Energy dependence of the electron shakeup and shakeoff: Evidence of different levels of nonseparability

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(Received 25 April 1988)

Electron shake processes are shown to be time independent, in contrast to collision processes, implying the existence of distinct levels of nonseparability (connection). The higher level of nonseparability, which occurs in the e^--p interaction, is capable of preventing time development of the electron system.

The nonseparable (indivisible) character and the related nonlocality of quantum processes are debated questions of quantum theory.[1,2] The recent spin-polarization experiment of Aspect *et al.*[3] and the investigation of energy transfer in β decay[4] have proved that nonseparability exists independently of the actual form of the theory and cannot be eliminated by the introduction of hidden variables into the theory.

Experimental information on nonseparability is rather sketchy: it is limited to the evidence of its existence quoted above. The aim of this report is to establish additional properties of nonseparability; I show that nonseparability may possess different properties when it operates between different particles. The outline of the paper is as follows. It is well-known[5] that the interaction of a bombarding particle (electron, proton, etc.) with an atom is rather well described by the time-dependent Schrödinger equation, in which the potential changes according to the speed of the particle. It will be shown below that the situation changes radically if the electron has been created in the nucleus (as in β decay) or a bound electron is knocked out of the atom (e.g., in the photoeffect). The transition of the atom, i.e., the shakeup and shakeoff probability, is then independent of the electron's speed. Clearly, it is useful to compare the two cases, where the Coulomb interaction is of the same magnitude.

The second case can be explained by nonseparability of quantum systems. Nonlocal transfer of energy and other quantities in a quantum system do not allow the determination of the time development of a subsystem in a nonseparable system (e.g., of an electron in the atom). The system consisting of the bombarding and atomic electrons is nonseparable also, which is emphasized by the antisymmetrization required to explain the experimental data.[6] Why is their behavior so different? A straightforward explanation is that the capacity of nonseparability (i.e., connection) is different, allowing the transfer of large energies and preventing normal time development of the system when the β electron or photoelectron is ionizing the atom. The connection in an electron-impact process is much weaker: The unity of the system can still be maintained, but the transfer of large amounts of energy, which would hinder the time development of the colliding systems is not possible. This notion is supported by additional experimental data that I hope to discuss in a separate paper.[7]

The general expression, valid for electron impact ionization and excitation, can be obtained by the method of variation of constants[5] from the time-dependent Schrödinger equation

$$[H^0+\mathcal{V}(t)]\Psi_n = i\hbar\frac{\partial\Psi_n}{\partial t} \ . \tag{1}$$

Writing

$$\Psi_n = \int_s a_{ns}(t)\phi_s \exp(-i\varepsilon_n t/\hbar) \ ,$$

where ϕ_s is the solution of the unperturbed equation, the following equation is obtained for the $n\rightarrow m$ one-electron transition amplitude:

$$i\hbar\frac{\partial a_{mn}}{\partial t} = \int_s a_{ns} V_{ms} \exp\left[\frac{i}{\hbar}\varepsilon_{ms} t\right] \ , \tag{2}$$

with

$$V_{ms} = \int \phi_m^* \mathcal{V}(t)\phi_s dt$$

and $\varepsilon_{ms}=\varepsilon_m-\varepsilon_s$. Approximate solutions are given by the first and second Born approximations, the distortion approximations, etc. The dependence of the excitation probability on the velocity v of the relative motion[5] is $\sim v^2$ in the first Born approximation (which is valid at high velocities) and it is proportional to v in the adiabatic limit ($v\rightarrow 0$). The experimental results are reproduced by these approximations fairly well.[6] Existing small differences are regarded as eliminable by increasing the accuracy of the approximations.

The experimental data[6] require us to take the exchange interaction into account as well; besides this the scattered and the atomic electrons are described by a common antisymmetric wave function, i.e., they form a common nonseparable system.

It is shown below that the situation is quite different from the foregoing when the ionizing electrons originate from the nucleus or the atom itself. Experimental shakeup and shakeoff probabilities are usually compared with theoretical values calculated in the projection approach. We therefore discuss here the time-dependent approach only.

