interference between electrons of the same energy but emitted at different instants of time from different states when several autoionization states are excited during the collision.[17] These oscillations can also be investigated by the method outlined above.

There are also other properties of the spectra such as inflections, which appear when a new autoionization channel is opened,[16] but these are difficult to observe.

In the analysis given above, the motion of the nuclei was described classically. A quantum-mechanical description is required for small relative velocities of the colliding particles and for the description of the scattering of light particles (an example of this is given by Ostrovskiĭ[18]).

The authors are indebted to Professor Yu. N. Demkov and Professor N. P. Penkin for their interest in this work.

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1) The quadratic approximation to the state energy was used previously by Ostrovskiĭ[4] to investigate spectrum features due to the turning point in the radial motion of the nuclei.

2) As already noted, $E_0(R)$ is the difference between the energy of the discrete term and the limit of the continuous spectrum.

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Theory of excitation of a quantum nonlinear oscillator by a harmonic force

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The first quantum corrections to the classical equations of motion of a nonlinear oscillator are derived. Experiments on the excitation and dissociation of molecules by laser radiation are discussed. It is shown that a molecule can be excited to considerably larger quantum numbers than is indicated by elementary theory: for typical values of the parameters this difference amounts to one and one-half orders of magnitude.

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Experiments on the excitation of molecular vibrations by laser radiation pose problems in the theory of vibrations whose solution requires that quantum effects must not be neglected. Even in the simplest case, however, that of a one-dimensional nonlinear oscillator, inclusion of quantum effects is an extremely complicated problem. There have been many papers[1-24] on attempts to solve this problem using various simplifying assumptions. Although a number of interesting results have been obtained in these papers, there still exists no consistent theory of such excitation, so that in many experimental researches on excitation of molecules the results are analyzed by means of the elementary theory, in which both nonlinear and quantum effects are essentially ignored. Accordingly, we feel it worth while to construct in this paper a comparatively simple consistent theory, providing a framework in which an answer to any question about excitation can be found. It takes nonlinear effects into account to a high degree of accuracy, and quantum effects are also included, but only approximately. The approximation we use is that corrections to the center of gravity of a wave packet and to its dimensions in a certain space (see Secs. 1 and 3) are considered only to and including the first nonvanishing order in $\hbar$; the spreading of packets is assumed to be small. We shall call this approximation semiquantal theory.$^{1)}$ In this theory quantum numbers can be comparable with unity.

Numerical estimates show that semiquantal theory cannot be applied to the quantitative description of experiments on the excitation of molecules, since for typical values of the parameters there is rapid spreading of the packets. Nevertheless, semiquantal theory is still of value in this situation, since it enables us to calculate a lower bound on the average vibrational quantum number to which a molecule can be excited. This lower bound is about one and one-half orders of magnitude larger than that found from the elementary theory. This greatly decreases the difficulties encountered in theoretical models for explaining the dissociation of molecules.

In the first section we write out the equation for the density matrix and the equations of semiquantal theory which can be derived from it. We shall not present the actual derivation, since it contains only cumbersome elementary calculations. We then discuss the results (Sec. 2) and the region of applicability (Secs. 3 and 4) of semiquantal theory, and use it to analyze the excitation of vibrations in molecules (Sec. 5). To demonstrate lucidly the difference between the semiquantal and elementary theories, we give in the Appendix a simple way to obtain the correct explicit expressions for the mean quantum number and the resonance width for a nonlinear oscillator.

1. Let us consider a one-dimensional nonlinear quantum oscillator with Hamiltonian $\hat{H}$. Let $|n\rangle$ be the stationary states: $\hat{H}|n\rangle = E(n)|n\rangle$; the energy spectrum $E(n)$ is of the form

$$E(n)=\hbar(\omega_{01}+{}^1/_2\alpha)n-{}^1/_2\hbar\alpha n^2, \tag{1}$$

where ω_{01} is the frequency of the transition $0\to 1$, and α is an anharmonicity constant. The Hamiltonian for the interaction with the laser field $E(t)=E\cos\omega_1 t$ is $-E(t)\hat{d}$, where $\hat{d}$ is the dipole moment operator.

