Shake-up processes accompanying electron transitions in atoms

V. I. Matveev and É. S. Parilis

U. A. Arifov Institute of Electronics, Academy of Sciences of the Uzbek SSR, Tashkent

Elementary processes in many-electron atoms—radiative and Auger transitions, photoionization, ionization by electron impact, etc.—are usually accompanied by relaxation of the electron shells. The conditions under which such an inherently many-electron problem can be solved in the shake-up approximation are examined, and the shake-up processes occurring as a result of electron transitions are described from a unified point of view. The features that are common both to this form of excitation and to the shake-up of atomic electrons following nuclear transformations are pointed out, and the distinguishing features are also noted. The various electron shake-up processes considered are the radiative Auger effect, the two-electron–one-photon transition, double ionization, spectral line broadening, the post-collision interaction, Auger decay stimulated by collision with a fast electron, and three-electron Auger transitions (the double and half Auger effects). These processes are classified according to the type of electron transition causing the shake-up, and the experimental data and methods of theoretical description are reviewed. Other effects of a similar nature that could accompany transitions in the electron shells of atoms are also mentioned. A derivation of the shake-up approximation is given, and it is pointed out that this approximation is to a large extent analogous to the distorted-waves approximation in scattering theory. It is shown that the shake-up approximation is rather effective for obtaining estimates of the probabilities of the various effects.

CONTENTS

INTRODUCTION

The change in the nuclear charge during K capture and α and β decay and the change in the momentum of the nucleus during collisions with neutrons or in radioactive decay are perceived as sudden by the comparatively slow atomic electrons and are accompanied by the shake-up of the electron shells, leading to their excitation and ionization. However, a shake-up of the electron shells occurs not only after nuclear transformations, but also after transitions in the electron shells, especially those in the inner shells, during which there is an abrupt change in the screening of the field of the nucleus and, hence, in its effective charge. A typical example of such a process is the shake-up accompanying an Auger transition, where the change in the screening of the nucleus upon the filling of a vacancy in an inner shell and the ejection of the Auger electron leads to the "shaking off" of yet another electron from the outer shell. Processes that can be discussed in terms of the shaking up of atomic electrons as a result

of electron transitions have been the subject of active experimental and theoretical research in recent years, but earlier review articles[1,2] on the use of the sudden approximation have not given them adequate attention.

At the same time, however, processes of the shake-up type play an important role in the electron transitions in many-electron atoms, particularly during collisions with electrons and other atoms. Practically all the elementary transitions in the electron shells of atoms are accompanied by a relaxation of the shells that is of the nature of a more or less intense shake-up leading to the excitation or decay of the system by ionization or dissociation processes. Without allowing for the shake-up processes one cannot describe completely the final state of the system nor even the elementary processes themselves that lead to excitation of the electron shells. For example, the ionization cross sections for the inner shells and the ionization thresholds as well depend on the subsequent shake-up processes. The spectra of the emitted photons and Auger

electrons are determined in an essential way by the shake-up processes, which cause a broadening and shifting of the peaks and also give rise to new peaks. The spectra observed in experiments cannot be interpreted correctly without taking the shake-up processes into account. It should be pointed out that processes of the shake-up type are by no means always small effects; in some cases they alter the whole picture of the event. For example, in post-collision interactions it becomes possible for the ionizing particle to be captured. Allowance for shake-up processes substantially alters the cascades of Auger transitions following ionization of an inner shell of a many-electron atom and, hence, causes changes in the relative abundances of the multiply charged ions formed and in the spectra of the Auger electrons. Unless the shake-up processes are taken into account, one cannot give a correct explanation for the appearance of highly charged ions.

In the present review we describe from a unified point of view the shake-up processes that occur in the electron shell of an atom as a result of the sudden perturbation due to electron transitions, pointing out both the similarities and differences between this form of excitation and the shake-up processes that accompany nuclear transitions. We examine the various electron shake-up processes and classify them, review the experimental data and theoretical descriptions, and mention other effects of a similar nature that could accompany transitions in the electron shells of atoms. We go through a derivation of the shake-up approximation and point out the high degree of analogy between this method and the distorted-waves method in scattering theory.

The sudden approximation is used in quantum mechanics to solve the time-dependent Schrödinger equation in the case where the external perturbation acting on the quantum system is rapidly changing in time. In that case, one can construct a perturbation theory in which the small parameter is not the magnitude of the perturbation but rather the ratio of the characteristic time for changes in the external perturbation to the characteristic period of the quantum system.[1-4] A rather wide group of problems which can be solved by this method are given in the reviews by Dykhne and Yudin.[1,2] However, the sudden approximation as formulated there cannot be directly applied to the shake-up of the atomic shells which accompanies radiative or Auger transitions in atoms, since in that case it is generally impossible to separate out a time-varying perturbation. Let us therefore consider how the sudden approximation (the shake-up approximation) must be modified for application to transitions in the electron shells of atoms. Radiative and Auger transitions are two-particle transitions, so we shall examine the shake-up of the electron shell during such transitions mainly as illustrated by the three-particle decay of autoionizing states. Examples of such transitions are the two-electron radiative Auger decay,[5-7] in which an Auger transition is accompanied by the simultaneous emission of a photon, and the two-electron–one-photon relaxation of states with two inner-shell vacancies, which results in the filling of the vacancies with all the excess energy being carried off by a single photon.[8-10] Three-electron Aug-

er transitions also occur. These are the double Auger effect,[11] in which the filling of one vacancy leads to the ejection of two electrons from the atom, and the half Auger effect,[12-14] in which the filling of two inner-shell vacancies leads to the ejection from the atom of a single electron, carrying off the entire transition energy. One can also include in the category of three-particle relaxation effects the post-collision interaction,[15-18] which arises in the scattering from an atom of an electron whose energy is slightly higher than the excitation energy of an autoionizing state, so that the decay of the autoionizing state excited in the collision occurs in the presence of a slow electron.

The excitation and ionization of atomic electrons during nuclear transformation can be interpreted as shake-up processes because the system admits a clear division into two subsystems—the nucleus and the atomic electrons. The "nucleus" includes the high-energy particles which interact through short-range forces and participate in the nuclear transitions. The change in the nuclear state occurs over a time which is much shorter than the characteristic atomic times, and so the nucleus can be considered the fast subsystem and the atomic electrons, the slow subsystem. The interaction between subsystems is well described by an average field—the Coulomb field of the nucleus, which changes quite rapidly on the atomic time scales during the emission or absorption of fast charged particles.

In contrast, the electron shells cannot be so clearly divided into fast and slow subsystems whose interaction can be well described by an average field. However, if the transitions in the inner shells involve rather fast particles or hard photons, the electrons of these shells can be considered a fast subsystem with respect to the electrons of the outer shells. In this case one can introduce an average field amounting to a central Coulomb field with a certain effective charge, the rapid change of which during transitions in the inner shells is "felt" by the outer electrons and causes their shake-up.

1. THE MECHANISM FOR SHAKE-UP AFTER ELECTRON TRANSITIONS

Just as the half-life for radioactive transformations of the nucleus (which often reach hundreds or thousands of years) cannot serve as the characteristic time determining the shake-up of the electron shells, the lifetime $\sim \Gamma^{-1}$ of a vacancy in an inner shell with respect to Auger or radiative transitions cannot serve the analogous purpose in a treatment of the shake-up accompanying these transitions.

The characteristic small time that governs whether a process is of a shake-up nature could be taken, for example, as the time of flight of a β particle or a fast Auger electron through the shell in question, or as the time of flight of a photon. We shall consider below the question of how and under what conditions the inherently many-particle problem of the relaxation of the electron shells following radiative and Auger transitions, photoionization, electron-impact ionization, etc., can be solved in the shake-up approximation.

a) Sudden change of average field

Let us examine how the average field changes during a one-electron radiative transition in a two-electron atom. As usual, we assume that the radiative transition occurs in a frozen core, i.e., for a fixed state of the electron which does not take part in the radiative transition. In accordance with this assumption, we seek a total wave function in the form

$$\Phi(r_1, r_2, t) = \eta(r_1, t)\, \xi(r_2, t), \tag{1.1}$$

where r_i are the coordinates of the electrons, $\eta(r_1, t)$ is the known wave function of the electron undergoing the radiative transition in the presence of a frozen state of the second electron, and $\xi(r_2, t)$ is the unknown wave function of the second electron, for which we easily obtain the equation

$$i\,\frac{\partial}{\partial t}\xi(r_2, t) = (H_2 + \widetilde{W}(r_2, t))\,\xi(r_2, t), \tag{1.2}$$

where H_2 is the Hamiltonian of the second electron without allowance for the interaction $W(r_1, r_2)$ between the electrons, and

$$\widetilde{W}(r_2, t) = \int d^3r_1 \eta^*(r_1, t)\, W(r_1, r_2)\, \eta(r_1, t) \tag{1.3}$$

is the time-varying average field acting on the second electron during the radiative transition of the first. If the radiative transition of the first electron is from state η_1 to state η_2, then

$$\eta(r_1, t) = a(t)\,\eta_1(r_1) + b(t)\,\eta_2(r_1), \tag{1.4}$$

where $|a(t)|^2 + |b(t)|^2 = 1$. If we neglect the products $\eta_1(r)\eta_2(r)$, we have for the time-varying average field during the radiative transition an expression of the form

$$\widetilde{W}(r_2, t) = \widetilde{W}_2(r_2) + |a(t)|^2 [\widetilde{W}_1(r_2) - \widetilde{W}_2(r_2)], \tag{1.5}$$

where

$$\widetilde{W}_i(r_2) = \int d^3r_1 W(r_1, r_2)\, |\eta_i(r_1)|^2 \tag{1.6}$$

is the average field acting on the second electron if the first electron is in state $\eta_i(r)$. Since $|a(t)|^2 \sim \exp(-\Gamma t)$, the probability of finding the atom in the excited state changes in time from unity to zero, and the average field (1.5) acting on the second electron due to the first electron changes in time from $\bar{W}_1(r_2)$ to $\bar{W}_2(r_2)$ with a characteristic time $\sim \Gamma^{-1}$.