Existing time-dependent calculations were made using

an exponential dependence of the potential change on the interelectron distance.[8] An exponential change is, however, much quicker than the change of the Coulomb potential, which depends on the interelectron distance as $1/r_{12}=1/vt$; v is the relative speed of the β particle or photoelectron. It is shown in a separate paper[9] that the error-function model used by Thomas[8] with reasonable parameters can yield shakeoff probabilities identical with those given by the projection approach; therefore, calculations with the correct dependence of perturbing potential on the interelectron distance are required to show whether the transition of the atom (shake processes) is described by the time dependent or the projection approach. The results of such calculations are reported below.

Solution of the time-dependent Schrödinger equation yields the following amplitude of a transition for persistent perturbations:[5]

$$d_{ai}=\int \frac{\partial}{\partial t}\frac{V_{ai}}{\gamma_{ai}}\exp\left[\frac{i}{\hbar}\int_0^{\infty}\gamma_{ai}dt\right]dt\ , \tag{3}$$

where V_{ai} is the same as V_{ms} in Eq. (2) for $m=a$, $s=i$, and

$$\gamma_{ai}=(\varepsilon_a+V_{aa})-(\varepsilon_i+V_{ii})\ .$$

The monopole nature of shake transitions, which were investigated experimentally, allows one to limit the multipole expansion of $1/r_{12}$ to the first term ($l=0$). The average change of the potential in this approximation is given as

$$\mathcal{V}(t)=\begin{cases}\dfrac{1}{R_{\max}}=\dfrac{1}{vt_0} & \text{if } t<t_0\\ \dfrac{1}{r}=\dfrac{1}{vt} & \text{if } t>t_0\ ,\end{cases} \tag{4}$$

where $R_{\max}=\max(R_i,R_n)$ and $t_0=R_{\max}/v$; n and i are the orbitals in which photoionization and shakeup occur, respectively, and R_n,R_i are their radii. Clearly, then, $R_n=0$ for β decay to an excellent approximation.

Substitution of Eq. (4) into (3) gives

$$d_{ai}=-\frac{V_{ai}}{\gamma_{ai}}t_0\int_{t_0}^{\infty}\exp(i\gamma_{ai}t)\frac{dt}{t^2}\ . \tag{5}$$

The term V_{ai}/γ_{ai} is the transition amplitude calculated in the projection approach by using first-order perturbation theory. The second part of Eq. (5) is the time-dependent correction, which was calculated by numerical integration. Details of the calculations will be published separately.[9]

The experimental results for 1s shakeoff in β decay are compared in Table I with the theoretical results calculated by Low and Suzuki[10] along with the present results which include time-correction of Eq. (5). The uncorrected theoretical values and the experimental results, which were also taken from Ref. 10, agree fairly well. This indicates that the time-dependent correction, which in many cases gives a 50% decrease of the shakeoff probability, is not correct. This means that shakeoff in β decay is not correctly described by the time-dependent Schrödinger equation.

TABLE I. 1s shakeoff probabilities in β decay in units of 10^{-4}. W_0 is the end-point energy, P(expt.) is the experimental probability, P(theor.) was calculated in the overlap approach by Low and Suzuki (Ref. 10), $P(t)$ is the time-corrected probability.

	W_0 (keV)	P(expt.)	P(theor.)	$P(t)$
Cl	710	22.1±3.8	43.77	38.1
Ca	252	24.3±3.9	26.82	19.6
Ni	65.9	4.6±0.4	5.25	2.73
Cu	573	11.8±0.8	13.43	9.8
^{89}Sr	1463	8.32±0.63	8.39	6.46
^{90}Sr	546	6.0±0.9	6.85	4.6
Y	2270	7.2±1.2	8.31	6.8
Nb	160	3.4±0.4	2.70	1.43
Tc	292	3.65±0.11	3.65	2.15
In	1978	5.40±0.14	5.05	3.79
Pr	930	2.89±0.14	2.70	1.7
Pm	225	0.91±0.05	0.73	0.34
Sm	76	0.022±0.003	0.019	0.006
Er	335	1.0±0.2	0.77	0.33
W	429	1.00±0.25	0.74	0.32
Hg	214	0.13±0.04	0.12	0.05
Tl	765	1.12±0.06	0.99	0.54
Bi	1160	1.30±0.07	1.29	0.76
Cu^+	656	13.23±0.65	7.03	5.5

