasing level is strongly coupled to the lowest level — the ground state — through the radiation reservoir. Therefore, the transitions from the lower lasing level to the ground state, causing non-adiabatic dephasing, are significant for the dephasing rate of the coherence of the laser. The latter is then to be compared with the decay rate of the population difference of the lasing levels. This decay rate, and not the transition rate, comes into play in the semi-classical model of the laser [11].

In dealing with many atomic levels interacting through a reservoir, we assume that all transition rates are known, since they can be calculated using the results of Section 2. Notice that the non-adiabatic dephasing rate contribution to  $1/T_2$  is given directly by equation (4) in terms of the transition rates. We are thus left with the problem of obtaining the rate  $1/T_1$ . Recall that the general rate equation for the populations,  $P_n$ , of the  $n$ th state is expressed as

$$\frac{d}{dt} P_n = \sum_{m \neq n} (P_m \Gamma_{m \rightarrow n} - P_n \Gamma_{n \rightarrow m}), \quad (70)$$

in terms of the transition rates. To describe the procedure of identifying the decay rates we first demonstrate it for a two-level atom, and then indicate how to extend it for a three-level atom.

We begin with a two-level system, denoting the levels as 1 and 2, and the transition rates between them as  $\Gamma_{1 \rightarrow 2}$



and  $\Gamma_{2 \rightarrow 1}$ , and writing equation (70) as

$$\begin{aligned}\dot{P}_1 &= -\Gamma_{1 \rightarrow 2}P_1 + \Gamma_{2 \rightarrow 1}P_2 \\ \dot{P}_2 &= \Gamma_{1 \rightarrow 2}P_1 - \Gamma_{2 \rightarrow 1}P_2.\end{aligned}\quad (71)$$

The symmetry of the transition rates in equation (71) results from the conservation of total population, i.e.,  $P_1 + P_2 = 1$ . Defining the population difference by  $D = P_2 - P_1$ , we get its evolution equation:

$$\begin{aligned}\dot{D} &= (\Gamma_{1 \rightarrow 2} - \Gamma_{2 \rightarrow 1}) - (\Gamma_{1 \rightarrow 2} + \Gamma_{2 \rightarrow 1})D \\ &\equiv -\Gamma_1 (D - D^0),\end{aligned}\quad (72)$$

where the steady state population difference is

$$D^0 \equiv \frac{\Gamma_{1 \rightarrow 2} - \Gamma_{2 \rightarrow 1}}{\Gamma_{1 \rightarrow 2} + \Gamma_{2 \rightarrow 1}},\quad (73)$$

and its rate of change in time is

$$\Gamma_1 \equiv (\Gamma_{1 \rightarrow 2} + \Gamma_{2 \rightarrow 1}).\quad (74)$$

Thus the inverse life time of the population difference for a two-level system is  $1/T_1 = \Gamma_1$ . Recalling the expression for the non-adiabatic dephasing rate,  $\Gamma_2 = 1/T_2$ , from equation (4),

$$\Gamma_2 = \frac{1}{2}(\Gamma_{1 \rightarrow 2} + \Gamma_{2 \rightarrow 1}),\quad (75)$$

we find that

$$T_2 = 2T_1.\quad (76)$$

We observe that for a two-level system, the non-adiabatic dephasing rate is smaller than the decay rate of the population difference. In passing we wish to remark that for a two level atom in a radiation reservoir, equation (76) holds, since there is no dephasing by adiabatic processes. Therefore, for a system of this kind, non-adiabatic processes of dephasing make the dominant contribution to  $1/T_2$ .

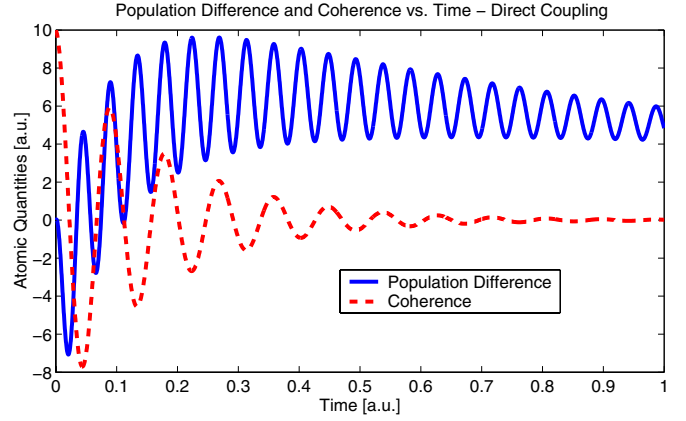
We turn on now to a three-level system, and write equation (70) in matrix form. For  $n, m = 1, 2, 3$ , we express

$$\frac{d}{dt}P_n = \sum_m W_{nm}P_m,$$

where the transition matrix is

$$W = \begin{bmatrix} -(\Gamma_{1 \rightarrow 2} + \Gamma_{1 \rightarrow 3}) & \Gamma_{2 \rightarrow 1} & \Gamma_{3 \rightarrow 1} \\ \Gamma_{1 \rightarrow 2} & -(\Gamma_{2 \rightarrow 1} + \Gamma_{2 \rightarrow 3}) & \Gamma_{3 \rightarrow 2} \\ \Gamma_{1 \rightarrow 3} & \Gamma_{2 \rightarrow 3} & -(\Gamma_{3 \rightarrow 1} + \Gamma_{3 \rightarrow 2}) \end{bmatrix}.\quad (77)$$