Let $|osc\rangle$ be the state vector (wave function) of the oscillator; we introduce the function $\xi_a(t;U,V)=\langle\beta|osc\rangle$, where $\beta=U+iV$ is an arbitrary complex number, and

$$|\beta\rangle=\exp\left(-\frac{|\beta|^2}{2}\right)\sum_{n=0}^{\infty}\frac{\beta^n}{(n!)^{1/2}}|n\rangle. \tag{2}$$

For the properties of the states $|\beta\rangle$ and their connection with coherent states for the linear oscillator see Sec. 3. Obviously,

$$p(t;\ U,\ V)=\pi^{-1}|\xi_a(t;\ U,\ V)|^2$$

are the diagonal elements of the density matrix in the representation of the states $|\beta\rangle$. The main advantage of this representation is that the equation for the diagonal elements of the density matrix does not contain the nondiagonal elements; this equation is[24]

$$\frac{\partial p}{\partial t}=[\delta\omega+\alpha n]V\frac{\partial p}{\partial U}-\left[(\delta\omega+\alpha n)U+\frac{f}{2}\right]\frac{\partial p}{\partial V}$$
$$-\frac{\alpha}{2}\left[UV\left(\frac{\partial^2 p}{\partial U^2}-\frac{\partial^2 p}{\partial V^2}\right)+(V^2-U^2)\frac{\partial^2 p}{\partial U\,\partial V}\right], \tag{3}$$

where $n=U^2+V^2$, $\delta\omega=\omega_1-\omega_{01}$ is the frequency detuning, and $f=Ed_{01}/\hbar$ is the field broadening. Equation (3) holds if

$$|\delta\omega|,\ \alpha,\ f^{2/3}\alpha^{1/3}\ll\omega_l.$$

In the classical limit the wave packet of the distribution p is localized in the neighborhood of a certain point on the β plane; that is,

$$p(t;\ U,\ V)=\delta(U-U_c(t))\delta(V-V_c(t)).$$

Equation (3) describes the motion and the diffusion (more accurately, the smearing out) of the wave packet in the β plane. The diffusion, caused by the presence of second derivatives in Eq. (3), occurs only for the nonlinear oscillator ($\alpha\neq 0$) when quantum effects are taken into account. This assertion becomes obvious if we express the anharmonicity constant α in terms of classical quantities; we have

$$\alpha=-\frac{d^2E}{dn^2}\frac{1}{\hbar}=-\hbar\frac{d^2E}{dI^2}=-\hbar\frac{d\omega_v(I)}{dI},$$

where $\omega_v(I)=dE/dI$ is the classical frequency, $I=\hbar n$ being the action variable.

Using Eq. (3), one can obtain equations describing the change with time of the quantities U_c and V_c, and also the quantum corrections to these quantities. The calculation must be made in the following way. From Eq. (3) we obtain equations for the coordinates U_c and V_c of the center of gravity of the packet and for the second moments of the distribution p, i.e., for

$$M_{UU}\equiv\int dU\,dV\,p(t;U,V)\,(U-U_c(t))^2$$

and for M_{VV} and M_{UV}, which are similarly defined. We neglect the higher-order moments. Suppose that initially ($t=0$) the oscillator is in the ground state. Then $U_c(0)=V_c(0)$, and the moments M can easily be shown to have the values $M_{UU}=M_{VV}=\frac{1}{2}$, $M_{UV}=0$. On the assumption that the moments $M(t)$ change only slightly during a period T of the motion of the point $\beta_c=U_c+iV_c$ in the β plane, i.e., that the wave function does not spread much in the time T, we find that the population p_n of the n-th level is given by the Poisson formula

$$p_n(t)=|\langle n|osc\rangle|^2=e^{-\bar{n}(t)}\frac{(\bar{n}(t))^n}{n!},\qquad(4)$$

