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# Orbital $K$-electron shakeoff in $\beta$ decay

J. Law and Akira Suzuki
*Guelph Waterloo Program for Graduate Work in Physics, Guelph Campus, University of Guelph, Guelph, Ontario Canada, N1G 2W1*
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The theory of shakeoff of inner-shell electrons in $\beta$ decay is reexamined. A resolution of the discrepancy that exists between theory and experimental data is provided in the $\beta^-$ decay cases. This comes about by considering the many-body aspects of the problem, and evaluating the wave functions involved in the initial and final states more exactly. The results indicate that agreement between the $K$-electron ejection probabilities $P_K$ and recent experimental results produced by different techniques is generally restored.

[RADIOACTIVITY $K$-vacancy creation in beta decay calculations.]

## I. INTRODUCTION

Despite the early work of Feinberg[1,2] and Migdal[3] which laid the theoretical foundation for the understanding of the process of atomic electron ejection in $\beta$ decay, most of the progress on detailed calculations and experimental measurements has come in recent years. The early calculations produced an agreement to a factor of 2 to 3 when confronted with measurements.

The incentive to do more detailed calculations came when high-resolution devices such as semiconductor detectors and magnetic spectrometers started producing experimental intensities of higher precision than hitherto available, as well as the measurements of the ejected electron spectrum. These high-precision data revealed serious disagreements with previous calculations and led to the development of a theoretical treatment which takes full account of the effect of the exchange between the $\beta$ particle and the ejected electron. The initial striking agreement between the new theory and data, including the ejected electron spectrum, in turn encouraged a spate of experiments of high quality. The history can be traced through various papers.[4–18] For example, Law and Campbell (LC) (Ref. 14) compared 33 measurements for $\beta^-$ decay with theory, and found the overall agreement was within a few percent. As has been pointed out by Isozumi, Mukoyama, and Shimizu (IMS),[19,20] however, the agreement is illusory, since the LC theory overcounts the 1$s$ shakeoff probability $P_K$ by a factor of 2. Since then, more precise experiments have been performed including two measurements for shakeoff in $\beta^+$ decay of Cu.[21,22] These experiments accentuated the discrepancy between theory and experiment.

There have been many suggestions to reconcile theory with experiment. The first such suggestion was from IMS who suggested that the $\sim 50\%$ difference could come from the "direct-collision" (DC) contribution, where the outgoing $\beta$ particle would physically knock out the $K$-shell orbital electron. However, IMS did not produce convincing estimates. The original calculation of Feinberg[1,2] underestimated DC even in the most favored cases for which the decay had small $Q$ values. The maximum DC contribution was estimated not to exceed $\sim 10\%$ of the shakeoff value. This small estimated value for DC has now been confirmed by a calculation by Intemann.[23] This author used a Green's function method adapted from his electron-capture-shakeoff theory to calculate the DC contribution and finds that in the most favored cases the value does not exceed $\sim 15\%$ of the shakeoff contribution.

The contributions from the effect that the process occurs in the presence of many electrons were examined by Cooper and Åberg[24] and by Mukoyama and Shimizu.[25] The many-body effects, estimated in different ways by the two groups, help in lessening the discrepancies between theory and data. However, DC does not account for the remainder.[23]

In a preliminary study, Law and Campbell[26] focused their attention on the configuration of the final-state electron, simulating the many-body effects, by using modified Dirac wave functions. It

 

was seen that one could resolve the discrepancy as far as the total probabilities $P_K$ were concerned; however, the shape of the ejected-electron spectrum could not be simultaneously fitted. We traced this to the use of Dirac wave functions. This gave us confidence to reexamine the problem from a many-body viewpoint focusing our attention on the wave functions involved in the shakeoff process. If one could ignore phase-space considerations as well as the presence of the $\beta^-$ particle, the most complete calculation taking the many-body aspect into account is that of Carlson *et al.*,[9] in which they use the completeness relationship to calculate the total probability for the $K$-shell electron not remaining after the nucleus suddenly acquires an extra charge. Yet this calculation, when confronted with experimental data, in the cases where phase-space effects may be neglected, still shows a discrepancy. For example, in the case of $^{114}$In, the experimental value is $5.4\pm0.14\times10^{-4}$ and this is greater than the Carlson *et al.* value of $4.10\times10^{-4}$ for the total $K$-ejection probability $P_K$. Since the Carlson *et al.* model should give an upper limit, this discrepancy points to a major difficulty even with a many-body scheme.