The period of revolution of an electron in an atomic orbit is in fact much shorter than the radiative decay time Γ^{-1}, but that does not mean that the electron follows the radiative decay adiabatically and that one may use the adiabatic approximation. The lifetime of the excited state has the meaning of the time during which the wave function flows from one orbital to another, i.e., the time in the course of which the electron will, with a high probability, undergo a quantum jump from one orbital to another and emit a photon.[19] The actual jump of the electron, which leads to an abrupt change in the wave function, takes place suddenly. In the present case a phenomenon occurs which is analogous to the collapse of the wave packet,[20] only here the "device" measuring the state of the electron undergoing the transition is the electron experiencing the shake-up

(the "shake-up electron"). Therefore, the change in the average field here is also sudden, and the shake-up approximation is suitable for solving the problem.

The average field acting on the shake-up electron changes over a time τ which characterizes the actual reorganization of the system after the quantum jump. The ratio of the time τ to the orbital period of the shake-up electron, or the quantity $\omega\tau$, where ω is its frequency, can serve as the criterion for the applicability of the shake-up approximation. If $\omega\tau \ll 1$, the perturbation is sudden, while if $\omega\tau \gtrsim 1$ it is adiabatic in character.

The applicability condition for the shake-up approximation is conveniently illustrated by the case of the Auger transition. The lifetime of an autoionizing state with respect to Auger decay is known to reach 10^{-13} s, but the Auger transition itself is sudden. Nevertheless, the change in the screening of the nucleus which causes the shake-up of the outer electron occurs over the finite time τ required for the Auger electron to leave the atom (or its inner shells). The condition $\omega\tau \ll 1$ necessary for the effect of the Auger transition on the outer electron to be of a shake-up character in this case reduces to the condition that the speed of the Auger electron be much higher than the speed of the outer electron, a condition that is usually well satisfied.

The approximate nature of the shake-up mechanism stems from the use of the concept of an average field for the system of interacting electrons, which is an external field for the system experiencing shake-up. In this case the transition energy is distributed between the photon and the shake-up electron. By measuring the photon energy one can therefore determine whether the radiative transition was accompanied by shake-up and, if so, find the energy acquired by the shake-up electron. The same can be said for the case in which one of the electrons is shaken down to a lower energy state. In the latter case the photon acquires a larger energy than it would if the transition were not accompanied by shake-up.

Sudden quantum jumps are also caused by transitions involving the simultaneous emission (absorption) of several quanta. A sequential shake-up is also possible in the case of the sequential emission (absorption) of quanta, where the system, in interacting with one quantum, undergoes a transition to a real (not virtual) stationary state in which it lives for some time before the absorption (emission) of the next quantum. An analogous sequential shake-up was examined by Smirnov and Firsov,[21] who described the sudden capture of an electron by a molecule and the subsequent excitation (shake-up) of the vibrational levels of the molecule, followed by a sudden decay and concomitant shake-up of the molecule.

It is of fundamental importance that the system can be divided into two subsystems whose interaction can be well described by an average field, with one of the subsystems undergoing a quantum jump and the other subsystem "feeling" this jump through the change in the average field and being "shaken up." Such a separation

of variables is possible when the system undergoing the transitions of interest consists of two interacting subsystems—a fast and a slow.

Generally speaking, the change in one of the subsystems can occur as a result of many quantum jumps, as when a rather strong external field is applied. For calculating such a change it is inconvenient to use the language of perturbation theory, i.e., to speak of quantum jumps, and it is necessary to solve the Schrödinger equation some other way. If the change in the first subsystem occurs over a time much shorter than the characteristic periods of the second subsystem, then one may use the shake-up mechanism, i.e., to examine the change in the first subsystem with the state of the second subsystem "frozen"; the second subsystem "feels" the change through a change in the average field and is "shaken up." But if we are considering a situation in which the change of state occurs through the absorption of soft quanta, i.e., a slow change brought about by a weakly varying field, then to solve the problem one must take into account the sequential absorption of a large number of soft quanta; although each quantum is absorbed suddenly, the accumulation of a sensible change of state requires the absorption of many quanta, and that takes a long time.

Thus, in the shake-up approximation one proposes to represent the amplitude of the process as a product[4,21] of the amplitude a_1 of the first, rapid stage in one of the subsystems and the amplitude a_2 of the shake-up stage of the other subsystem, i.e., $a = a_1 a_2$.

b) Shake-up efficiency

We have seen that every quantum transition in an electron shell causes a sudden change in the average field (in the screening of the nucleus) and may be accompanied by the shake-up of the remaining atomic electrons. The shake-up will be the entire effect if the interaction among the atomic electrons is well described by the approximation of an average field characterized by an effective charge.

One can introduce a shake-up parameter N, which serves as a measure of the shake-up efficiency:

$$N = \frac{\Delta z^*}{z^*}, \tag{1.7}$$

where Δz^* is the change in the effective charge z^* of the nucleus.

In treating the shake-up of atomic electrons accompanying a sudden change in the momentum of the nucleus, Dykhne and Yudin[1] introduced as a measure of the shake-up efficiency the parameter $N = \Delta v/v$, where Δv is the speed imparted to the nucleus by a sudden impact and v is the orbital speed of the shake-up electron. The parameter N introduced above in (1.7) can be put in the same form by considering that the speed of an electron in its orbit is $v = z^*/n$, where n is the principal quantum number, while the speed of an electron in an orbit with the same value of n but in the field of a nucleus of charge $z^* + \Delta z^*$ is equal to $v + \Delta v = (z^* + \Delta z^*)/n$, and therefore $N = \Delta z^*/z^* = \Delta v/v$.

According to the sudden approximation,[3,4] the shake-up probability upon an instantaneous change in the Hamiltonian is proportional to the square of the overlap integral of the wave functions of the shake-up electron describing the stationary state of the Hamiltonian before and after the change. But the overlap integral turns out to be directly proportional to the shake-up parameter [see (3.7) and (3.8) below]. Therefore. in accordance with our qualitative arguments, the shake-up probability increases with increasing N.

c) Selection rules for shake-up processes

Expressing the shake-up probability in terms of the overlap integral leads to monopole selection rules for the quantum numbers characterizing the state of the shake-up electron,[3] namely, that the orbital angular momentum and its projection should be preserved during shake-up: $\Delta l = \Delta m = 0$. These selection rules correspond to the physical situation that the interaction of the subsystems can be validly described with the aid of an average field which undergoes a sudden change but remains central before and after the change. The application of the shake-up approximation to transitions in the electron shells of atoms therefore leads to monopole selection rules. However, experiments show that it quite often happens that an electron which can be interpreted as a shake-up electron has changed its orbital angular momentum and projection. Such a change in the selection rules for shake-up can be explained by the inherently many-electron nature of the problem. It is clear that it is especially important to take this circumstance into account in cases where the electrons involved in the transition responsible for the shake-up and the electrons experiencing the shake-up are located in the same shell. It is shown below that it is necessary to take into account the change in the angular momentum and its projection during the shake-up process in order to describe the majority of the effects listed in the Introduction. The probabilities of such transitions can be estimated in the average-field approximation by introducing appropriate multiplicative factors to take into account the possibility of shake-up processes involving a change in the angular momentum and its projection.

d) Shake-up approximation for electron transitions

In essence, all the qualitative arguments given above constitute an interpretation of the expressions for the transition probabilities in many-electron atoms. Let us consider, for example, the single-photon decay of the excited state $\psi_a(r_1, r_2)$ of the helium atom. According to perturbation theory the decay rate to state $\psi_b(r_1, r_2)$ is of the form

$$\Gamma \sim |(\psi_b(r_1, r_2), (r_1 + r_2)\psi_a(r_1, r_2))|^2. \tag{1.8}$$

Let $\psi_a(r_1, r_2)$ describe the 2s2p state. In the single-electron approximation for distinguishable electrons we have $\psi_a = \varphi_{2p}(r_1)g_{2s}(r_2)$, $\psi_b = \varphi_{1s}(r_1)g_b(r_2)$. The decay rate is given by

$$\Gamma = \Gamma_r I_b, \tag{1.9}$$

where Γ_r is the rate for the one-electron–one-photon transition 2p→1s for a frozen state of the 2s electron,

and $I_b = (g_b, g_{2s})$ is the overlap integral of the initial and final states of the 2s electron. If the electrons are assumed to be noninteracting, then I_b is zero in all cases except that in which the 2s electron stays in the same state. However, if the interaction between the electrons is taken into account, such as by a self-consistent field, then the overlap integral is nonzero for transitions involving a change in the state of the 2s electron as well. We shall treat these transitions as resulting from the shake-up of the 2s electron due to a one-electron radiative transition. The fact that the rate (1.8) for one-photon decay involving a change of state for two electrons has the typical form for the shake-up approximation[1] is a consequence of expressing the two-electron wave function as a product of single-electron functions. Such an approximation is, of course, valid in the case that the shake-up electron is slow compared to the electron involved in the emission of the photon. However, in atomic physics the representation of many-electron wave functions as products of single-electron functions is used even in cases where the speeds of the electrons are comparable. The best one-electron representation is obtained in the solution of the Hartree-Fock equations. They are based on a variational principle, and there are no simple criteria for the domain of applicability. For this reason the domain of applicability of formulas such as (1.9) in the shake-up approximation is determined in a more complex way (see below).

Formula (1.8), just as (1.9), has the form of an expression in first-order perturbation theory. However, formula (1.8) contains the two-electron wave functions which are the exact wave functions for the helium atom. Of course, the exact wave functions are unknown, but there are various methods of obtaining the approximate form of the two-electron wave functions. It is natural to consider expressions of type (1.8) as a generalization of the shake-up approximation. In particular, an approximation of this type which incorporates the interelectron correlations enables one to make allowance for the exchange of angular momentum during the shake-up process. In the next section we consider a more rigorous derivation of the shake-up approximation for electron transitions.