where $\bar{n}(t)=U_c^2(t)+V_c^2(t)$ [cf. Eq. (2)]. Let us substitute constant values of the moments M in the equations for U_c and V_c; we thus find the first quantum corrections to the quantities U_c and V_c. Next, we can derive from the equations for U_c and V_c an equation in closed form for the one quantity in which we are interested—the average quantum number $\bar{n}(t)$, which according to Eq. (4) completely describes the excitation of the oscillator. This last equation has the potential form[12]

$$d^2\bar{n}(t)/dt^2=-dV/d\bar{n}.\qquad(5)$$

The potential V depends on $\bar{n}$ and on the frequencies $\delta\omega$, f and α. Moreover, it depends on the initial values $\bar{n}(0)$ and $d\bar{n}(0)/dt$ and the parameters. Excitation of the oscillator from the ground state corresponds to the initial conditions $\bar{n}(0)=d\bar{n}(0)/dt=0$; in this case the potential V is given by

$$V=\frac{f^2}{2}\left[-\bar{n}+\frac{\bar{n}^2}{4f^2}(\alpha\bar{n}+2\delta\omega)^2\right].\qquad(6)$$

2. Let us consider some semiquantal-theory results that can be derived easily from Eqs. (4)–(6). For excitation from the ground state the quantity $\bar{n}(t)$ reaches its maximum value at $t=T/2$, where T is the period of the motion in the potential V. If the frequencies α and f are given, the maximum value of $\bar{n}$ depends only on $\delta\omega$; we denote it by $\bar{n}_{\max}(\delta\omega)$ and write it in the form

$$\bar{n}_{max}(\delta\omega)=\bar{n}_{max}F_1(x),\qquad(7)$$

where $x=\delta\omega/\delta\omega_c$ and

$$\delta\omega_c={}^3/_2f^{2/3}\alpha^{1/3},\quad \bar{n}_{max}=4(f/\alpha)^{2/3}.\qquad(8)$$

Figure 1 shows the potential $V(\bar{n})$ for the case $\delta\omega=-\delta\omega_c$ (i.e., $x=-1$). If $\delta\omega>-\delta\omega_c$, the inner maximum lies below the axis $V=0$; if, on the other hand, $\delta\omega<-\delta\omega_c$, the maximum is higher and the second well is inaccessible. Accordingly, the function $F_1(x)$ has a discontinuity at the point $x=-1$, and takes its maximum value 1 to the right of $x=-1$: $F_1(-1+0)=1$; to the left of $x=-1$ we have $F_1(-1-0)=\frac{1}{4}$; for $|x|\gg1$ the form is $F_1(x)=9/x^2$. The curve of $F_1(x)$ is shown in Fig. 2. The quantity $\bar{n}_{\max}$ is the maximum average quantum number to which the oscillator can be excited for given values of the anharmonicity α and the field broadening f; $\delta\omega_c$ has the meaning of a resonance width for the nonlinear oscillator.

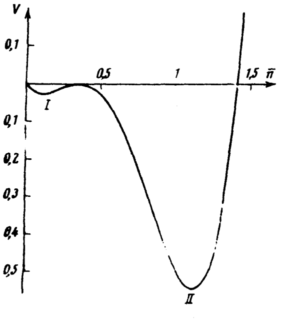

FIG. 1. The potential $V(\bar{n})$ which describes the excitation of the oscillator from the state of rest when the frequency detuning is $\delta\omega=-\delta\omega_c$. The axes are marked with scales in accordance with Eqs. (6) and (13).

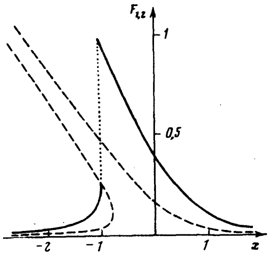

FIG. 2. The function $F_1(x)$. The dashed curves show the function $F_2(x)$.