Experimental energy dependences of shakeup and shakeoff probabilities measured in the photoionization of the 1s shell of nitrogen, neon, and argon are compared with the theoretical results in Figs. 1(a), 1(b), and 2, respectively. Experimental results were obtained by Stöhr *et al.*[11] for nitrogen, by Carlson and Krause[12] for neon, and by Armen *et al.*[13] for argon. Curve A, in each case, is calculated in the projection approach. The result of Sachenko and Burtsev[14] were adopted for the neon by Carlson *et al.*[15] Accurate calculations by using Hartree-Fock wave functions were made for the argon by Armen *et al.*[13] They found that theoretical shakeup probability levels off about 60 eV above the threshold [see Fig. 2(a)]. This property was used to estimate the theoretical energy dependence of the shakeup probability for nitrogen [Fig. 1(a)]. The calculated time-dependent correction was multiplied by the asymptotic value of the corresponding shakeup or shakeoff probability, i.e., an upper limit was obtained. The result was calculated by using the parameters given in the inset of each figure and displayed as time-corrected probability by curves B and C.

It should be noted that the experimental data were obtained for mixtures of shakeup or shakeoff transitions, therefore an accurate treatment would require separate correction of the components. The time-corrected curves in Figs. 1 and 2 disagree with the experimental results even for the most favorable situation; therefore, the above complicated procedure is unnecessary for our purposes. At the same time the disagreement indicates that shake processes are time-independent processes.

The energy dependence of Ne 2p satellite intensities

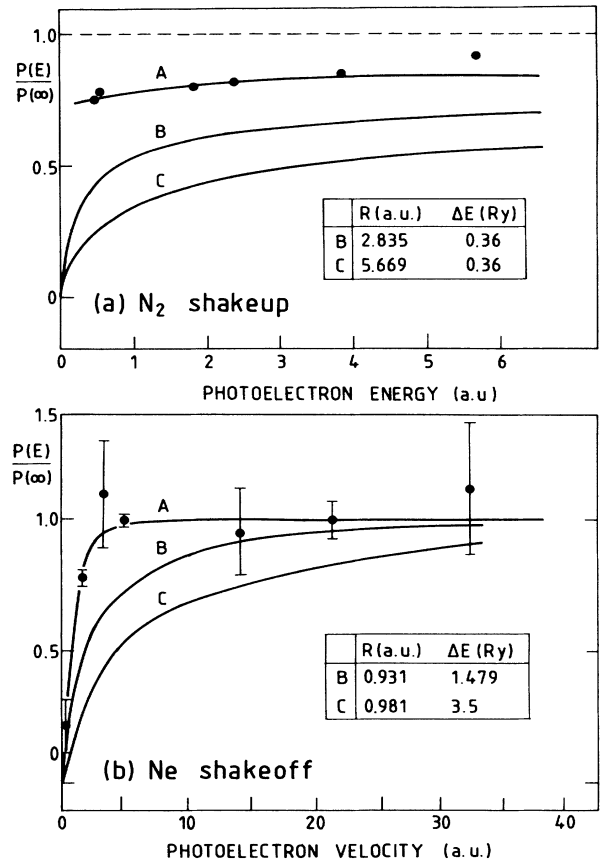

FIG. 1. Comparison of the normalized experimental shakeup probabilities in 1*s* photoionization of nitrogen (a) and shakeoff probabilities in 1*s* photoionization of neon (b) with the theoretical curves calculated in the overlap (curve *A*) or in the time-dependent approach (curves *B* and *C*). Agreement between the experimental points and curve *A* proves the time independence of shake processes. Time-dependent curves *B* and *C* were calculated with parameters given in the inset. The time-corrected shake probability is overestimated by curves *B*.

