Modeling Electromagnetic Interactions in Quantized Electronic Systems

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1 Introduction

We have been developing a density-matrix approach [1] that provides a convenient framework for the systematic computer simulation of the electromagnetic spectra emitted or absorbed by a quantized electronic system. A quantized electronic system is characterized by discrete energy-level structures, which correspond to bound or quasi-bound states, and by radiative transitions that produce line-like spectral features, which are advantageous in the development of sources of coherent electromagnetic radiation.

Extensive applications of our density-matrix approach have been made to radiative transitions of many-electron atomic systems in strong fields [2, 3], and detailed spectral simulations have been provided for K-alpha dielectronic satellite spectra of highly charged atomic ions in electron-ion beam interactions [4] and in high-temperature plasmas [5]. In these simulations, it has been necessary to assemble a very large data base of atomic energy levels and transition probabilities. We have also been interested in applications to radiation processes involving energetic electron beams propagating in strong electric and magnetic fields, as in free-electron lasers and electron cyclotron masers or gyrotrons, and in crystal fields, giving rise to electron channeling radiation and coherent bremsstrahlung [6]. Currently, we are adapting our density-matrix approach to coherent electromagnetic interactions in low-dimensional semiconductor microstructures [7], such as quantum wells, quantum wires, and quantum dots. These structures have been referred to as quantum-confinement systems, because they can give rise to discrete or quasi-discrete levels and to radiative transitions that are closely analogous to the spectral-line transitions in atomic systems. In contrast to natural atomic systems, which may be treated as identical, the quantum dots that are often referred to as "artificial atoms" may occur in arrays, and their geometric and physical properties may vary in a random manner. Consequently, our microscopic description is expected to be most appropriate for the investigation of the properties of a single microstructure, where the homogeneous line-broadening mechanisms and elementary relaxation processes may be examined.

The numerous device applications of the electromagnetic processes of interest include laser systems, electro-optical components, optical communications technologies, and radiation detectors. New quantum-optics applications include quantum computing, coherent control, and quantum cryptography. In addition, this fundamental study forms the basis for the spectroscopic investigation of basic material properties and interactions.

2 Density-Matrix Organization of the Spectral Simulation

The starting point for a detailed spectral simulation should be a realistic determination of the quantized electronic structure for the single-electron or many-electron subsystem of interest. The complete spectrum of electronic states may include discrete bound states, continuum states, and quasi-bound states or autoionization resonances. These electronic states may be taken to be eigenstates of a Hamiltonian in the presence of an external (classical) electric or magnetic field or an intemal crystal field that can be represented by a local potential function. The correct treatment of coherent electromagnetic interactions usually involves the self-consistent determination of the radiation fields, as solutions of the coupled dynamical equations governing the interacting quantized electronic subsystem and the electromagnetic field.

The effects of many-particle interactions can be treated as self-energy corrections to the single-particle energy levels. In the description of many-electron atomic systems, the starting point is usually a many-electron approximation, which must be systematically improved. In the treatment of electrons (or holes) in ideal crystals or in semiconductor microstructures, the initial single-particle description must also be systematically improved to take into account the effects of the electrostatic interaction between charged particles, which are referred to as correlation effects. The inclusion of these effects leads to dielectric screening and to band-gap renormalization. The effects of lattice vibrations may be described, within the framework of many-body quantum field theory, in terms of electron-phonon collisional interactions.

The total probabilities for the various radiative transitions can be evaluated using the familiar Fermi Golden-Rule formula, which is obtained from the lowest-order perturbation theory describing the interaction of the electronic subsystem of interest with the quantized electromagnetic field. The familiar radiation parameters include the (Einstein) spontaneous emission rates and the cross sections for the induced emission and absorption processes. In order to describe the spectral line shapes, it is necessary to employ a high-order, non-perturbative description of the interaction of the electronic system with the quantized electromagnetic field and with the multitude of perturbing particles or quasi-particles. In order to accomplish this objective, it is necessary to adopt a quantum statistical description of the interaction of electromagnetic radiation with the charged particles.

A complete non-perturbative statistical description of the interaction between the quantized electronic subsystem of interest and the quantized electromagnetic field, as well as its interaction (or entanglement) with a much larger quantum system representing the surrounding environment, is provided by the density-matrix approach. In the time domain, the equation of motion for the density operator representing the combined, enlarged system provides the starting point for the general quantum dynamical description. It is often desirable to introduce a transformation to the frequency domain, in which the basic quantity is the Liouville-space resolvent operator. In order to obtain a practical formulation, it is necessary to introduce reduced density-matrix descriptions, in which the interactions of the subsystem of interest with the environment are treated stochastically, as collisional and radiative relaxation processes. In this manner, reduced density operators are defined for the electronic subsystem and for the electromagnetic radiation field. If coherent interactions are of interest, the reduced system must be defined to include the coherently coupled subsystems.

Our density-matrix description [1] may be viewed as a comprehensive framework for the systematic organization of the basic collisional-interaction and radiation-transition data. In order to obtain the electronic-level populations from the traditional data set of transition probabilities and cross sections, it is necessary to simplify the equations of motion for the reduced density

operators. The Markov or short-memory-time approximation leads to the conventional rate or Master equations for the electronic-level populations, together with the electronic-state coherences. In the case of free or quasi-free particles, non-equilibrium distribution functions can be determined. A separate reduced density-matrix equation for the radiation field must be included in order to provide a self-constant treatment of the non-linear behavior that is characteristic of coherent electromagnetic processes.

In the frequency-domain formulation of the density-matrix description, it is convenient to introduce a generalized Fermi Golden-Rule formula for the evaluation of the spontaneous radiative emission rate, as well as for the various cross sections of interest. This formula is expressed in terms of the initial-state density operator for the electronic subsystem and the final-state projection operator appropriate to the relevant photon detection process. The Liouville-space reduced transition operator occurring in this formula is defined in terms of a Liouville-space resolvent operator, which may be evaluated to give the spectral-line shape produced by an array of radiative transitions. This is a standard procedure in the isolated-line approximation, but it may be necessary to employ an overlapping-line description. The Liouville-space self-energy operator provides the open-system description of the collisional and radiative relaxation processes. In order to include Stark and Zeeman broadening, it is necessary to evaluate the line-shape formula using the "atomic" data that has been determined from electronic eigenstates in the presence of static or dynamic external electric and magnetic fields. In order to make comparisons with experimental observations, it is usually necessary to include either thermal or turbulent Doppler broadening.

3 Spectral Simulations

Spectral simulations have been carried out for many-electron atomic systems in electron-ion beam interactions [4] and in high-temperature plasmas [2, 3, and 5]. An ultimate goal in these simulations has been to employ the same set of atomic data consistently in the description of the non-equilibrium atomic-population kinetics and in the determination of the spectral-line shapes. These atomic spectral simulations have been found to be useful in determinations of electric-field and magnetic-field distributions and for diagnostics of plasma densities and temperatures. Spectral simulations for coherent radiation processes of energetic electrons in crystal lattices, such as coherent bremsstrahling and channeling radiation [6], can provide information on the elementary microscopic interactions and on the local crystal environment. Our density-matrix approach [1] may provide a comprehensive framework for detailed and systematic spectral simulations of electromagnetic interactions in low-dimensional semiconductor electronic systems [7], such as quantum wells, quantum wires, and quantum dots.

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