2. THE SHAKE-UP APPROXIMATION

Suppose that at some instant of time an unstable system is formed in a state φ_a which is an eigenfunction of the approximate Hamiltonian K, i.e., $K\varphi_a = \varepsilon_a \varphi_a$. The total Hamiltonian is $H = K + U$, where the interaction responsible for the decay is the sum of two operators: $U = V + W$. The system decays to a state φ_b such that $K\varphi_b = \varepsilon_b \varphi_b$ and $(\varphi_b, U\varphi_a) = 0$, i.e., the transition $\varphi_a \to \varphi_b$ is due to an effect of higher than first order in perturbation theory. According to Goldberger and Watson,[22] the initial decay rate is

$$\Gamma = 2\pi \, d\rho \, (\varepsilon_a) \mid R_{ba}^+ (\varepsilon_a) \mid^2, \tag{2.1}$$

where $d\rho(\varepsilon_a)$ is the density of final states, and the matrix element of the operator for the shift and width of the level is

$$R_{ba}^- (\varepsilon_a) = \lim_{\eta \to 0} (\varphi_b, \ R (\varepsilon_a + i\eta) \, \varphi_a) = (\varphi_b, \ U\psi_a); \tag{2.2}$$

here the function ψ_a satisfies the equation

$$\psi_a = \varphi_a - (\varepsilon_a + i\eta - K)^{-1} (1 - \Lambda_a) \, U \psi_a, \tag{2.3}$$

where Λ_a is the operator for the projection onto state φ_a. By introducing a function ψ_b in accordance with the equation

$$\psi_b = \varphi_b + (\varepsilon_a - i\eta - K)^{-1} (1 - \Lambda_a) \, W\psi_b, \tag{2.4}$$

we can write expression (2.2) in the more convenient form[23]:

$$R_{ba} (\varepsilon_a) = (\psi_b, \ V\psi_a) + (\psi_b, \ W\varphi_a). \tag{2.5}$$

We shall assume that the operator V is small enough that it may be taken into account only once; then in (2.3) we have $U \simeq W$, and Eqs. (2.3) and (2.4) can usually be written in the form

$$\begin{aligned} (E_a - K - W) \, \psi_a &= 0, \\ (\varepsilon_a - K - W) \, \psi_b &= 0. \end{aligned} \tag{2.6}$$

Here $\psi_{a,b} \to \varphi_{a,b}$ upon the adiabatic switching off of W; $E_a = \varepsilon_a + R_{aa}(\varepsilon_a)$ is the energy of the quasistationary state ψ_a; $\mathrm{Re}\, E_a = \varepsilon_a + \mathrm{Re}\, R_{aa}(\varepsilon_a)$, $\mathrm{Im}\, E_a = \mathrm{Im}\, R_{aa}(\varepsilon_a)$; and $R_{aa}(\varepsilon_a)$ is the width and shift of level ε_a.

The shake-up approximation is obtained from the exact two-potential formula (2.5) by substituting the solution of Eqs. (2.6) into it. The situation is thus analogous to the case of scattering by two potentials[22] when only the linear terms in the small potential are retained and the strong potential is taken into account exactly by the change in the initial and final states (the distorted-waves method in scattering theory). The problem of evaluating the transition probability in a higher order of perturbation theory is thus replaced by a formula having a form typical of the first order in perturbation theory. We note that in (2.6) one can usually assume E_a to be a real quantity equal to $\varepsilon_a + \mathrm{Re}\, R_{aa}(\varepsilon_a)$, since, according to Baz' et al.,[24] for $\mathrm{Im}\, E_a \ll \varepsilon_a$ such a change has a negligible effect in a matrix element of the type in (2.5), except in the case when the wave functions are those of the continuum (see Sect. 4a below).

Taking the strong potential into account exactly leads to a substantial improvement in the results of calculations in scattering theory in comparison with the Born approximation.[25]

3. TWO-ELECTRON RADIATIVE TRANSITIONS

A two-electron radiative transition involves a change of state for two electrons and the simultaneous emission or absorption of a γ photon. In this case V is the interaction with the electromagnetic field, and W is the interaction between the electrons. Since the small operator V is taken into account only once, the functions $\psi_{a,b}$ are products of the electron wave functions $\Phi_{a,b}$ and the photon wave functions $\Omega_{a,b}$. We then obtain from (2.6) the equations for just the electron parts of the wave functions

$$\begin{aligned} (\varepsilon_a - K - W) \, \Phi_a &= 0, \\ (\varepsilon_b - K - W) \, \Phi_b &= 0, \end{aligned} \tag{3.1}$$

$\varepsilon_b = \varepsilon_a \pm \omega$, where ω is the energy of the γ photon (the

V. I. Matveev and É. S. Parilis   885

plus sign corresponds to absorption of the photon and the minus sign to emission). The boundary conditions for Eqs. (3.1) are that the functions $\Phi_{a,b}$ tend toward the states of an atom with noninteracting electrons as the interaction between the electrons is adiabatically turned off. It is these states that we take as the zeroth approximation (see the beginning of Sec. 2) for the excited states, while Eqs. (3.1) describe the atomic states that should be obtained when the interaction between the electrons is taken into account exactly. Such a choice for the zeroth approximation enables one to show clearly that allowance for the interaction between electrons even in the average-field approximation [in the solution of Eq. (3.1)] and allowance for the interaction with the electromagnetic field in the first order of perturbation theory lead to a nonzero amplitude for the two-electron—one-photon transition.

The second term in (2.5) is equal to zero, since the state φ_a does not contain a photon but ψ_a does, and so the transition amplitude is of the form

$$R_{ba} = (\Phi_b, \, V_r \Phi_a), \tag{3.2}$$

where $V_2 = (\Omega_b, V\Omega_a)$ is proportional to the dipole moment d. The amplitude for the two-electron radiative transition is thus of the same form as the amplitude for the one-electron transition, with the distinction that the dipole-moment matrix elements are taken between many-electron wave functions $\Phi_{a,b}$ satisfying Eqs. (3.1).

If it is assumed that the operator W for the interaction between electrons is small, then Eqs. (3.1) can be solved using perturbation theory. In that case, of course, we obtain all the diagrams for the amplitude R_{ba} that would appear in a direct perturbation-theory solution of the problem, as was carried out in Refs. 8, 9, and 10 for the case of two-electron—one-quantum relaxation; in those papers the diagrams were calculated which appear in the second order of perturbation theory. On the other hand, solution of Eqs. (3.1) is equivalent to taking all the terms of the series in powers of W into account. The advantages of the shake-up approximation are realized in cases where Eqs. (3.1) can be solved, because then the transition amplitude is calculated from an expression which is formally identical to the formula which appears in the first order of perturbation theory.

Let us illustrate this for the case when Eqs. (3.1) are solved in the average-field approximation. In this case we seek functions $\Phi_{a,b}$ of the form

$$\Phi_{a,b} = f_{a,b}(1) \, X_{a,b}(2), \tag{3.3}$$

where $f_{a,b}(1)$ are states of the first electron which are coupled together by the radiation operator with the position of the second electron frozen. In other words, $f_{a,b}$ are the known functions used in calculating the one-electron—one-quantum relaxation under the assumption that the transition does not affect the second electron. We note that state f_a is orthogonal to state f_b, i.e., $(f_a, f_b) = 0$. Substituting (3.3) into (3.1), we obtain equations for the unknown functions $X_{a,b}$ of the second electron:

$$\begin{aligned} \{\varepsilon_{a2} - K_2 - (f_a, Wf_a)\} \, X_a(2) &= 0, \\ \{\varepsilon_{b2} - K_2 - (f_b, Wf_b)\} \, X_b(2) &= 0, \end{aligned} \tag{3.4}$$
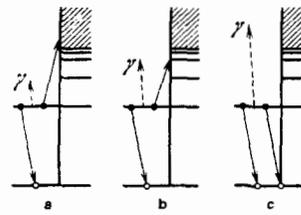
FIG. 1. Radiative Auger effect. a) Auger electron in the continuum; b) Auger electron in bound state; c) two-electron-one-photon transition.

where ε_{a2} and ε_{b2} are the energies of the second electron before and after the transition, and $(f_{a,b}, Wf_{a,b})$ is the average field acting on the second electron before and after the one-electron transition. It is this approach that is generally taken when the shake-up approximation is used. The simplest way of taking the average field into account reduces to the method in which the charge of the nucleus is screened by the first electron.[23] The average field can be taken into account *more exactly by using self-consistent wave functions* $f_{a,b}$, as was done, for example, by Åberg.[6] The transition amplitude in the average-field approximation is of the form

$$R_{ba} = (f_b, V_r f_a)(X_b, X_a), \tag{3.5}$$

where the states X_a and X_b are not orthogonal since they are solutions of Eqs. (3.4) with different Hamiltonians. It is customary to say that as a result of the radiative transition $f_a \rightarrow f_b$, the second electron, which we assumed to be frozen, remains in a state X_a which is not an eigenfunction of the new Hamiltonian, and the overlap integrals (X_a, X_b) with the eigenfunctions of the new Hamiltonian determine the shake-up amplitude. The error in such a method can be estimated by taking stock of all the diagrams in a perturbation theory in W that do not contain the average field.

a) Radiative Auger effect

The radiative Auger effect is the two-electron—one-photon decay of an autoionizing state involving the emission of a photon, the filling of an inner-shell vacancy by one of the electrons, and a transition of the other electron either into the continuum (Fig. 1a) or into a bound state (Fig. 1b). The first theoretical estimates of the probability of such a transition were made back in 1935 by Bloch[7] using perturbation theory, while
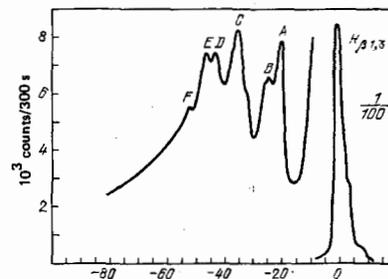
FIG. 2. Low-energy part of the γ-ray spectrum emitted in K—MM radiative Auger transitions in the argon atom.

the experimental proof of the existence of the effect was obtained relatively recently.[26-28]

