

# Scientific session of the Division of General Physics and Astronomy of the USSR Academy of Sciences (February 15–16, 1978)

Usp. Fiz. Nauk 126, 334–342 (October 1978)

PACS numbers: 01.10.Fv

A scientific session of the Division of General Physics and Astronomy of the USSR Academy of Sciences was held on February 15 and 16, 1978, at the Lebedev Physics Institute in Moscow. This session heard the following reports:

1. *V. M. Galitskiĭ, E. E. Nikitin, and B. M. Smirnov*, Theory of quasiresonant processes in the collision of atomic particles.
2. *Yu. N. Demkov and L. P. Presnyakov*. An asymptotic approach in the theory of atomic collisions.
3. *G. A. Smolenskiĭ*, The electroacoustic phonon echo.
4. *B. P. Zakharchenya, V. A. Novikov, and V. G. Fleisher*, States and resonances of optically pumped electron and nuclear spins in a semiconductor.

Abstracts of the reports follow.

*V. M. Galitskiĭ, E. E. Nikitin, and B. M. Smirnov*, *Theory of quasiresonant processes in the collision of atomic particles*. Two paths for the development of the theory of atomic collisions have been delineated. One is based on numerical solutions of the Schrödinger equation without invoking any additional physical arguments. The other is based on the use of qualitative physical considerations to convert to approximate calculation methods and models. Progress by the first approach depends on the use of computers to integrate the hundreds of coupled scattering equations, if some kind of physical arguments are used beforehand to choose a basis set of electron states. In other words, of the infinite number of states of the colliding atoms, those which are considered inconsequential for the given process are eliminated.

The second approach is more attractive, since it can lead to a general picture of various types of collisions, and it is based on approximations which exploit the natural "small parameters" of the system. In particular, in a study of transitions for the group of quasiresonant processes with which we are concerned in the present paper, the small parameter is the ratio of the characteristic dimension of the colliding particles to the characteristic distance between the particles at which the transition occurs. This is the basis for the theory of quasiresonant processes, which have large cross sections and thus determine the properties of, and the processes which occur in, various gas and plasma systems.

A common procedure in the derivation of theories for various processes involving the collisions of atomic particles is to make use of the fact that the mass of the nuclei is large in the scale of atomic units and the fact

that any inelastic process involves only a change in the state of the system of light particles (the electrons). For transitions between valence states of the atoms, the fact that the ratio  $m/M$  is small ( $m$  is the electron mass and  $M$  is the nuclear mass; their ratio is typically  $m/M \sim 10^{-4}$ ) means that up to comparatively large energies of the nuclei ( $10^3 - 10^4$  eV) the motion of the electrons in the system of two colliding atomic particles  $A$  and  $B$  is adiabatic. In other words, the ratio of the typical frequency of the electron motion,  $\Delta E/\hbar$  ( $\Delta E \sim 1 - 10$  eV), to the frequency of the nuclear motion which is characteristic of the collision,  $v/R_0$  ( $R_0$  is the characteristic distance at which the transition occurs, and  $v$  is the velocity of the nuclei), is large ( $\Delta E R_0/\hbar v \gg 1$ ). Then for problems of this type it may be a reasonable first step to use the adiabatic approximation, i.e., to choose as the electron basis set the electron wave functions of the system of colliding particles found for the case of fixed nuclei. Associated with each such wave function is an adiabatic electronic energy of the quasimolecule made up of the colliding particles, but with fixed nuclei. Transitions between adiabatic electronic states are caused by the dynamic interaction of the electrons and nuclei due to the nuclear motion, which is ignored in the construction of the adiabatic basis set.

It is a much simpler matter both to formulate the theory and to solve specific problems if we also make use of the semiclassical nature of the collision, i.e., the fact that the wavelength of the relative motion,  $\lambda$ , is small in comparison with  $R_0$ . When the condition  $\lambda/R_0 \ll 1$  is used, the system of second-order equations can be reduced to a first-order system, the concept of a classical nuclear trajectory can be introduced, and it is thus possible to learn much more about the general properties of the solutions of the system of equations.