In this paper, we attempt a resolution of this difficulty. Our major contribution is based on a treatment of the inital and final states of the $\beta$ decay shakeoff process that is more accurate than predecessors. Section II gives a brief resume of the extension to the LC/IMS theory of shakeoff. Section III discusses the self-consistent-field models used for bound and continuum states. Section IV gives a discussion of the results obtained for shakeoff. Section V discusses the relative size of shakeup and DC. The conclusions follow in Sec. VI.

## II. THEORY OF THE SHAKEOFF PROCESS

We shall present only a very brief account of the main aspects of earlier theoretical work. Much of this has been detailed elsewhere[11,12,14,20] and need not be repeated here. We shall concentrate on the main theme of the LC/IMS theory. Furthermore, only the shakeoff process in which the orbital electron and the $\beta$ particle are both in continuum states will be considered in this section.

The one "active" electron model is given in detail in the paper by Law and Campbell.[14] Here we will extend the LC theory to account for exchanges between the electrons in the bound initial state and similarly in the final state. The initial state (using the notation of LC and leaving out the neutrino and nuclear variables) is

$$\Phi_i=\mathscr{A}\{e_{K\uparrow},e_{K\downarrow},e_{L\uparrow},\cdots\}\,, \tag{1}$$

where $\mathscr{A}$ stands for the antisymmetrization operator and can be written as

$$\mathscr{A}\{---\}=\frac{1}{\sqrt{Z!}}\det\{---\}$$

if there are $Z$ electrons. $\Phi_i$ is a Slater determinant. Similarly the final state is

$$\Psi_{f\sigma}=\mathscr{A}\{e'_{p\sigma},e'_{s\uparrow},e'_{K\downarrow},e'_{L\uparrow},---\}\,, \tag{2}$$

where $\sigma=\uparrow$ or $\downarrow$. In the matrix element $\langle f\,|\,H_\beta\,|\,i\rangle$,[14] the part that deals with the electrons may be factored out as $\langle\Psi_{f\sigma}\,|\,\psi_e^+\,|\,\Phi_i\rangle$, which can be reduced following standard methods to

$$\begin{aligned}
&\langle\mathscr{A}\{e'_{p\sigma}(x_0)e'_{s\uparrow}(x_1)e'_{K\downarrow}(x_2)---\}\,|\,\psi_e^+(x)\,|\,\mathscr{A}\{e_{K\uparrow}(x_1)e_{K\downarrow}(x_2)---\}\rangle\\
&\quad=\sqrt{(Z+1)!}\langle e'_{p\sigma}(x_0)e'_{s\uparrow}(x_1)e'_{K\downarrow}(x_2)---\,|\,\mathscr{A}\{\delta^3(x-x_0)e_{K\uparrow}(x_1)e_{K\downarrow}(x_2)---\}\rangle\\
&\quad=e'_{p\sigma}(x)\langle e'_{s\uparrow}(x_1)e'_{K\downarrow}(x_2)---\,|\det\{e_{K\uparrow}(x_1)e_{K\downarrow}(x_2)---\}\rangle\\
&\qquad-e'_{s\uparrow}(x)\langle e'_{p\sigma}(x_1)e'_{K\downarrow}(x_2)---\,|\det\{e_{K\uparrow}(x_1)e_{K\downarrow}(x_2)---\}\rangle+\text{"other terms."}
\end{aligned} \tag{3}$$

The first two terms above correspond to creating one electron in the continuum state $p\sigma$, while the other is shaken off from the $K$ shell into the state $s\uparrow$, together with the Pauli-exchange process. The "other terms" would correspond to creating an electron into a bound state with two electrons shaken off (but still leaving only one $K$ vacancy). These are much higher order processes, and one can estimate them in specific decay cases. Our numerical estimates put them at least an order of magnitude less than the *shakeup* contributions.