In the radiative Auger effect the transition energy is distributed between the electron and the photon, and so radiative Auger transitions are manifested in the low-energy part of the photon spectrum emitted during the filling of an inner-shell vacancy in an atom. Figure 2 shows the low-energy side of the $(1s)^{-1}\,{}^{1}S \to (3p)^{-1}\,{}^{2}P^{0}$ line in argon.[5] It consists of several peaks (A, B, C, D, and E), a low-energy tail, and a bump F at 55 eV. Peaks A and B arise from transitions to the final states $(3p)^{-2}np^{2}P^{0}$, peak C is due mainly to the discrete transitions $(1s)^{-1}$ $\to [(3s)^{-1}(3p)^{-1}, {}^{3}P, {}^{1}P]ns, nd$, ${}^{2}P^{0}$ (see Fig. 1b), the position of peaks D and E corresponds to the onset of the transitions $(1s)^{-1} \to (3s)^{-1}(3p)^{-1}\varepsilon s, \varepsilon d$, ${}^{2}P^{0}$ (see Fig. 1a), and the position of bump F corresponds to the onset of transitions to the $(3s)^{-2}\,{}^{1}S$ states. The relative intensity of the low-energy part of the spectrum amounts to 5% of the intensity of the entire spectrum, in fair agreement with the results of calculations[6] in the shake-up approximation (7.3%). The spectrum shown in Fig. 2 was obtained by observing radiative Auger transitions in the free argon atom, whereas the first observations of these transitions were made in atoms of Mg, Al, Si, and S in solid compounds.[26] It has been found that the ratio of the intensity of the K–LL radiative Auger transition to that of the Kα line of the one-electron radiative transition falls off as the atomic number increases from 12 to 16, the average value of the intensity ratio being 0.007. The spectrum of Auger electrons emitted in the radiative Auger transition turns out to be similar to the spectrum of electrons "shaken off" from the L shell as a result of photoionization of the K shell.[29] On this basis it is assumed that the radiative Auger transition is a consequence of the shaking off of an outer electron as a result of a one-electron radiative transition. According to this interpretation, the observed spectrum should not depend on the way in which the K vacancy was formed. A study was therefore undertaken[27] to compare the spectra of the K–LL transitions for the cases in which the K-shell vacancy was produced by an electron and by a photon. The spectra were found to be identical to within 0.4%. The probabilities for K–LL and K-MM radiative Auger transitions calculated[6] in the shake-up approximation with self-consistent wave functions are in fair agreement with experiment.

As we have seen, the radiative-Auger transition probability can be calculated using the formulas of second-order perturbation theory. However, calculations of this kind are generally rather awkward, whereas the shake-up approximation yields relatively easy estimates that are in satisfactory agreement with experiment. Let us consider, for example, the radiative Auger decay of the 2s2p state of a heliumlike ion. For simplicity, we treat the electrons as distinguishable and the wave functions as hydrogenic, and we introduce an effective charge to take care of the average field. Since the amplitude of the two-electron radiative transition is of the same form as that of the one-electron radiative transition, the probability for the emission of a photon of energy ω_b in a two-electron transition is (cf. Ref. 30)

$$\Gamma = \Gamma_r \frac{1}{\omega^3} \sum_b \omega_b^3 \, |\, I_b\,|^2, \tag{3.6}$$

where Γ_r is the probability for the one-electron radiative transition 2p $\to$ 1s when the state of the second electron is frozen, ω is the energy of the photon which would be emitted under this condition, I_b is the overlap integral of the 2s state with the states into which the 2s electron is "shaken" as a result of the one-electron radiative transition, and $\sum_b$ calls for a summation over the final states. For a shake-up into a state ψ_n of the discrete spectrum, the overlap integral is evaluated as

$$I_n = \frac{1}{2} \left(\frac{2}{n}\right)^{3/2} N \frac{\left(\frac{1}{2} - \frac{1}{n}\right)^{n-3}}{\left(\frac{1}{2} + \frac{1}{n}\right)^{n+3}} \left(\frac{2}{n^2} - \frac{3}{2}\right), \tag{3.7}$$

where N is the shake-up parameter introduced earlier (see Sec. 1b). For shake-up ("shake-off") into a state ψ_k of the continuum we have

$$I_k = \frac{\sqrt{2}}{\sqrt{1 - \exp(-2\pi/k)}} \frac{N}{z^*} \frac{\exp[-(2/k)\,\mathrm{arcctg}\,(1/2k)]}{[(1/4) + k^2]^3} \left(\frac{3}{2} + 2k^2\right), \tag{3.8}$$

where $k = \sqrt{2\varepsilon}/z^*$ and $z^* \gg \Delta z^*$. The effective charge can be evaluated using the Slater rules[31] or some more detailed rules.[32] Performing the summation in (3.6) over all the bound final states of the Auger electron (see Fig. 1b), we obtain the following transition probability:

$$\frac{\Gamma}{\Gamma_r} = 6.95 \cdot 10^{-1} (z^*)^{-2}. \tag{3.9}$$

Analogously, for transitions into the continuum (see Fig. 1a) we have

$$\frac{\Gamma}{\Gamma_r} = 3.87 \cdot 10^{-2} (z^*)^{-2}. \tag{3.10}$$

The combined relative probability for radiative Auger transitions for $z^* = 14$ is equal to 0.004, in rather good agreement with experiment (see Ref. 26).

As another example, let us consider the radiative Auger decay of the autoionizing state $2p^2\,{}^{3}P$ of the helium atom. In light atoms, the autoionization probability (where such is possible) is known to be significantly higher than the probability of a radiative transition.[33] Exceptions to this are states of double excitation, for which autoionization is forbidden by selection rules. The double excited $2p^2\,{}^{3}P$ state of the helium atom is just such a state.[34] We take the wave function Φ_a of the initial state in the form proposed by Wu[35]:

$$\Phi_a = \frac{\beta^5}{4!} r_1 r_2 \exp\left[-\frac{\beta}{2}(r_1 + r_2)\right] Q(\hat{r}_1, \hat{r}_2), \tag{3.11}$$

where $Q(\hat{r}_1, \hat{r}_2)$ is the known[58] angular part of the $2p^2\,{}^{3}P$ wave function, and $\beta = 1.68$ is a variational parameter. The final state

$$\Phi_b = \frac{1}{\sqrt{2}} [\varphi(r_1)\psi(r_2) - \varphi(r_2)\psi(r_1)], \tag{3.12}$$

where $\varphi(r)$ is the wave function of the ground state of He$^+$, and $\psi(r)$ is the wave function of the electron in the excited state or in the continuum in the field of the He$^+$ ion, whose effective charge for all such states we take to be unity. The ratio of the width of the two-electron radiative transition to the width of the one-electron transition is then found to be 6.6%, of which 3.0% is due

to the radiative Auger effect with shake-off into the continuum, and 3.6% with shake-up into the discrete spectrum.[23]

b) Two-electron–one-photon transition

A study[36] of the decay of autoionizing states with two inner-shell vacancies revealed transitions in which both vacancies were filled and all the energy was carried off by a single photon (see Fig. 1c). Such a transition can be regarded as a particular case of a radiative Auger transition for which the final bound state is one of the vacancies. In the spectrum of photons emitted as a result of the radiative decay of states with two inner-shell vacancies, the two-electron–one-photon transition is detected by the presence of a bump on the high-energy part, located at a photon energy approximately equal to the sum of the energies of the one-electron radiative transitions to the inner-shell vacancies. Figure 3 shows the spectra of photons emitted in the decay of states having two inner-shell vacancies in atoms of Ni and Fe. The lower part of the figure shows blowups of the energy regions in which the bumps are observed in the high-energy parts of the spectra. It is seen that this region contains peaks $X1$, $X2$, $X3$, and $X4$ at energies corresponding to the two-electron–one-photon transitions. The peak $X1$ is located at an energy that is slightly higher than twice the energy of the $K\alpha$ satellite in Ni; the peak $X3$ corresponds to the same transition in Fe. The energies of peaks $X2$ and $X4$ are slightly higher than the sum of the energies of the $K\alpha$ and $K\beta$ transitions in Ni and Fe, respectively. The probability of the two-electron–one-photon transition turns out to be smaller by a factor of $\sim 10^{-4}$ than the probability of the corresponding one-electron radiative transition.[36] A two-electron–one-photon transition involving the filling of vacancies in the L shell of Cl and Ar atoms has been observed in experiments.[37] The state with two inner-shell vacancies was produced by the hard collision of Cl and Ar ions with Ar atoms at a projectile-ion energy of 48 keV. It was determined that the probability for two-electron–one-photon decay is $\sim 10^{-6}$ of the total decay probability.
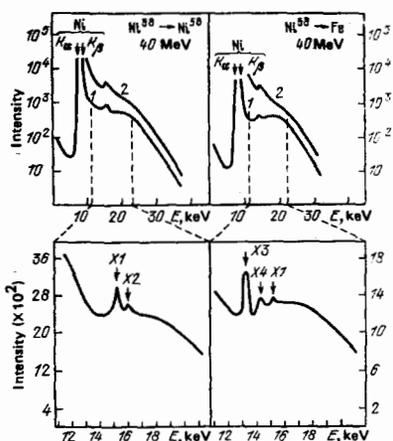
FIG. 3. High-energy part of the spectrum of $K\alpha$ and $K\beta$ satellites arising as a result of the radiative decay of states having two inner-shell vacancies formed during ^{58}Ni–^{58}Ni and ^{58}Ni–Fe collisions.

The use of collision experiments to study the decay of states with inner-shell vacancies was motivated by the relatively large cross section for ionization of the inner shells, which can reach values of the order of the geometric dimensions of these shells. For other methods of ionizing the inner shells—photoionization and electron- and proton-impact ionization—the cross section for the formation of two inner-shell vacancies is much smaller. A discussion of the quasimolecular mechanism for the formation of two inner-shell vacancies and the energy dependence of the one-photon decay can be found in the paper of Greenberg et al.[38] (for Ni-Ni collisions in the energy range from 17.6 to 91.5 MeV).