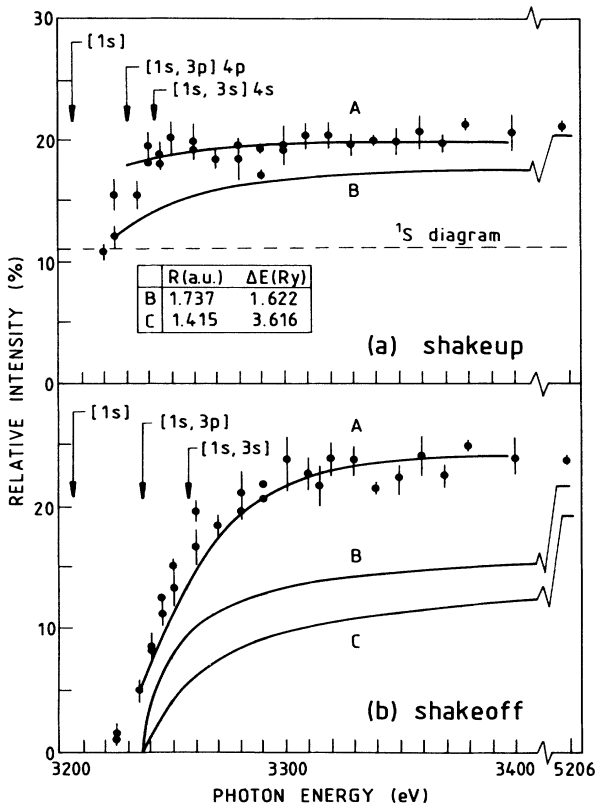

FIG. 2. Comparison of the experimental shakeup (a) and shakeoff (b) probabilities in 1*s* photoionization of argon with the theoretical results. See caption of Fig. 1 for details.

measured by Becker *et al.*[16] corroborate this conclusion, because the measured intensities reaches the sudden limit at much lower energies than predicted by the time dependent calculations [cf. Fig. 1(b) in this paper and Fig. 3 in Ref. 16].

The time-independent nature of the shake processes results from the nonseparability in the atom-nucleus-leptons system during β decay. It has been shown[4] that significant amounts of energy, ~ 20 keV in the case examined in Ref. 4, can be transfered in a nonlocal manner. This transfer cannot be explained by the change of the Coulomb field. Therefore, one cannot expect that the rearrangement of the atom follows the change of the potential.

It is clear from the foregoing that atomic electrons behave differently depending on the origin of the electron perturbing the atom: The effect of a bombarding electron is well described by the time-dependent Schrödinger equation. On the other hand, the e^--atom interaction appears to be time independent even at low relative speed if the electron originates from inside the atom or the nucleus.

The situation is further complicated because, whether or not separability is valid, the electrons are indistinguishable and the wave function is antisymmetric in both cases. This apparent contradiction seems to be unsolvable in the domain of known particles and fields; therefore, we outline here a possible solution of the problem, a solution supported by additional experimental evidence[7].

The existence of nonseparability, independent of theory, requires the existence of some physical entity underlying nonseparability. We term this entity a connective string. The differing nature of e^--e^- processes discussed above imply that connective strings have different effects in electron-proton and electron-electron interactions. Experimental results indicate that e^--p connective strings are amenable to nonlocal transmission of energies up to tens of keV or higher (cf. the energy transfer in β decay[4]), while the capacity of the connective strings between electrons is probably limited to subatomic (e.g., molecular) energies.

Finally, it is important to note that the string structure underlying nonseparability is not deduced from the experimental results discussed here; additional information is used to make this conclusion[7].

In summary, then, the main achievements of this paper are the following. (1) Time-dependent calculations were made for electron shakeup and shakeoff. (2) It was shown that shake processes are time independent in contrast to collision processes. (3) It has been concluded that (a) distinct types of nonseparability (connection) exist for the electron-atomic nucleus and the electron-electron systems, respectively; (b) the electron-nucleus connection is strong enough to prevent time development of the system.

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