The truncation of the overlap integral in Eq. (3) to the active electron would reduce it to the case considered by LC/IMS. Except for the interpretation of the wave functions the LC/IMS model is recovered fully.

In the above derivation one assumed that the exact initial state $\Phi_i$ can be written as a single Slater determinant and the exact basis states $e_i(x_i)$ are known. Similarly, the exact final state $\Psi_{f\sigma}$, consisting of a $K$ vacancy and 2 continuum electrons, can also be written as a single Slater determinant and the corresponding basis state $e_j'(x_j)$ are also assumed known. In the LC/IMS works, these basis states were approximated by Dirac wave functions. This assumption is equivalent to switching off all the mutual interactions between the electrons. The numerical results for $\beta^-$ decay shakeoff indicate that this is a very poor approximation. The Carlson *et al.* work replaces the initial basis states by Dirac-Fock-Slater (DFS) wave functions. This reintroduces the mutual interactions between the electrons, and thus the basis states should be a much better approximation to the exact ones. The problem seems to arise in the final state. Rather than solve for the state with one $K$ vacancy and 2 electrons in the continuum, Carlson *et al.* invoke completeness, and replace the final state $\Psi_{f\sigma}$ by the ground state $\Psi_{fg}$, in which both electrons are present in the $K$ shell. The other electron that is in the continuum may either be neglected or placed into a higher level configuration making the final state again a neutral atom. Again the Dirac-Fock-Slater procedure is invoked and the basis states solved for. Then from the completeness theorem,

$$1-|\langle\Psi_{fg}^{\mathrm{DFS}}|\Phi_i^{\mathrm{DFS}}\rangle|^2 \tag{4}$$

would correspond to at least one $K$ electron not remaining plus higher order processes. From this they find that even in cases where phase-space effects may be neglected, the results, which should be upper limits, fall below the measurements in most cases. We think that the problem is not so much in the completeness relationship as in the approximation of $|\Psi_{fg}\rangle$ by a DFS wave function. In fact, the DFS wave function $|\Psi_{fg}^{\mathrm{DFS}}\rangle$ is not orthogonal to $|\Psi_{f\sigma}\rangle$, i.e., $\langle\Psi_{fg}^{\mathrm{DFS}}|\Psi_{f\sigma}\rangle\neq 0$, while of necessity $\langle\Psi_{fg}|\Psi_{f\sigma}\rangle=0$. In other words the DFS wave function $|\Psi_{f\sigma}^{\mathrm{DFS}}\rangle$, which is orthogonal to the DFS ground state $|\Psi_{fg}^{\mathrm{DFS}}\rangle$, is not the correct wave function for the many-body system. The physical state corresponds to a fully relaxed system (after rearrangement) with a $K$ vacancy, while $|\Psi_{f\sigma}^{\mathrm{DFS}}\rangle$ corresponds to a "frozen orbital" state with a $K$ vacancy, so that $\langle\Psi_{f\sigma}|\Psi_{f\sigma}^{\mathrm{DFS}}\rangle\neq 1$. The results indicate that the importance of rearrangement effects of the rest of the electrons may not be negligible. It also suggests that with approximate wave functions, the more direct approach of solving for $|\Psi_{f\sigma}\rangle$ may be more appropriate. We shall present a model in the next two sections based on the Dirac-Fock-Slater approach to solve this problem.