The two-electron–one-photon transition probability has been evaluated in second-order perturbation theory[8–10,39] and also by methods that do not make use of the assumption that the interaction between electrons is small.[23,40–42]

The shake-up approximation permits an extremely simple estimate of the transition probability for $(1s)^{-2} \rightarrow (2s)^{-1}(2p)^{-1}$. From (3.6) we have

$$\frac{\Gamma}{\Gamma_r} = \left(\frac{\omega_b}{\omega}\right)^3 I^2(2s,\ 1s) = (17.7 \cdot z^2)^{-1}, \tag{3.13}$$

where $I(2s,1s)$ is the overlap integral of the 2s and 1s states (3.7). This estimate is in rather good agreement with the results $[\Gamma/\Gamma_r = (8.3 \cdot z^2)^{-1}]$ of second-order perturbation-theory calculations.[9] A similar, but somewhat more complex, calculation scheme was employed by Åberg et al.[40] to evaluate the $(1s)^{-2} \rightarrow (2s)^{-1}(2p)^{-1}$ transition probability in the shake-up approximation with Hartree-Fock wave functions. The discrepancy between the calculated and experimental results can be attributed to the fact that the average-field approximation does not adequately describe the interaction between electrons located in the same shell. Nussbaumer[41] has proposed a method of incorporating the interelectron correlations whereby the wave functions of the initial and final states—the solutions of Eqs. (3.1)—are sought by a method involving the superposition of configurations. Moiseev and Katriel[42] proposed a different way of of taking the interelectron correlations into account—they introduced a factor $(1 - \lambda \cos\theta_{1,2})$ in the hydrogenic wave functions, where λ is a variational parameter and $\theta_{1,2}$ is the angle between the radius vectors of the electrons.

The use of single-electron wave functions leads to rigid selection rules for the angular momentum and its projection, but it has been shown[9] that transitions involving a change in the angular momentum of the shake-down electron give a contribution to the amplitude that is comparable to that from transitions without a change in angular momentum. In other words, in the two-electron–one-photon transition the two electrons participate on equal footing, effectively doubling the number of final states. This explains why the relative probability (3.13) is roughly half that calculated by Safronova and Senashenko.[9]

We can thus formulate a general rule for applying the average-field approximation in calculating shake-up effects when the shake-up and transition electrons are

both in the same shell: Use the single-electron approximation to estimate the probability for the allowed transitions (shake-ups) preserving the angular momentum and its projection and then multiply by the number of transitions which are allowed by the many-electron selection rules.

c) Two-electron transitions involving absorption of a photon. Photoionization with simultaneous excitation

Let us for simplicity consider the effects which occur upon the absorption of a photon by the helium atom in its ground state as the photon energy ω increases. When $\omega \gtrsim 58$ eV, the probability of exciting the first autoionizing state begins to appear against the background of single ionization. At $\omega \gtrsim 65.4$ eV one begins to see ionization accompanied by the simultaneous excitation of the He^+ ion into states with $n = 2$ and higher, and at $\omega \gtrsim 79$ eV, double photoionization of the helium atom begins.

The probabilities for these transitions are nonzero only when the interaction between electrons is taken into account. Photoionization with simultaneous excitation has been studied in the helium atom by a number of authors (see, for example, Refs. 43–47), with different choices for the wave functions of the initial and final states. Let us examine in some detail the paper by Brown.[45]

The initial state Φ_a—the solution of the first of Eqs. (3.1)—is the wave function of the ground state of the helium atom. Here, as in the study of radiative Auger-type transitions, the average-field method is inadequate and the interaction between electrons must be considered more exactly.[48] For treating the photoionization and simultaneous excitation of the helium atom, Brown[45] therefore chose the following variational wave function for the ground state:

$$\Phi_a = \frac{1}{4\pi} \sum_l F_l(r_1, r_2) P_l(\cos\theta_{1,2}), \qquad (3.14)$$

where $P_l(\cos\theta_{1,2})$ are Legendre polynomials, $\theta_{1,2}$ is the angle between the directions of the vectors r and r_2, and the parameters of the function $F_l(r_1, r_2)$ are found from a variational principle. On the other hand, the wave function of the final state can be adequately represented in the framework of the effective-charge method, i.e., in the form of a symmetrized product of the wave function of the bound state in the field of charge z = 2 (the state of the He^+ ion) and the continuum wave function in the field of charge $z = 1$ (in the field of the He^+ ion). When functions of this kind are used to evaluate the amplitude (3.2) there is no overlap integral, and in this approach one cannot single out a "shake-up" electron. Nevertheless, this approximation is the shake-up approximation (see Sec. 1d), namely, the approximate treatment of the weak potential of the interaction with the electromagnetic field in the first order of perturbation theory and the "exact" treatment of the strong interaction between electrons (see Sec. 2).

d) Double photoionization

In evaluating the double photoionization of the helium atom, Brown[49] used a six-parameter Hylleraas wave function for the ground state of the atom:

$$\Phi_a \sim \exp(-\beta s)(1 + c_1 u + c_2 t^2 + c_3 s + c_4 s^2 + c_5 u^2), \qquad (3.15)$$

where $s = r_1 + r_2$, $t = r_1 - r_2$, and $u = |r_1 - r_2|$; this wave function gives a deeper energy minimum than the function in (3.14). The final states were taken to be the symmetrized product of two Coulomb wave functions in the field of a charge $z = 2$, i.e., it was assumed that the interaction of the electrons in the continuum could be ignored. The interaction between electrons in the continuum becomes important near the double-photoionization threshold and can be taken into account by perturbation theory.[50]

In complex atoms it is also necessary to incoporate the interelectron correlations if the photoelectron and shake-up electron are in the same shell.[48] However, if the photoelectron is ejected from an inner shell by a hard enough photon, the one-electron shake-up approximation, as we mentioned earlier, works rather well. The escape of the fast photoelectron is felt by an outer electron as a sudden change in the screening of the nucleus or, what is the same, as a change in the effective nuclear charge. The situation is thus similar to the shake-up of atomic electrons that accompanies nuclear β decay. One can therefore estimate the shake-up probability P for this case using the shake-up probability P_β for the case of β decay.[51] Considering that during photoionization the effective charge changes by an amount ΔZ, we have $P = (\Delta Z)^2 P_\beta$, as was shown by Carlson and Krause.[52,53] Calculations with this formula give results which are similar to those obtained by direct evaluation of the overlap integrals for Hartree-Fock wave functions of the shake-up electron. Since the overlap integral falls off rather rapidly as the energy of the shake-up electron increases, the energy spectrum of the electrons shaken off from an atom is maximum at zero energy; this result is in full accord with experiment.[29]

The shake-up approximation with relativistic Hartree-Fock wave functions has been used to calculate the double photoionization of noble-gas atoms.[54]

It becomes necessary to include in the calculations the interelectron correlations in the final state when the energy of the γ photons is low, since the low speed of the photoelectron in this case does not allow one to neglect its interaction with the shake-up electron.[55]

The shake-up processes which accompany photoionization have a substantial effect on the photoelectron spectra[56] and must therefore be taken into account in atomic shell-structure studies based on analysis of these spectra. The shake-up mechanism plays an essential role in the formation of multiple vacancies during the reorganization of the atomic shells after photoionization; a review of the corresponding experimental results can be found in the paper by Krause.[57] The literature cited[43-57] also contains experimental data on two-electron transitions accompanying the photoionization of various atoms, discussions of these data, and comparisons with theory.

889   Sov. Phys. Usp. 25(12), Dec. 1982

V. I. Matveev and É. S. Parilis   889

e) Spectral line broadening

Electrons scattered by radiating atoms interact differently with the upper and lower states of the radiative transition. Therefore, the atom and the projectile electron exchange energy during the emission of the photon, thereby affecting the photon energy.[58] In this case we are dealing with a two-electron radiative transition, and so the photon-emission probability per unit time is

$$\Gamma = \frac{4}{3}\alpha^3\omega^3 |d_{ba}|^2 = \Gamma_r \sum_b (X_b, X_a), \qquad (3.16)$$

where Γ_r is the emission probability for an isolated atom, and X_b and X_a are the wave functions of the projectile electron before and after the emission of the photon, i.e., the transition is of the typical form for the shake-up approximation.

4. THREE-ELECTRON TRANSITIONS

In the case of the two-electron radiative transitions the choice of the small potential is rather simple: The interaction with the electromagnetic field is weak [an exception (see Sec. 1a) is the emission or absorption of soft quanta, as in the scattering of charged particles[3]], and the interaction between the electrons is strong and must be taken into account exactly. For three-electron transitions, on the other hand, the separation of the perturbation into weak and strong parts is determined by the form of the final and initial states. As an illustration, let us consider the post-collision interaction (see Sec. 4a below). In this case the interaction of a slow electron with electrons in an autoionizing state must be treated exactly, since the low energy of the electron makes perturbation theory inapplicable, while the Auger-decay amplitude can be calculated by perturbation theory. This is the approach that has been taken[16-18] in applying the shake-up approximation to this effect. We face opposite situation in considering autoionization in the field of a fast charged particle[59] (see Sec. 4b below), where the interaction of this fast particle with the electrons in the autoionizing state can be treated by perturbation theory.

The transition amplitude (2.5) consists of two terms, and, while the second of these was exactly zero in the case of the radiative transition (see the beginning of Sec. 3), for three-electron transitions this term is non-zero. However, this second term is quite often small. In fact, in the post-collision interaction, for example, the strong potential W is the interaction of the slow electron with the electrons in the autoionizing state, while the second term—the matrix element between bound states and the continuum—is small, since there is little chance that a slow particle will cause one of the electrons to go into the continuum with a high velocity and the other electron to go into a deeper bound state. For the case of Auger decay in the field of a fast particle the second term in (2.5) is zero, since the matrix element is taken between different states of the fast particle, and its coordinates do not appear in the operator W. Thus, in applying the shake-up approximation to three-electron transitions, one must, generally speaking, make allowance for both terms in (2.5). However, in cases where the second term is small,

the transition amplitude in the average-field approximation will be of the form

$$R_{ba} = (\psi_b(\mathbf{r}_1, \mathbf{r}_2), \ r_{12}^{-1}\psi_a(\mathbf{r}_1, \mathbf{r}_2))(X_b(\mathbf{r}_3), X_a(\mathbf{r}_3)), \qquad (4.1)$$

where the overlap integral (X_b, X_a) determines the shake-up probability of the third electron. This formula also works fairly well for the shake-up of outer electrons accompanying an Auger transition in an inner shell of a complex atom.