For an instantaneous application of the field, with $E(t<0)=0$, the average quantum number $\bar{n}$ undergoes beats. If, on the other hand, the field E is turned on adiabatically, there are no beats, and $\bar{n}$ increases along with the increase of the field amplitude. Let us denote the average value of n for the case of adiabatic application of the field by $\bar{n}_{ad}$. This quantity is given by the equation

$$(\delta\omega+\alpha\bar{n}_{ad})^2\bar{n}_{ad}={}^1/_4f^2,\qquad(9)$$

where $f=Ed_{01}/\hbar$ and $E=E(t)$ is the varying amplitude of the field. We note that this is precisely the sort of equation that holds for the quantity $I/\hbar$, where I is the action variable of a classical nonlinear oscillator executing forced vibrations in the presence of a small friction. The solution (9) can be put in the form $\bar{n}_{ad}=\bar{n}_{\max}F_2(x)$. The function $F_2(x)$ is three-valued for $x<-2^{-1/3}$ and is shown as the dashed curve in Fig. 2. Analytic expressions for $F_{1,2}(x)$ are given in[25].

In classical language, the period T of the motion in the potential V is the beat period of the oscillator amplitude. For excitation from the ground state the period T is

$$T=F_4(x)/\delta\omega_c,$$

where

$$F_4(x)=6(F_1(x))^{1/2}\int_0^1\frac{dy}{[y-y^2F_1(x)(4F_1(x)y+3x)^2]^{1/2}}.$$

The function $F_4(x)$ has a singularity of the type of $-\ln|1+x|$, with $F_4(-1+\varepsilon)=2F_4(-1-\varepsilon)$ for $\varepsilon\to0$. For $|x|\gg1$, $F_4(x)=2\pi/|x|$. Values of $F_4(x)$ are given in Table I.

3. Let us discuss the region of applicability of the semiquantal theory. The spreading of the packet during a beat period T will be small if the anharmonicity constant $\alpha\ll1/T$. In fact, since in Eq. (3)

$$|\delta\omega+\alpha n|\sim|\delta\omega+\alpha n+f/2U|\sim1/T,$$

we can neglect the second derivatives in (3) when αT

TABLE I.

x	F_4	x	F_4	x	F_4	x	F_4
−6	1,05	−1,25	5,86	−0.999	31,6	−0.5	11.2
−4	1.58	−1,10	7,60	−0.99	23.6	0	9,16
−2	3,33	−1.01	11.8	−0.90	16.1	2	3,06
−1,5	4,42	−1,001	15,8	−0,75	13,2	4	1.56

$\ll 1$. Therefore, for the semiquantal theory to be applicable over times of order T the inequality

$$\alpha T = \hbar \frac{d\omega_v(I)}{dI} T \ll 1 \tag{10}$$

must be satisfied. This condition can also be derived in a more rigorous way from the system of equations for U_c, V_c and the moments M.

If $\alpha T \gtrsim 1$, the wave packet spreads a great deal during even a single beat period. This restricts the region in which Eqs. (4)–(6) can be applied, since they are derived from Eq. (3) along with the condition $\alpha T \ll 1$, which does not apply however, to the validity of (3) itself. The fact that the wave packet spreads also does not limit the possibility of expanding an arbitrary state in terms of the system of states $|\beta\rangle$. In fact, for $\alpha = 0$ the states $|\beta\rangle$ are the well known coherent states of the linear oscillator, in terms of which one can expand any state, since the completeness condition

$$\hat{1} = \int \frac{dU\,dV}{\pi} |\beta\rangle\langle\beta| \tag{11}$$

is satisfied. However, according to the definition (2) the relation (11) holds also for $\alpha \neq 0$, since it requires only that the stationary states $|n\rangle$ that appear in Eq. (2) be a complete set. We need the condition $\alpha T \ll 1$, and the associated slowness of the spreading of the packet only to let us get from the complicated equation (3) to the comparatively simple semiquantal theory (4)–(6).