## III. SELF-CONSISTENT-FIELD MODEL

A review of relativistic self-consistent-field (SCF) calculations may be found, for example, in the article by Lindgren and Rosén.[27] In our calculations for the ground state of the parent atoms before $\beta$ decay, we have used the Dirac-Fock-Slater model with optimized potentials for the exchange-interaction part as introduced by Lindgren and Rosén (including a Latter tail correction). We shall refer to this scheme as the optimized Dirac-Fock-Slater (ODFS) scheme, subsequently. A check of this scheme and the program is afforded by calculating the shakeoff plus shakeup probability following Carlson *et al.*'s procedure. We obtain the numbers given in Table I. We find a small $\sim 2\%$ increase for the probability $P_K$ for lower $Z$ values using ODFS under the $\Psi_g$ column as compared to Carlson *et al.* This is probably due to the optimized exchange potential being different from the Slater exchange. In fact, in the case of Cu, when we revert to using the Slater exchange, the result obtained is $10.99\times 10^{-4}$ under the $\Psi_g$ column. The $\Psi_g$ column under ODFS + LC/IMS simply means solving for the electron continuum

TABLE I. Comparison of ODFS and Carlson *et al.* values for the $K$-shell vacancy creation probability $P_K\times 10^{+4}$. See text for the differences between $\Psi_g$ and $\Psi_v$.

| | Carlson *et al.* | ODFS | | ODFS + LC/IMS | |
|---|---|---|---|---|---|
| | $\Psi_g$ | $\Psi_g$ | $\Psi_v$ | $\Psi_g$ | $\Psi_v$ |
| Cu ($\beta^-$) | 10.9 | 11.1 | 17.1 | 9.13 | 14.3 |
| In ($\beta^-$) | 4.10 | 4.12 | 6.35 | 3.51 | 5.42 |
| Cu ($\beta^+$) | 11.5 | 12.8 | 6.72 | 11.4 | 5.80 |
| Co ($\beta^+$) | 12.3 | 14.8 | 7.79 | 13.0 | 6.70 |

state on the assumption that the final continuum electron moves in the SCF potential defined from the solution of the final ground state ion (namely the SCF potential that emerges from the Carlson *et al.* procedure), and inserting the overlap integral into the LC/IMS theory. The results indicate that the exchange effect between the continuum electrons in the $\beta^-$ decay case tends to suppress the probability. This is most noticeable in the In $\beta^-$ decay case, where a probability of $3.51\times10^{-4}$ emerges in comparison with the experimental value of $5.4\times10^{-4}$. The Cu $\beta^-$ values are larger than the Dirac wave function predictions; however, they too tend to be below the experimental values. This trend continues in most of the $\beta^-$ decay cases that have been measured. This underestimation leads us to question the validity of the final-state configuration. We thus introduce the columns marked $\Psi_v$. The differences between the columns labeled $\Psi_g$ and $\Psi_v$ occur as follows: In the physical situation, the parent atom $\beta$ decays to a final state consisting of a $K$ vacancy and two continuum electrons. For concreteness we have

$$\mathrm{Cu}\rightarrow\mathrm{Zn}^{++}+e^-+e^-+\bar{\nu}\,, \tag{5}$$

$$\{\,[\mathrm{Ar}]3d^{10}4s\,\}_{29}\rightarrow\{\,[\mathrm{Ar}]1s^{-1}3d^{10}4s\,\}_{30}+e_p+e_s+\bar{\nu}\,, \tag{6}$$

where we have written down the configurations in the second form. The subscript is the nuclear charge. The argon core [Ar] in $Zn^{++}$ has a $K$ vacancy, hence the $1s^{-1}$; $e_p$, $e_s$ are the electron continuum states. In all calculations done so far, the argon core and outer orbitals $3d^{10}$ and $4s$ basis states are solved for in the configuration

$$\Psi_g=\{\,[\mathrm{Ar}]3d^{10}4s\,\}_{30}\ \text{for}\ \mathrm{Zn}^+\,, \tag{7}$$

as was done, for example, in creating Table I column $\Psi_g$ above, so that with the ODFS (or other equivalent scheme), the $K$-shell occupation number is 2. However, the physical state insists that the $K$-shell occupation be 1, and one should solve for the configuration

$$\Psi_v=\{\,[\mathrm{Ar}]1s^{-1}3d^{10}4s\,\}_{30}\ \text{for}\ \mathrm{Zn}^{++}\,. \tag{8}$$