For the case of three-electron Auger transitions (see Secs. 4d, e below) in which all three electrons are in nearby shells, the two terms in (2.5) are comparable, since one cannot separate the weak and strong parts of the potential. However, the transition amplitude can be represented in the form of (4.1), since allowance for the second term has the physical meaning that it is necessary to take into account the different pairings of the three electrons involved in the transition, and this can be done in averaging the transition rate over the initial states and summing over the final states. Here we neglect the interference terms in the transition rate.

We also note that Eq. (4.1) assumes rigid selection rules on the angular momentum and its projection for the shake-up electron. But here, as in Sec. 3, these restrictions stem from the use of the average-field approximation and do not occur in the three-electron solution of Eqs. (2.6). Kishinevskii et al.[13] therefore estimated the matrix elements which do not preserve the angular momentum of the shake-up electron using perturbation theory and included them in the calculation, even though the overlap integral in (4.1) was zero by virtue of the different angular parts of the functions X_b and X_a.

a) Post-collision interaction

The post-collision interaction was discovered by Hicks et al.[15] in a study of the reaction

$$e_s + A \to A^{**} + e_s \to A^+ + e_a + e_s, \qquad (4.2)$$
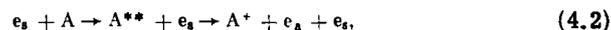
when the electron e_s scattered by atom A has an incident energy ε_0 that is slightly higher than the excitation energy of autoionizing state A^{**}. In that case, in exciting the autoionizing state the scattered electron loses almost all its energy, and, if the lifetime of the autoionizing state is less than or comparable to the characteristic separation time, the Auger decay occurs in the field of the slow electron. Here energy can be exchanged between the decaying atom and the scattered electron, and the shape of the spectrum of the emitted Auger electron e_a depends on the initial energy ε_0 of the scattered electron, being shifted toward higher energies as ε_0 decreases. This means that the excitation of the autoionizing state begins not at a value of ε_0 equal to the excitation threshold of an isolated atom, but rather at higher energies. In other words, the post-collision interaction (following the excitation of the autoionization state) causes the fast (Auger) electron to be accelerated and the slow (scattered) electron to be slowed. Experiment has shown[60] that the increase in the energy of the fast electron is equal to the decrease in the energy of the slow electron. Figure 4 shows the

V. I. Matveev and É. S. Parilis
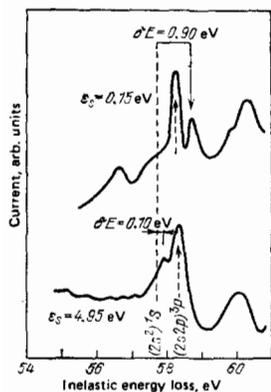
FIG. 4. Inelastic scattering spectra for electrons on atomic helium; the electron energies are close to the excitation threshold of the $(2s^2)\,^1S$ and $(2s2p)\,^3P$ states.

spectra[60] for the inelastic scattering of electrons by the helium atom for two final energies ε_s of the scattered electron, plotted as a function of the initial energy ε_0 of this electron (what is actually plotted is the current of inelastically scattered electrons versus the inelastic energy loss $\varepsilon_a = \varepsilon_0 - \varepsilon_s$). The autoionizing states appear in the spectrum as resonant line shapes and are indicated by arrows in Fig. 4. Also shown here is the displacement δE of the excitation threshold from its position in the isolated atom.

The post-collision-interaction effect is also observed[61] in the Auger decay of an atom with an inner-shell vacancy produced by absorption of a photon whose energy is slightly above the threshold for ionization of the inner shell, since here the Auger decay occurs in the presence of a slow photoelectron. Figure 5 shows the spectrum of Auger electrons emitted at various photon energies. It is seen that as the photon energy approaches the inner-shell ionization threshold (67.5 eV), the threshold shifts toward higher energies and becomes asymmetric. The dashed curves show the peaks in the isolated atom.

Interestingly, the energy of the slow electron can be decreased by the post-collision interaction to such an
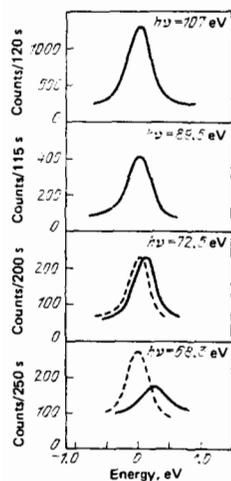
FIG. 5. The $N_5-O_{2,3}O_{2,3}\,^1S_0$ Auger peak in xenon for various photon energies.
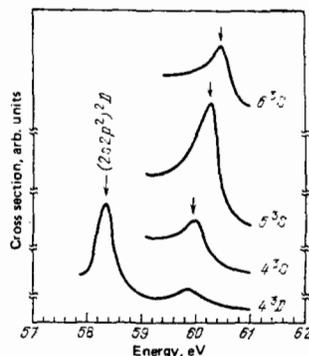
FIG. 6. Cross sections for the excitation of the 4^3D, 4^3S, 5^3S, and 6^3S states of the helium atom as functions of the initial energy of the scattered electron.

extent that this electron can be captured into a bound state by the positively charged residual ion. Such a resonant population of the high-lying bound states was discovered simultaneously by two groups of authors.[62-65] The corresponding cross sections are shown in Fig. 6. Experimental data and discussions can also be found in Refs. 16, 66, and 67.

Several theoretical models have been proposed[16-18,68] to explain this effect, in essence consisting of sudden-approximation calculations of the three-electron transition probability for reaction (4.2).

Let us begin by considering the so-called "shake-down" model,[16,69-71] in which the three-electron transition amplitude is evaluated by formula (4.1), i.e.,

$$R = AI\,(\mathbf{k}_s, \mathbf{k}_f), \qquad (4.3)$$

where A is the Auger transition amplitude of the isolated atom, $\mathbf{k}_s$ is the momentum of the scattered electron after excitation of the autoionizing state, $\mathbf{k}_f$ is the momentum of the scattered electron in the final state, ψ_{k_s} and ψ_{k_f} are the corresponding wave functions of the scattered electron, and

$$I\,(\mathbf{k}_s,\ \mathbf{k}_f) = \int d^3r\, \psi^*_{k_f}(\mathbf{r})\,\psi_{k_s}(\mathbf{r}) \qquad (4.4)$$

is the overlap integral of the wave functions of electron e_s before and after the Auger transition. In particular, ψ_{k_f} can be taken as a bound-state wave function in the field of ion A^+. In evaluating this integral it must be kept in mind that the energy E_a in the first of Eqs. (2.6) contains an imaginary part; the energy of electron e_s after excitation of the autoionizing state is then

$$\tfrac{1}{2}k_s^2 = \varepsilon_0 - \varepsilon_a + \tfrac{1}{2}\,i\gamma, \qquad (4.5)$$

where γ is the width of the autoionizing state in the isolated atom. This damping makes it possible to evaluate the overlap integral.

Another theoretical model, based on a semiclassical approach,[75] has been proposed by Niehaus and co-workers.[68,72-74] According to this model, the observable spectrum of the Auger electrons differs from that of the isolated atom because the Auger transition occurs at different distances between the atom and slow electron, the motion of the latter being described classically, i.e., a definite trajectory is assumed. It has been

shown by Van de Water and Heideman[76] that this model reduces to the shake-up approximation if the final state of the scattered electron is described semiclassically.

A more systematic application of the adiabatic approximation to the post-collision interaction, in which the scattered electron is described quantum mechanically, has been set forth by Ostrovskii.[17] In the adiabatic approximation the solution of Eqs. (2.6) is of the form

$$\Phi_{a,b} = \psi_{a,b}(r_1, r_2; R) X_{a,b}(R), \qquad (4.6)$$

where $\psi_{a,b}$ are the known wave functions for the two-electron Auger transition $\psi_a \to \psi_b$ in the quasimolecule formed for a fixed position R of the slow electron, and $X_{a,b}$ are the unknown wave functions of the initial and final states of the slow electron, which are found by solving a system of equations analogous to (3.4). As a result, the two-electron Auger transition rate is dependent on R, i.e., $\Gamma_a \equiv \Gamma_a(R)$, and the amplitude for a three-electron transition which leaves the atom ionized and the scattered electron in state X_b is of the form

$$R_{ba} = \int d^3R \sqrt{\Gamma_a(R)} (X_b^*(R), X_a(R)). \qquad (4.7)$$

Finally, one can solve system (2.6) using perturbation theory, taking into account the diagrams containing the average field in all orders, as was done by Amus'ya et al.[18]

Since calculation of the quasimolecular states is a separate and rather complicated computational problem,[77,78] it was assumed by Ostrovskii[17] that the presence of the slow electron affects only the energy of the Auger electron, just as in the semiclassical model, the width of the autoionizing state in (4.7) was assumed to be independent of R and equal to the width in the isolated atom.

