DESCRIPTION OF NONRADIATIVE MULTIPHONON TRANSITIONS
IN THE STATIC COUPLING SCHEME

I. FOUNDATIONS

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Nonradiative multiphonon transitions generated by the interaction of the electronic system with quantized normal oscillation modes are described quantum-theoretically on the basis of the static coupling scheme which is an essential, physically plausible alternative model to the adiabatic coupling scheme predominantly used in earlier papers. Putting emphasis on the mathematical correctness of the calculations we obtain a generally valid expression for nonradiative multiphonon transition rates which is based on the concept of temperature-averaged overlap factors. In the case of a single phonon energy this result is reduced to very compact expressions not given in original papers published so far. For non-vanishing phonon dispersion a simple standard formula is given which is suited for approximative numerical calculations.

1. INTRODUCTION

In the last two decades nonradiative multiphonon transitions of charge carriers in semiconductors have been studied theoretically by many authors. Consequently, considerable progress in the development of suitable quantum-theoretical and mathematical procedures has been achieved. At the same time, some fundamental problems of the theory of nonradiative multiphonon processes remain still unsolved (cf. e.g. STASIW [1], STUMPF [2], BOŃCH-BRUEVICH and LANDSBERG [3], LANDSBERG [4], HAUG [5, 6], SCHLAG, SCHNEIDER and FISCHER [7]).

From a purely quantum-theoretical point of view, these difficulties are connected in the first line with certain ambiguities in choosing an appropriate basis set of both initial and final quasistationary states of the coupled electron-phonon system (see e.g. KOVARSKIY, CHAYKOVSKIY and SINYAVSKY [8], SCHLAG, SCHNEIDER and FISCHER [7]). Since any actual choice of such a basis set corresponds to a certain coupling scheme, i.e. to a certain decomposition of the Hamiltonian $H$ of the total electron-phonon system into a "zero"-Hamiltonian $H'$ associated with these quasistationary states and the "rest"-Hamiltonian $V'$ inducing nonradiative transitions between them, any significant modification of the basis set is connected with corresponding changes in the numerical values of the theoretically predicted nonradiative transition rates. The general consequence is a striking non-equivalence of different basis sets and hence coupling schemes in the quantum-theoretical description of nonradiative multiphonon transitions.

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Proceeding from the fundamental work of Huang and Rhys [9], most of the original papers after 1950 dealing with the subject in question were based on the well-known adiabatic coupling scheme (see e.g. the review by Perlin [10] and the papers cited there). A basically different quantum-theoretical model of nonradiative multiphonon transitions which may be called adequately the static coupling scheme was considered for the first time by Helmis [11] in 1956 (cf. also Markham [12]). This scheme is based on the physically reasonable idea that in multiphonon relaxation processes the quasistationary states of charge carriers in semiconductors are affected only by some effective average lattice potential, whereas the fluctuations of the actual electron–lattice interaction potential connected with the vibrations of the ion cores around their equilibrium positions are considered entirely as a transition-inducing perturbation (see Haug [5, 13]).

In comparison with corresponding values calculated on the basis of the adiabatic coupling scheme and in connection with the well-known Condon-approximation, the alternative use of the static coupling scheme leads, according to Helmis [11], to an increase of theoretical transition-rate values by a factor of $10^3$ to $10^4$ for typical nonradiative multiphonon transitions in semiconductors, the latter calculation procedure thus permitting a much better theoretical understanding of experimental nonradiative transition-rate data in general.

After a period of about 10 years characterized by the predominant use of the adiabatic coupling scheme Kovarskiy, Chaykovskiy and Sinyavskiy [8], Howgate [14], Haug [5] and Päßler [15] employed, without referring to the earlier work of Helmis [11] an independently of each other, coupling schemes that are essentially identical with the static coupling scheme introduced by Helmis. Thus, the latter has been definitively established as an alternative model for the quantum-theoretical description of nonradiative multiphonon transitions in semiconductors, with the problem of the applicability and limitations of both fundamental coupling schemes remaining generally unsolved so far. Recently, similar problems were also discussed in molecular physics, as it may be seen e.g. from the review by Schlag, Schneider and Fischer [7].

In the adiabatic coupling scheme, more or less drastic approximations such as the Condon approximation (see e.g. Meyer [16]) or the so-called Non-Condon approximation (see Kovarskiy [17], Kovarskiy and Sinyavskiy [18]) cannot be avoided in any actual transition-rate calculations. Similar approximations are not required in the static coupling scheme, due to the simplicity of the basis set of quasistationary states. Therefore, it becomes both possible and meaningful to treat in a more careful manner, as compared with previous papers, the general mathematical procedures of transition-rate calculations as well as the approximations to be made when phonon dispersion is taken into account. This will be the main purpose of our bipartite treatise.

In this first paper, after presenting shortly the foundations of quantum-theoretical calculations of multiphonon transition rates in the static coupling scheme, we indicate