In this case, the basis state emerges different from that above, and in fact the $K$-shell basis wave functions from $\Psi_v$ and $\Psi_g$ do not overlap to unity. This gives rise to column $\Psi_v$ in Table I which is much larger than Carlson *et al.* values in the case of $\beta^-$ decay. This can be explained by the rearrangement effect. Owing to the $K$ vacancy, the occupied $K$ orbital is pulled in, hence, sees less shielding from the outer electrons. The absence of the other $K$ electron thus effectively cancels off the order of $0.3\sim0.4$ charge. Simulating this using Dirac wave functions gives the same increase in $P_K$ (see Law and Campbell[26]). However, in the case of $\beta^+$ decay, the trend is in the opposite direction. The state tends to decrease the shakeoff probability. Although this now tends to set the theoretical value for Cu $\beta^+$ decay shakeoff at about half the experimental value, it does point to the sensitiveness of the choice of final state SCF potential. In the corresponding case of shakeoff in electron-capture-decay we find the above trend also goes towards bringing theory into line with most experiments.

Although, in $\beta^-$ decay cases, the increase goes in the correct direction to realign theory with experiment, it neither takes the shakeoff electron, the $\beta$ particle, phase space, nor Pauli exchange into account. For these to be included, we would need to calculate the continuum wave function by reintroducing both continuum electrons. Again taking Cu $\beta^-$ decay for concreteness, we should solve for the states $e_p$, $e_s$ in the configuration

$$\Psi_c=\{\,[\mathrm{Ar}]1s^{-1}3d^{10}4s\,\}_{30}+e_p+e_s=\Psi_v+e_p+e_s\,. \tag{9}$$

This is quite formidable unless one uses successive approximation. One method that can be adopted is to apply ODFS to $\Psi_v$ to obtain the basis states, and using them to create the central potential for one of the continuum electrons and then solve for the continuum electron state. In principle, one should then bring in the other continuum electron and obtain the central potential for it. This latter potential is identical to the former if we switch off the mutual interaction between the continuum electrons (i.e., ignore direct collisions). For the model to be tractable, we will proceed by ignoring the mutual interactions of the continuum electrons as a first approximation, and produce a first approximation to the central potential felt by a continuum electron in the field of the other bound electrons (i.e., the state with a $K$ vacancy). This will then allow us to solve for a realistic continuum state in the physical final-state configuration.

The basis functions are solved for in the configuration (for example in $Zn^+$ daughter state)

$$\{\,[\mathrm{Ar}]1s^{-1}3d^{10}4s^2\,\}_{30}\,, \tag{10}$$

where a $K$ vacancy is created in the neutral Zn configuration. This is equivalent to placing the continuum electron in the first available high $s$ state. (We restrict ourselves to $s$ states since the overlap matrix elements we need only project out the $s$ continuum state.) In fact, this state corresponds to the first shakeup state of the system. This has the advantage of taking some effect of the continuum electron into account in the SCF procedure. (We note in passing that whether we use $4s^2$ or $4s^1$ configuration affects the final results by less than 1%. The use of the latter configuration is equivalent to neglecting the continuum electron from the ODFS calculation.) However, it must be stated that this of course does not completely simulate the situation. In solving for the continuum state, we then use the ODFS potential that emerges above.