The above models agree fairly well with experiment, but, as we mentioned earlier, the single-electron sudden approximation cannot account for the transfer of angular momentum in a shake-up process, whereas experimentally[64-67,77] one observes transitions which involve a change in the angular momentum of the slow (shake-up) electron. Furthermore, it happens that the displacement of the excitation threshold (see Fig. 4) is not described by $\delta E \sim v^{-1}$ for all the autoionizing states, as is implied by the semiclassical model.[61] The deviations can evidently be explained using a quasimolecular approach (4.7). Qualitative agreement can be achieved[79] by incorporating the deviations of the autoionizing terms from Coulomb terms and taking into account the R dependence of the width of the autoionizing state, using the mixing of the autoionizing states of the isolated atom by the field of the slow electron,[59,80,81] which is analogous to the Stark effect. In addition, the quasibound states of the He$^-$ ion lying near the autoionizing states of the helium atom apparently contribute to the exchange of angular momentum.[64,65,67]

b) Auger decay stimulated by collision with a fast electron

Let us consider for the sake of definiteness the scattering of an electron by a helium atom in the autoioniz-

ing state $2p^2{}^3P$, the Auger decay of which is forbidden by selection rules.[34] The presence of the scattering electron lifts this restriction on Auger decay (cf. Sec. 3a), and one can characterize the process by a cross section. The transition is accompanied by a change of state of three electrons—the projectile electron and two atomic electrons; one of the atomic electrons fills the 1s state, the other goes either to a state of the discrete spectrum or to a continuum state in the field of the He$^+$ ion, and the projectile electron is scattered. The perturbation responsible for the transition is

$$U \cdot -\frac{2}{R} + \frac{1}{|R - r_1|} + \frac{1}{|R - r_2|} + \frac{1}{r_{12}} \approx \frac{R}{R^3}(r_1 + r_2) + \frac{1}{r_{12}}, \qquad (4.8)$$

where r_i are the coordinates of the atomic electrons and R the coordinates of the projectile electron. We have retained in (4.8) only the dipole terms, as is the usual practice in considering the scattering of fast electrons by atoms.[4] To apply the shake-up approximation, we can separate the perturbation (4.8) into strong $W = r_{12}^{-1}$ and weak $V = R(r_1 + r_2)R^{-3}$ parts. However, let us first treat the problem by perturbation theory. To get a nonzero three-electron transition amplitude one must go at least to the second order of perturbation theory in the potential U. Then, of the products of matrix elements UU, only VW and WV will appear in the states of the three particles. The transition amplitude is thus

$$R_{ba} \cdot \cdot (\varphi_b(R), \frac{R}{R^3} \varphi_a(R)) B, \qquad (4.9)$$

where

$$B = \sum_s \frac{(\Psi_b, r_{12}^{-1}\Psi_s)(\Psi_s, (r_1 + r_2)\Psi_a)}{\varepsilon_b - \varepsilon_s + i\delta} + \sum_s \frac{(\Psi_b, (r_1 + r_2)\Psi_s)(\Psi_s, r_{12}^{-1}\Psi_a)}{\varepsilon_a - \varepsilon_s + i\delta}, \qquad (4.10)$$

where ψ_a, ψ_s, ψ_b and $\varepsilon_a, \varepsilon_s, \varepsilon_b$ are the wave functions and energies of the atom in the initial, intermediate (s), and final states, respectively, and $\varphi_{a,b}(R) = \exp(ip_{a,b}R)$ are the states of the projectile electron. Integrating over the angles of the scattered electron, we obtain the cross section of the transition as[69]

$$\sigma = \frac{8\pi}{v^2}\left(\ln \frac{q_{max}}{q_{min}}\right) \frac{|B|^2}{3}, \qquad (4.11)$$

where q is the momentum transfer in the collision and, as usual,[4] $q_{min} = |\varepsilon_b - \varepsilon_a|v^{-1}$, while $q_{max} \sim r_0^{-1}$ is found from the conditions for applicability of the dipole expansion (4.8), which is valid at distances down to around the atomic dimensions $\gtrsim r_0$. Amplitude (4.9) formally coincides with the amplitude for the two-electron radiative Auger transition (see Sec. 3a), so we shall estimate the amplitude in the shake-up approximation rather than using the somewhat complicated formula (4.10); in other words, the projectile electron causes a transition of the atom from state $2p^2$ to state $2p1s$, and the electron remaining in the $2p$ state is shaken up to either a bound state or continuum state. This approach enables one to compare the cross section for the three-electron transition with that of the two-electron transition in which the projectile electron is scattered and the atom goes from $2p^2$ to $2p1s$; Landau and Lifshitz[4] give the latter cross section as

$$\sigma_s = \frac{8\pi}{v^2}\left(\ln \frac{q_{max}}{q'_{min}}\right) \frac{|(2p^2, d, 1s2p)|^2}{3}, \qquad (4.12)$$

where $q'_{min} = |\varepsilon'_b - \varepsilon_a|v^{-1}$, with ε'_b being the energy of the 2p1s state.

In the shake-up approximation

$$B \quad (2p, d, 1s)(X_b, X_{2p}).\qquad(4.13)$$

The ratio of the cross sections for the three-electron (4.11) and two-electron (4.12) transitions, after cancellation of the slowly varying logarithmic functions, will be of the form

$$\frac{\sigma}{\sigma_e} \approx |(X_b, X_{2p})|^2,\qquad(4.14)$$

i.e., will be simply the overlap integral of the 2p state with the final state of the shake-up electron. Consequently, in a certain percentage of cases, scattering involving the transition $2p^2 \to 2p1s$ will be accompanied by the transition $2p^2 \to (n \text{ or } \varepsilon)p1s$.

c) Excitation of atoms by fast electrons

When a fast electron is scattered by a many-electron atom, the possible effects include double ionization and single ionization with simultaneous excitation. Here, as in Sec. 4b, the interaction between the projectile and atomic electrons is considered small and only the dipole terms in the expansion of the potential (4.8) are taken into account. The problem then becomes analogous to photoionization. If it is considered that the projectile electron is adequately described by plane waves, then the wave functions of the atomic electrons in the initial and final states can be chosen in the form described in Secs. 3c,d. The transition amplitude

$$R_{ic} = \left(\varphi_i, \frac{R}{R^3}\varphi_c\right)(\Phi_i(r_1, r_2)\cdot(r_1 + r_2)\Phi_n(r_1, r_2))\qquad(4.15)$$

in this case is proportional to the photoionization amplitude and has the typical form for the shake-up approximation.

d) Three-electron Auger transitions. The double Auger effect

The term "three-electron Auger transition" is applied to transitions involving three bound electrons which result in the filling of an inner-shell vacancy and the transition of an electron to the continuum, with the remaining electron being either "shaken off" into a continuum state (the double Auger effect; Fig. 7a), "shaken up" to a bound excited state (Fig. 7b), or else, if there is another inner-shell vacancy, "shaken down" into it (the half Auger effect; Fig. 7c). This last effect was first observed experimentally by Afrosimov et al.,[12] who called it a "three-electron Auger transition," a name which unfortunately does not distinguish it from the double Auger effect, for example. To describe the many-electron Auger transitions it is convenient to use
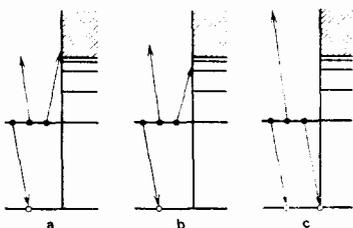
a fraction, with the number of Auger electrons emitted in the numerator and the number of vacancies filled in the denominator. Following this principle, Kishinevskii and the present authors, in giving the theory for the effect illustrated in Fig. 7c, called it the "half Auger effect."[13]

If one of the electrons is in a highly excited orbital (i.e., is slow), then the three-electron Auger transitions would be more correctly treated in the shake-up approximation, as in the case of the post-collision interaction, while second-order perturbation theory would not give as good results on account of the small electron energy. As a rule, however, the three electrons involved in the transition are all in the same shell, and it is more correct to calculate the transition amplitude using second-order perturbation theory.[14] Such calculations are rather complex and can be done only numerically, whereas the shake-up-approximation calculation can easily be done analytically and is extremely easy to interpret. For this reason, the first calculations for the three-electron Auger effect were done in the shake-up approximation (for both the double[82-84] and half[13] Auger effects).

The double Auger effect was first detected[82] in an analysis of the charge state of neon ions following photoionization of the K shell by γ rays at a photon energy too low to cause two vacancies simultaneously in the K and L shells. At such energies, Ne^{3+} ions can only result from the double Auger effect. More careful measurements have since been made[83] by analysis of the energy spectrum of the Auger electrons emitted in the decay of vacancies in the L shell of argon. In the double Auger effect the energy of the Auger transition is divided between the two emitted electrons (Fig. 8). The authors of these papers offered a shake-up mechanism to explain the existence of the double Auger effect, but calculations of the overlap integral with Hartree-Fock wave functions for the shake-up electrons gave a value for the probability (0.6%) that differed by more than an order of magnitude from the experimental value (10%). This led those authors to conclude that the interelectron correlations must be taken into account. Here it is necessary to take the correlations into account not only in the initial state, in which all three electrons are in nearby shells, but also in the final state, since in this

FIG. 7. Three-electron Auger transition. a), b) Double Auger effect; c) half Auger effect.
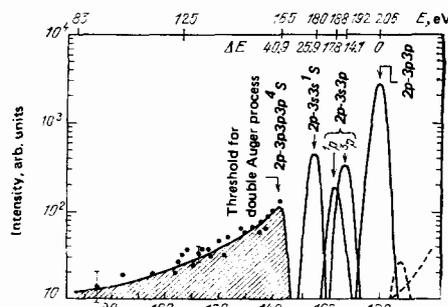
FIG. 8. Spectrum of Auger electrons emitted in the decay of $L_{2,3}$ vacancies in argon. The hatched part of the spectrum is due to Auger electrons emitted as a result of the double Auger effect. The threshold energy for the onset of the double Auger effect is 165 eV.

case there are two slow electrons in the continuum. In particular, it is necessary to take into account the terms in perturbation theory that describe the double Auger effect as the knocking out of another electron by the outgoing Auger electron. One can nevertheless estimate the probability of the double Auger effect using single-electron wave functions. If it is considered that the electrons participating in the double Auger transition have comparable velocities in both the initial and final states, the operative angular-momentum selection rules are not the monopole rules but the less stringent three-electron selection rules. This circumstance makes it possible for the shake-up electron to exchange angular momentum during the shake-up process. Since the three electrons all participate in the transition on equal footing, it is to be supposed that shake-up involving a change in angular momentum is about as probable as shake-up without a change in angular momentum. This leads to a substantial increase in the number of final states of the shake-up electron, and in order to obtain a correct estimate of the probability of the double Auger effect, one must multiply the probability in the single-electron approximation by the number of final states. This results in a value for the transition probability that agrees in order of magnitude with the value found in experiment.