Near a resonance, i.e., when $|\delta\omega + \delta\omega_c| \lesssim \delta\omega_c$, the beat period $T \sim 1/\delta\omega_c \sim 1/f^{2/3}\alpha^{1/3}$. In this case the condition $\alpha T \ll 1$ takes the form $(f/\alpha)^{2/3} \sim \bar{n}_{\max} \gg 1$. Far from resonance, i.e., when $|\delta\omega + \delta\omega_c| \gg \delta\omega_c$, the function $F_4(\delta\omega/\delta\omega_c) = 2\pi\delta\omega_c/|\delta\omega|$, and the condition $\alpha T \ll 1$ takes the form $\alpha \ll |\delta\omega|$. This condition can be satisfied, independently of whether the quantity $\bar{n}_{\max}(\delta\omega)$ is small or large relative to unity. Accordingly, the application of the semiquantal theory is not restricted to the case of large quantum numbers.

We note that the expressions (7) and (8) are obtained if we write the corresponding formulas of classical theory[12] in quantum notation and make the substitution

$$\omega_v(I) \to \omega_v(I) + \hbar\, d\omega_v(I)/dI. \tag{12}$$

The result (12) was obtained in a special case in[26].

Although the expressions (7) and (8) are of essentially classical nature, the semiquantal theory does not reduce to classical theory, since besides Eqs. (7) and (8) it enables us to derive the nontrivial relations (4) and (10), and also the formula (12), which is of some methodological importance.

4. Let us discuss qualitatively the excitation of the oscillator in the case in which the wave packet spreads appreciably during a single beat period, i.e., for $\alpha T \gtrsim 1$. Numerical calculations[25, 27–30] show that if $\delta\omega < -\delta\omega_c$, then during a time of a few periods T an excess population appears on levels with $n \gtrsim \bar{n}_{\max}$; this excess can be orders of magnitude larger than the population calculated from Eq. (4). This phenomenon can be regarded as tunneling[20] into the second potential well of the potential $V(\bar{n})$ (region II in Fig. 1), which for $\delta\omega < -\delta\omega_c$ is separated from the first well (region I) by a potential barrier. It is clear from general considerations that the tunneling can only increase the population on levels with $n \geqslant \bar{n}_{\max}$, and this is confirmed by the numerical calculations. An analytical investigation of the population of levels with $n \gtrsim \bar{n}_{\max}$ in the case $\delta\omega < -\delta\omega_c$ is a very complicated problem, since quantum effects must be completely taken into account.

In this case the semiquantal theory is useful, whether or not the condition $\alpha T \ll 1$ is satisfied, because by using the formulas (4) and (8) we can estimate a lower limit on the actual values of p and $\bar{n}_{\max}$. In the case $\delta\omega > -\delta\omega_c$, numerical calculations[25] show that the semiquantal theory gives much larger values of p_n.

5. We shall now discuss experiments (see[31–36]) on the excitation of vibrations in polyatomic molecules in the field of a CO_2 laser. It is well known that in these experiments, in a field of intensity $I = cE^2/8\pi = 10^8$ W/cm^2 and over a time of $\tau \leqslant 10^{-8}$ sec dissociation of molecules has been observed; this is a purely radiative effect, since τ is smaller than the collision time. The characteristic values of the dipole moment d_{10}, the field broadening f, and the anharmonicity α for the excited vibrational mode are of the order of

$$d_{01} = 0.3 \cdot 10^{-18} \text{ cgs esu} = 0.3 \text{ D}, \quad f \approx 1 \text{ cm}^{-1}, \alpha = 5 \text{ cm}^{-1}. \tag{13}$$

From this we have $\delta\omega_c = 2.6$ cm^{-1}. Values of the frequency detuning $\delta\omega$ varied from 0 to -20 cm^{-1}.