This procedure may overemphasize the exchange ($V_{\rm ex}$) part of the potential. This may be seen from say the Slater approach to derive the exchange potential. As is well known, within the uniform electron gas approximation the average exchange potential from the Hartree-Fock-Slater approach reduces to

$$V_{\rm ex}=-2(6\rho_s/\pi)^{1/3}F(\eta)\ , \tag{11}$$

where $\rho_s$ is the uniform electron density and

$$F(\eta)=(\tfrac{1}{2})+\frac{1-\eta^2}{4\eta}\ln\left|\frac{1+\eta}{1-\eta}\right| \tag{12}$$

and $\eta=k/k_F$. $k$ is the local momentum and $k_F$ the Fermi momentum. The usual method of translation from uniform electron gas to finite system involves (a) the local density approximation

$$\rho_s\rightarrow\rho_s(\vec{r})=\rho(\vec{r})/2=\rho(r)/8\pi r^2 \tag{13}$$

for spin saturated systems, (b) averaging $F(\eta)$ over the Fermi sea

$$F(\eta)\rightarrow\langle F\rangle=\int_0^1 F(\eta)\eta^2 d\eta=\tfrac{3}{4}\ , \tag{14}$$

which implies all states have $k$ less than $k_F$, and (c) that the Lindgren and Rosén optimized potential introduces a further modification in an attempt to bridge the gap between the Slater and Kohn-Sham approaches.

Their approach is to write

$$V_{\rm ex}^{\rm LR}=-2\tfrac{3}{4}C\left[\frac{3r^{n-3}\rho^m(r)}{4\pi^2}\right]^{1/3}\ , \tag{15}$$

where $C$, $n$, and $m$ are chosen via an optimization procedure.

In our case, our continuum electrons have momenta greater than $k_F$, so that procedure (b) may be too drastic. To see the effect of this we have replaced the exchange potential by

$$V_{\rm ex}^c=-2F(\eta)C\left[\frac{3r^{n-3}\rho^m(r)}{4\pi^2}\right]^{1/3}\ , \tag{16}$$

which takes the Lindgren and Rosén optimization parameters into account. If we were to apply it to bound states and replace $F(\eta)$ by the Fermi average of $\frac{3}{4}$, we regain the Lindgren and Rosén potential. For continuum states, we can proceed further within two approximations to the above, both of them guided by discussions on the approximations to use in the corresponding problem of electron scattering from atoms.[28–33] A possible choice is to use the local density approximation for the Fermi momentum in $F(\eta)$, namely,

$$k_F(r)=[3\pi^2\rho(r)]^{1/3}\ , \tag{17}$$

and insert also the local momentum

$$k(r)=\left\{\frac{2m}{\hbar^2}[E_0-V_s(r)-V_{\rm ex}^c(r)]\right\}^{1/2}\ . \tag{18}$$

$E_0$ is the energy of the electron and $V_s$ is the direct central potential. Since $k(r)$ depends on $V_{\rm ex}^c(r)$, which in turn depends on $k(r)$, some sort of self-consistency iterative scheme should in principle be used. Various approximations have been studied in electron scattering and it has been found that they essentially do not differ at high energies. Differences do occur at lower energies. In our case, since the region of interest in the overlap integral tends to fall in the intermediate energy region, we have to test out two approximations, both of which sets the local momentum to

$$k^2=p^2+k_F{}^2\ , \tag{19}$$

where $p$ is the physical momentum. This approximation goes by the name of "asymptotically adjusted free electron gas exchange approximation."[28] Our two approximations thus depend on how $k_F$ is chosen. The first is to define $k_F(r)$ as above in Eq. (17), where the density $\rho(r)$ is obtained from ODFS [this will be labeled as the local density approximation (LDA) subsequently]. The second is to obtain $k_F$ as the average Fermi momentum in our bound system by relating the average kinetic energy $E_{\rm av}$ to the Fermi energy

$$E_{\rm av}=\frac{3}{5}\frac{\hbar^2k_F{}^2}{2m}\ . \tag{20}$$

Again $E_{\rm av}$ is obtained from the ODFS. This ap-

TABLE II. Shakeoff probabilities in units of $10^{-4}$. See text for description of the various shakeoff columns.