Finally, if the change in the kinetic energy of the atoms due to the inelastic collision,  $\delta\epsilon$ , is small in comparison with  $\Delta E$ , then the multiple-channel problem can be approximated well by a problem with few channels (as few as two). The reason for this situation is that the condition  $\delta\epsilon \ll \Delta E$  actually means that the nonadiabatic interaction between the molecular terms frequently occurs at distances  $R^*$  much larger than  $R_0$ . In turn, this circumstance can be utilized for an asymptotic calculation (i.e., a calculation which is accurate for large values of  $R$ ) of the interaction of the terms in the range of interest,  $R \sim R^*$ .

The three conditions  $\Delta E R_0/\hbar v \ll 1$ ,  $\lambda \ll R_0$ , and  $\delta\epsilon \ll \Delta E$  define a special part of the theory of collisions, which deals with slow, semiclassical, quasiresonant collisions. This is the part of the theory which has been studied in most detail. The basic processes of this type

TABLE I. Quasiresonant processes in collisions of atomic particles.

| Process   | Effect or system in which the given process occurs  |
|---|---|
| 1. Resonant charge exchange   | Charge transfer in an atomic gas or plasma (gas discharges, fusion plasmas, electrode effects, etc.)  |
| 2. Nonresonant charge exchange  | The solar wind in the upper atmosphere; aurorae; astrophysics; the diagnostics of hot plasmas; the formation of population inversions in lasers; etc.   |
| 3. Transfer of excitation   | Spectral-line broadening and the formation of population inversions in lasers   |
| 4. Spin exchange and transitions between hyperfine-structure states             | The hydrogen and rubidium maser   |
| 5. Depolarization (change in the direction of angular momentum) in collisions   | Fluorescence of an atomic gas, spectroscopic effects (e.g., the Hanle effect), laser spectroscopy   |
| 6. Transitions between fine-structure states                                    | Sensitized fluorescence, spectroscopy of gases  |
| 7. Ionization in a collision with a highly excited atom                         | Formation of charged particles in an excited gas, in particular, an irradiated gas  |
| 8. Mutual neutralization in the collision of a positive ion with a negative ion | Charge recombination in a low-density electronegative gas, in particular, in the earth's atmosphere; formation of population inversions in lasers; etc. |
| 9. Destruction of a negative ion in a collision with an atom or molecule        | Formation of electrons in an electronegative gas and the inverse process  |
| 10. Deactivation of metastable atoms in collisions                              | Kinetics of excited states in an excited gas  |

are listed in Table I. In the resonant processes, transitions between states occur when the nuclei are far apart in comparison with the dimensions of the colliding particles. This circumstance has two consequences. First, the cross sections of the quasiresonant processes are large, so these processes are important in various effects in gases and plasmas (Table I). Second, there is a small parameter, which can be exploited to derive a rigorous asymptotic theory for each process.

An asymptotic theory for a quasiresonant process consists of several elements.<sup>1</sup> The transitions which occur in long-range collisions involve a limited number of channels, and for each of these channels the energy of the corresponding state of the quasimolecule must be calculated as a function of the distance between nuclei in an asymptotically exact manner (i.e., in the limit of large distances between nuclei). Then the dynamical problem for the transition probability amplitudes must be solved. Ultimately, it is possible to determine the transition cross section or other parameters of the collision (in particular, the density matrix of the system for given conditions).

The asymptotic theory of quasiresonant processes (like any approach which is based on a small parameter) has the advantage that the accuracy of the result can be estimated. Let us illustrate this point with the case of

resonant charge exchange of an ion with an atom of the same species, in which the small parameter of the theory is about 0.1 for collision energies up to the kiloelectron-volt range. Most of the error in the calculation of the cross section for resonant charge exchange is due to the inexact value of the wave function of the valence electron in the atom far from the nucleus. This uncertainty in the electron wave function is 10–30% for most elements, and the corresponding error in the cross section is 3–10%. This 3–10% value is larger than that due to other factors (the approximations made regarding associated processes, such as depolarization, a change in the fine-structure state of the colliding particles, and inelastic transitions; and the neglect of those effects in short-range collisions which lead to oscillations in the cross section). It follows that the asymptotic theory can lead to a cross section for resonant charge exchange which is more accurate than the results which can presently be found experimentally (the error in the absolute experimental cross sections is 10–30%). These considerations demonstrate the possibilities of asymptotic approaches in the theory of atomic collisions.

<sup>1</sup>E. E. Nikitin and B. M. Smirnov, *Usp. Fiz. Nauk* **124**, 201 (1978) [*Sov. Phys. Usp.* **21**, 95 (1978)].