The eigenvalues of  $W$  are the exponential decay rates of the atomic populations. It is clear that one of these eigenvalues is zero, giving the steady-state solution, and the slower of the other two rates is the decay rate of the population difference,  $\Gamma_1$ . In general the expression for  $\Gamma_1$  is



**Fig. 2.** Population difference and coherence vs. time in a three-level atom. The figure depicts a case in which the coherence decays quickly, while the population difference rises abruptly, and then decays slowly. The rates chosen for this example were  $\Gamma_{1 \rightarrow 3} = \Gamma_{3 \rightarrow 1} = 0$ ,  $\Gamma_{1 \rightarrow 2} = \Gamma_{2 \rightarrow 1} = 100$ ,  $\Gamma_{2 \rightarrow 3} = \Gamma_{3 \rightarrow 2} = 1$ .

quite complicated, and it depends on the various transition rates between the three levels. Therefore, the significance of the non-adiabatic dephasing rate compared to the population difference decay rate varies according to the relative magnitudes of these transition rates. An interesting case is when  $\Gamma_{1 \rightarrow 3}$ , and  $\Gamma_{3 \rightarrow 1}$ , are completely negligible, while  $\Gamma_{1 \rightarrow 2}, \Gamma_{2 \rightarrow 1} \gg \Gamma_{2 \rightarrow 3}, \Gamma_{3 \rightarrow 2}$ . Here we find that  $\Gamma_1/\Gamma_2 \propto \Gamma_{2 \rightarrow 2}/\Gamma_{1 \rightarrow 2} \ll 1$ , i.e. non-adiabatic dephasing is significant. This effect is presented in Figure 2.

The derivation given here consists of a simple, yet comprehensive method for calculating the rates  $1/T_1$  and  $1/T_2$ , which can be applied to similar systems. We emphasize that, in the context of a complete description of dephasing of an atomic system, the non-adiabatic dephasing rate must be calculated, since for certain parameters of a physical problem, it can be significant.

## 5 Summary and conclusions

In this paper, we have developed a *Hamiltonian-based* model for describing the evolution of a small atomic system interacting with hot plasma. The motivation for our work stems from X-ray laser research, in which the gain medium of the laser is usually a small part of a hot, dense plasma. Understanding the evolution of atomic states due to such interactions is relevant to other physical problems as well, such as emissions in stellar configurations.

We define our problem in terms of different interactions between the atomic system and electron, ion and radiation reservoirs, which model the plasma. Since treatment of a radiation reservoir is given in the literature (e.g. [6]), and since the effect of the ion reservoir is negligible, we focus on interaction with the electron reservoir.

In our work we use the density matrix method to derive the evolution rates, describing the reservoir states through second quantization. These techniques enable us to derive a *general* formulation, and verify it against results appearing in literature. This formulation is extensible to different

reservoirs, in similar physical setups. In contrast to previous work, this approach does not rely on the notions of scattering theory, and is free of the limitations therein. Therefore, our research provides added insight as to the differences between reservoirs, and their associated interactions.

Our description of the interaction with an electron reservoir yields exact expressions for the transition rate (Eq. (44)) and for the adiabatic dephasing rate (Eq. (55)). We find that the adiabatic dephasing rate component does not vanish (as in the case of a radiation reservoir), since the interaction potential is composed of terms in every order of the multipole expansion. We then derive approximate expressions for the rates to the first contributing term (Eqs. (46), (56)). Studying these simpler analytic expressions, we learn that the adiabatic dephasing rate is much larger than the transition rate, and therefore significant for understanding the radiation emitted by the atom.

We also check the effect of motion of the atomic center of mass, which is responsible for the Doppler phenomenon, on the rates calculated earlier. We show that the correction to the rates is negligible, following a derivation using a power series expansion (Eqs. (68), (69)).

We then explore the effect of a multitude of energy levels on the dephasing mechanisms. This more complicated system requires that we compare the dephasing rate of two levels with the decay rate of their population difference, which is the relevant quantity (instead of the transition rate). We derive the relationships for this effect for the case of a two-level atom and for the case of a three-level atom, and find that certain parameters of the system could enhance the relative significance of non-adiabatic dephasing.

In conclusion, this research has focused on deriving *generalized* relationships for the evolution rates of an atomic system interacting with plasma, which is modeled using an electron reservoir. Employing the density matrix formalism, we were able to derive the master equation and all the relevant rates based on an *integral Hamiltonian* model. Our formulations for the transition rates are validated by partial results found in the literature. We also show that beyond familiar Doppler dephasing, adiabatic dephasing caused by the electron reservoir, and non-adiabatic dephasing in the case of a many-level atom, could be significant.

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