| | $E_0$ (keV) | $B_K$ (keV) | $P$(exp) | $P$(ODFS) | $P$(LDA) | $P$(AKF) | $k_F$ (mc) |
|---|---|---|---|---|---|---|---|
| beta minus decay | | | | | | | |
| Cl | 710 | 3.21 | 22.1 ±3.8 | 46.09 | 43.77 | 39.81 | 0.10 |
| Ca | 252 | 4.49 | 24.3 ±3.9 | 28.57 | 26.82 | 24.44 | 0.11 |
| Ni | 65.9 | 8.98 | 4.6 ±0.4 | 5.54 | 5.25 | 4.81 | 0.13 |
| Cu | 573 | 9.66 | 11.8 ±0.8 | 14.27 | 13.43 | 11.95 | 0.14 |
| $^{89}$Sr | 1463 | 17.04 | 8.32 ±0.63 | 8.97 | 8.39 | 7.54 | 0.17 |
| $^{90}$Sr | 546 | 17.04 | 6.0 ±0.9 | 7.30 | 6.85 | 6.12 | 0.17 |
| Y | 2270 | 18.00 | 7.2 ±1.2 | 8.89 | 8.31 | 7.52 | 0.17 |
| Nb | 160 | 20.00 | 3.4 ±0.4 | 2.88 | 2.70 | 2.46 | 0.18 |
| Tc | 292 | 22.12 | 3.65 ±0.11 | 3.88 | 3.65 | 3.34 | 0.18 |
| In | 1978 | 29.20 | 5.40 ±0.14 | 5.42 | 5.05 | 4.54 | 0.20 |
| Pr | 930 | 43.57 | 2.89 ±0.14 | 2.90 | 2.70 | 2.42 | 0.23 |
| Pm | 225 | 46.84 | 0.906±0.047 | 0.78 | 0.73 | 0.66 | 0.23 |
| Sm | 76 | 48.52 | 0.022±0.003 | 0.020 | 0.019 | 0.018 | 0.24 |
| Er | 335 | 59.39 | 1.0 ±0.2 | 0.81 | 0.77 | 0.70 | 0.26 |
| W | 429 | 71.68 | 1.00 ±0.25 | 0.78 | 0.74 | 0.67 | 0.27 |
| Hg | 214 | 85.53 | 0.13 ±0.04 | 0.13 | 0.12 | 0.11 | 0.29 |
| Tl | 765 | 88.01 | 1.12 ±0.06 | 1.05 | 0.99 | 0.88 | 0.29 |
| Bi | 1160 | 93.11 | 1.30 ±0.07 | 1.38 | 1.29 | 1.15 | 0.30 |
| beta plus decay | | | | | | | |
| Cu | 656 | 8.33 | 13.23 ±0.65 | 5.80 | 7.03 | 8.25 | 0.13 |
| Co | 474 | 7.11 | | 6.70 | 7.96 | | |

proximation will be referred to as the average Fermi momentum approximation (AKF).

The set of equations to solve is given by Eq. (97) in Lindgren and Rosén,[27] where for the case of the continuum electron the energy is taken to be

$$\epsilon_a + c^2 = (p^2c^2 + c^4)^{1/2} \tag{21}$$

using Hartree atomic units, where $p$ is the electron momentum. These equations were numerically integrated outwards and matched at a point, where the ODFS potential healed to the Latter tail.

## IV. RESULTS FOR SHAKEOFF

Our shakeoff results are shown in Table II. We label by $P$(ODFS), the result obtained simply from using the potential that emerges from the ODFS calculation to calculate the continuum electron state; $P$(LDA), that obtained from the local density treatment of $k_F(r)$ as explained in Sec. III, and $P$(AKF), that which arises from using an average $k_F$ in the treatment of the exchange potential.