The experimenters' interpretation[31–36] of their results encounters difficulties in basing the discussion on the following widely accepted scheme. It is well known[37] that the maximum value of $\bar{n}$ to which a linear oscillator can be excited is

$$\bar{n}_{max} = f^2/(\delta\omega)^2. \tag{14}$$

Since $f \ll \alpha$, "the field broadening cannot overcome the anharmonicity." Therefore in the most favorable case the effective value of $\delta\omega$ cannot be smaller than α, and for an order-of-magnitude estimate we can replace $\delta\omega$ with α in Eq. (14); we then have

$$\bar{n}_{max} \approx f^2/\alpha^2. \tag{15}$$

For the values (13) the quantity $\bar{n}_{\max}$ calculated from (15) is 0.04. Meanwhile, for dissociation of the molecule we must have populations comparable with unity on levels with $n = 3$–4 (it is at present generally believed that the further excitation and the dissociation of polyatomic molecules occurs through a quasicontinuous segment of their energy spectrum[11]). Since according to Eq. (15) $\bar{n}_{\max} \ll 3$, the dissociation of such molecules cannot be explained in this way.

Concerning this we can say the following. Equation (14) is true; it follows from the general formula (7) when $\alpha \to 0$. In fact, for $|x| \to \infty$ we have $F_1(x) = 1/9x^2$ and we obtain (14). Equation (15) is not true. According to Eq. (7) the maximum value of $\bar{n}$ is attained at $\delta\omega = -\delta\omega_c$ and is

$$\bar{n}_{\max} = 4(f/\alpha)^{2/3}. \qquad (16)$$

In the Appendix we show why the transition from Eq. (14) to Eq. (15) cannot be justified even in the case $f \ll \alpha$, and give a simple derivation of the correct explicit expression for $\bar{n}_{\max}$.

With the values (13) we find from Eq. (16) that $\bar{n}_{\max}$ is equal to 1.4. This is one and one-half orders of magnitude larger than the value given by Eq. (15), which was derived in the framework of the elementary theory. Actually the value 1.4 is probably an over-estimate, since the laser spectrum cannot be entirely concentrated at the detuning value $\delta\omega = -\delta\omega_c$; it has a finite width, usually of the order of 0.05 cm^{-1}. Therefore we follow the table and take $F_4(x) = 20$, $F_1(x) = 0.7$ (see[25]); then $\bar{n}_{\max} = 1$, and the beat period is $T = 0.26$ nsec. The value of the parameter αT in Eq. (10) is 38, so that in only the time T there is a strong spreading of the wave packet and the semiquantal theory cannot give an accurate quantitative description. Therefore the values of p_n given by the Poisson formula (4) must be regarded as a lower limit on the actual values of p_n.

According to the semiquantal theory, at time $T/2 = 0.13$ nsec after the beginning of the excitation $\bar{n}(t)$ reaches the value $\bar{n}_{\max} = 1$; the value of p_3 is then 0.06 [cf. Eq. (4)]. We can suppose that molecules on levels with $n \geqslant 3$ are rapidly excited further and dissociate. Then after one beat period $T = 0.26$ nsec there will again be a fraction $p_3 = 0.06$ of the molecules on levels with $n \gtrsim 3$, and so on. The characteristic dissociation time found in the experiments is 5–10 nsec.[31–36] In 10 nsec $\bar{n}(t)$ has about 40 beats. Since at every beat maximum $p_3 = 0.06$, during a time of 10 nsec at least 90 percent of the molecules get excited to the level $n = 3$. This is probably sufficient to explain the observed luminescence.

We thank V. L. Ginzburg for a helpful discussion.

The table was computed with a Wang 2200-B computer, and the figures were drawn by the machine's plotting device.