The shake-up accompanying Auger transitions, as in the case of radiative transitions, has an important effect on the relative abundances of the ions obtained as a result of the reorganization of the electron shells following the formation of inner-shell vacancies and also on the energy spectrum of the electrons emitted in the process. Therefore, shake-up processes must be taken into account in calculating the cascades of transitions which arise in the decay of inner-shell vacancies in many-electron atoms. Table I, which was taken from Ref. 84, gives the relative probabilities (in %) for the shake-off of electrons from the various shells of krypton as a result of photoionization and Auger transitions, as calculated in the sudden approximation with self-consistent wave functions. The probability for shake-off of an electron from state $\psi_{i,nl}$ into all the other states was evaluated by the formula

$$P_{nl} = 1 - \{|(\psi_{f,nl}, \psi_{i,nl})|^2\}^N - NP_F, \qquad (4.16)$$

where N is the number of shake-off electrons, P_F is the probability of a transition to levels which are forbidden by the Pauli principle, and $\psi_{f,nl}$ is the wave function de-

scribing the state of the shake-off electron that has the same quantum numbers n and l as the initial state, but after the photoionization or Auger transition. The data in Table I should be considered correct if the initial states of the shake-off electron (column 1) lie above the states of the electrons involved in the photoionization or Auger transition. If the shake-up occurs from the same shell one must, as we mentioned earlier, allow for the exchange of angular momentum. The calculated charge spectra of krypton ions formed as a result of the cascade decay of an inner-shell vacancy are in fair agreement with experiment.

e) Half Auger effect

The three-electron Auger decay of states having two inner-shell vacancies, wherein the vacancies are filled by two outer electrons and all the excess energy is carried off by the third electron, was discovered[12,85-87] in studies of the high-energy part of the spectrum of electrons emitted during atomic collisions. The existence of the half Auger effect is detected by the appearance of a bump in the high-energy part of the Auger-electron spectrum at an energy roughly twice that of the Auger electron emitted in the ordinary Auger decay of a single inner shell vacancy. Figure 9 shows the spectrum of Auger electrons emitted in the decay of two K vacancies formed in nitrogen during N^+-N_2 collisions. The intense peak at an electron energy of 345 eV corresponds to the ordinary K–LL Auger transitions. The peak at 765 eV corresponds to KK–LLL three-electron Auger transitions. A review of the experimental data on the half Auger effect has been given by Shergin and Gordeev.[87] The transition probabilities have been calculated in second-order perturbation theory by Ivanov et al.[14] Such calculations require some rather awkward numerical computations. Let us therefore consider how one might estimate the probability for the half Auger effect in the shake-up approximation.[13]

Suppose we have a three-electron ion whose K shell is empty and whose L shell contains the three electrons, with an initial configuration of $2s^22p$ and a final configuration of $1s^2\epsilon p$. According to (3.7), the overlap integral of the 2s and 1s states is given by

$$I^2 = 0.31 \left(\frac{\Delta z}{z}\right)^2 = \frac{0.012}{z^2}. \qquad (4.17)$$

TABLE I. Electron shake-off probabilities due to photoionization and Auger processes in krypton.

State	Photoionization			Auger transition		
	1s	2s	2p	1s – 2p2p	2p – 3p3p	2p – 3d3d
1s	0.004	0.000	0.000	0.003	...	...
2s	0.053	0.003	0.007	0.019	0.002	0.008
2p	0.27	0.026	0.034	0.016	0.032	0.03
3s	0.25	0.085	0.100	0.042	0.019	0.012
3p	1.22	0.523	0.59	0.22	0.05	0.067
3d	3.66	3.39	3.48	2.88	0.16	0.112
4s	2.23	1.85	1.98	1.46	0.95	1.00
4p	13.90	12.18	12.37	7.23	5.09	5.38
Totals	21.6	18.1	18.6	11.9	6.3	6.59

FIG. 9. Spectrum of Auger electrons emitted in the decay of two K vacancies in the nitrogen atom.

One can immediately arrive at a very simple estimate by considering the fact that according to (4.1) the ratio of the three-electron transition frequency Γ to the two-electron Auger-transition frequency Γ_a is described by the relation

$$P = \frac{\Gamma}{\Gamma_a} \sim I^2. \qquad (4.18)$$

Then for $z = 6$ we have $P = 3.3 \cdot 10^{-4}$ and for $z = 7$ we have $P = 2.4 \cdot 10^{-4}$, in rather good agreement with the results of Afrosimov et al.[12]

To obtain more exact estimates, we must perform the averaging over the initial and summation over the final states of the electrons involved in the three-electron Auger transition. Since the electron shells of all the atoms for which the three-electron transition probabilities have been measured[37] contain only s and p electrons, we introduce the following notation for the rates of the two-electron Auger transitions: w_{ss} for the transition involving two s electrons, w_{sp} for that involving s and p electrons, and w_{pp} for that involving two p electrons. Because of the large number of Auger transitions, one can use the average values of the two-electron Auger transition rates and of the overlap integrals. Furthermore, in the three-electron transition all the electrons may participate on an equal footing, and only the spin selection rules need be considered. The probability ratio for the half Auger effect compared to the two-electron Auger transition is therefore of the form[13]

$$P = \frac{\sum_{i=1}^{N} (n_i w_{ss} + m_i w_{sp} + k_i w_{pp})}{\sum_{i=1}^{N} (N_i w_{ss} + M_i w_{sp} + K_i w_{pp})} \bar{I}^2 \equiv \beta \bar{I}^2. \qquad (4.19)$$

where N is the number of initial states; n_i, m_i, and k_i are the numbers of possible Auger transitions accompanied by the shake-up of a third electron which involve two s electrons, an s and a p electron, or two p electrons, respectively; N_i, M_i, and K_i are the corresponding numbers for all the possible two-electron Auger transitions from the initial state i; $\bar{I}$ is the average value of the overlap integral, which for KK–LLL transitions is taken from (3.7), while the overlap integrals of the 2s and 3s and of the 2p and 3p states are given by

$$\bar{I}^2(2s, 3s) = 0.78 \left(\frac{\Delta z}{z}\right)^2,$$
$$\bar{I}^2(2p, 3p) = 1.1 \left(\frac{\Delta z}{z}\right)^2. \qquad (4.20)$$

In this case there are many possibilities for transitions to vacancies in the L shell or into ss, sp, and pp holes; simply taking the average value for Δz according to the

FIG. 10. Dependence of the relative probability for three-electron transitions on the number n of electrons in the outer shells of neutral atoms. The points are experimental values; the curve, theoretical.

rules of Burns,[32] we find that

$$\bar{I}^2(2s, 3s) \approx \bar{I}^2(2p, 3p) \approx 9 \cdot 10^{-2} z^{-2}. \qquad (4.21)$$

The results of the calculations are given in Table II. Figure 10 shows how the relative probability of the three-electron transition depends on the number n of electrons in the outer shells of neutral atoms. It is seen that the dependence is linear. Such a dependence is easily explained by the following qualitative arguments: Because essentially all n electrons can participate in the three-electron transition, the probability for such a transition goes as $n(n - 1)(n - 2)$, while the probability for the two-electron Auger transition goes as $n(n - 1)$; their ratio then goes as $(n - 2)$, as was observed experimentally.[12]

Thus the calculated results agree with experiment.[12] Furthermore, the coefficient β in formula (4.19) turns out to depend very weakly on the probability ratios for the two-electron Auger transitions, being given for all configurations of three electrons as $\beta \approx 3/4$, for four electrons as $\beta \approx 1$, for five electrons as $\beta \approx 1.6$, and for six electrons as $\beta \approx 2$.

5. CONCLUSION

In this short review of the various shake-up effects accompanying transitions in the electron shells we have seen that these effects are rather widespread and are, in fact, manifestations of the reaction of a many-electron system to a sudden change in the state of a part of the system. The fact that complex relaxation processes can be reduced to a physically clear and easily calculated shake-up effect is a great convenience for theorists and also for experimentalists who wish to interpret and estimate effects of this type.

The shake-up approximation for atomic transitions provides a unified method of examining three-particle transitions whose amplitudes are nonzero in perturbation theory only in orders higher than the first. In cases where one can separate the perturbation responsible for the transition into weak and strong parts, the shake-up approximation has a wider domain of applicability than perturbation theory, since the weak part is treated by perturbation theory while the strong part is taken into account exactly with the aid of the different wave functions for the initial and final states. In cases where the potentials causing the three-particle transi-

TABLE II. Relative probabilities of three-electron Auger transitions.

Atom with two inner vacancies	Transition	Experiment (×10⁴)	Theory (×10⁴)	Atom with two inner vacancies	Transition	Experiment (×10⁴)	Theory (×10⁴)
C	KK–LLL	2.2	2.5	S	LL–MMM	5.4	5.9
N	KK–LLL	3.4	2.8	Cl	LL–MMM	6.2	6.5
Si	LL–MMM	2.5	2.6	Ar	LL–MMM	9.7	9.8

tion can be considered weak, the shake-up-approximation results go over to the perturbation-theory results.

The method employing a change in the average field permits a substantial simplification of the calculations for transitions and can be used to estimate the probabilities of various effects.

We have examined three-particle transitions whose amplitudes are nonzero in the second-order of perturbation theory. In this case, one can, as a rule, carry out direct calculations of the transition amplitudes by perturbation theory, and the shake-up approximation is an alternative method. However, for treating transitions involving four or more particles a direct perturbation-theory solution would be prohibitively complex. For example, transitions to three inner-shell vacancies are possible (three-electron–one-photon or four-electron Auger transitions), in which the three inner-shell vacancies are filled by three outer electrons and all the excess energy is carried off by a single photon or electron. More than double ionization by a photon or by an electron is also possible. In the cases just mentioned, the transition amplitude will be nonzero only in the third and higher orders in perturbation theory. Here the shake-up approximation is the only practical way of calculating these effects.

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