APPENDIX

We shall estimate the characteristic value of the quantum number n to which the oscillator can be excited. We introduce the expression for the frequency detuning as a function of n

$$\Delta\omega(n) = [\hbar n\omega_l - E(n)]/\hbar;$$

for the spectrum of Eq. (1), $\Delta\omega(n) = [\hbar n\omega_l - E(n)]/\hbar$. Excitation will continue to the point at which, with increasing n, the detuning $\Delta\omega(n)$ becomes comparable with the characteristic frequency of a dipole transition in the range of quantum numbers near n. This frequency is given by $Ed_{n\,n+1}/\hbar \approx n^{1/2}f$. Comparing the values

$$|\delta\omega + {}^1\!/_2\alpha n|n \quad \text{and} \quad n^{1/2}f, \qquad (17)$$

we readily see that the estimate $n \sim (f/\delta\omega)^2$ holds only far from resonance, where $\delta\omega \gg f^{2/3}\alpha^{1/3}$. If, on the other hand, $|\delta\omega| \lesssim f^{2/3}\alpha^{1/3}$, we get from Eq. (17) the value $n \sim (f/\alpha)^{2/3}$.

We have obtained the correct explicit expressions for $\bar{n}_{\max}$ and the characteristic value of the frequency detuning $\delta\omega_c$ [cf. Eq. (8)].

In going from Eq. (14) to Eq. (15) by the replacement $\delta\omega \to \alpha$ one incurs an error, since this does not allow for the fact that for the nonlinear oscillator the transition frequency $\omega_{n\,n+1} = \omega_{01} - \alpha n$, and along with it the difference $\omega_l - \omega_{n\,n+1} = \delta\omega + \alpha n$, will depend on n. From the latter expression it can be seen that the effective value of $\delta\omega$ is the term αn. When we use the value $\delta\omega \to \alpha n$ in Eq. (14), we again obtain the correct value for $\bar{n}_{\max}$ without the (significant) factor 4.

1)The term "semiquantal theory" is adopted from Bloembergen.[10] (Translator's note: Actually Bloembergen did not use this term in the paper cited. Kuz'min and Sazonov have coined this name, apparently, by their misunderstanding (or a translator's misunderstanding) of Bloembergen's calling his calculations "semiquantitative.")

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One-photon decay of two-hole states in atoms

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The techniques of many-body theory are used to make calculations with Hartree-Fock wave functions of the probability of one-photon decay of two-hole states in the first nonvanishing approximation in the interaction of vacancies. Specific results are obtained for two $1s$ vacancies in neon, two $2p$ and $2s$ vacancies in doubly ionized argon, and two $4d$ vacancies in xenon. The results agree extremely well with recently obtained experimental data on neon and argon. An experimental study is proposed of one-photon decay in a process in which a two-hole state is formed as the result of an Auger process following the removal of an electron from an inner shell by a photon or fast electron.

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1. There have recently appeared both experimental[1–5] and theoretical[6, 7] investigations of the mechanisms of decay of highly excited atomic states produced by the removal of two electrons from an inner shell—two-hole states. These phenomena are interesting because their study can give additional information about the interaction between electrons in atoms; in the case of simultaneous decay of two vacancies this is the only information available.

Two-hole states can decay either owing to the ordinary Auger effect, in which the two vacancies are destroyed independently with the emission of two or more photons, or by a radiative process in which one vacancy decays via the Auger effect, and the other in a radiative transition.

There is, however, also a different and extremely interesting possibility for the decay of a two-hole state, in which both vacancies are simultaneously filled by electrons from the outer shells, and the energy released is carried away by a single electron or photon. In the case of emission of an electron the process has received the name of the three-electron Auger effect[1]; the other case, with a photon emitted, is called one-photon decay of a two-hole state.[2–6] Both processes are possible only because of the existence of an interaction between electrons (or holes) in an atom, and consequently are essentially many-electron phenomena. Therefore in theoretical studies on the decay of two-hole states the interaction between vacancies must be taken into account from the beginning.

In the present paper we make an investigation of the one-photon decay of two-hole states in atoms by means of the techniques of the quantum theory of many-bodies.[8] The probabilities of one-photon decay are calculated for two-hole states of several atoms: $(1s)^{-2}$ in Ne, $(2s)^{-2}$ and $(2p)^{-2}$ in Ar^{++}, and $(4d)^{-2}$ in Xe. A preliminary note on the theoretical interpretation and results for this process has been published earlier.[6]