It is interesting to note that for $\beta^-$ decay the results for $P$(ODFS) tend in most cases to be quite close to the experimental numbers. There is only a slight tendency to be greater for the lower $Z$ elements. This suggests that the exchange potential used for the continuum state may be a little too strong. On the other hand the $P$(LDA) results mostly fall slightly below the experimental numbers, this time suggesting some weakening of the exchange potential. The use of an average $k_F$ indicated by $P$(AKF) was included as it took considerably less computing time. This gives a slightly smaller value for the shakeoff probability. As will be seen in the next section, the shakeup and direct-collision processes probably play an insignificant role in enhancing the $K$-vacancy creation probability, at least in $\beta^-$ decay. On this basis, the $\beta^-$ decay model of LC/IMS can now be said to agree with experiment very reasonably. This is also borne out with the spectrum shapes shown in Figs. 1 and 2, where we have compared the shapes obtained with ODFS versus the use of Dirac wave functions. We have compared the shapes without shape factor, as we expect that inclusion of shape factor would simply merge them onto the data, as for example in the $^{89}$Sr case; the solid curve through the data points corresponds to the Dirac wave function result with shape factor included.

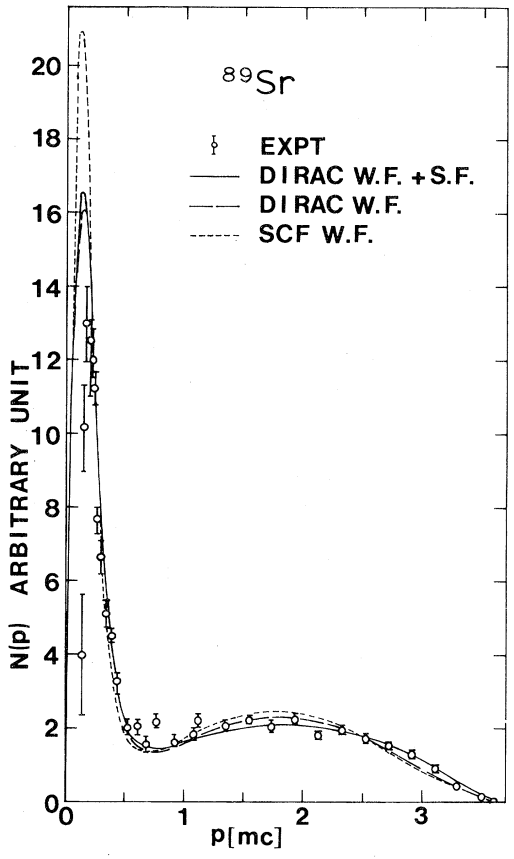


FIG. 1. $K$-shell ejected electron spectrum measured in coincidence with $K$ x rays in the $\beta$ decay of $^{89}$Sr. The curves ( — — ) Dirac w.f., and (----) SCF w.f. do not include the shape factor corrections. The theoretical curves are normalized to the data point at $p=2.5$ mc.

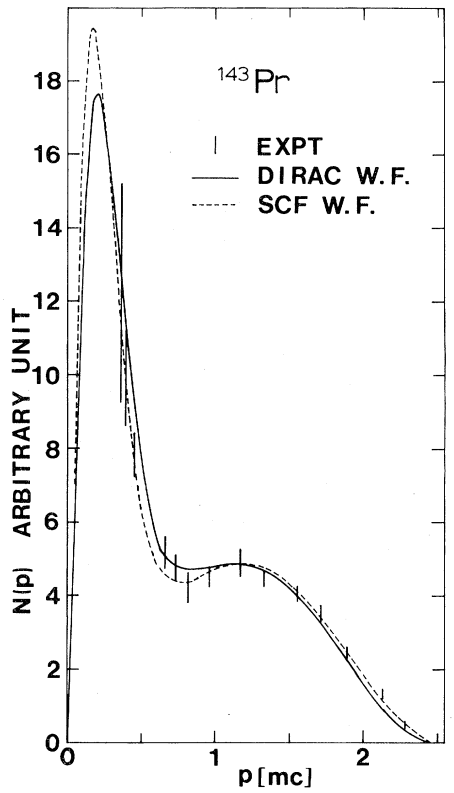


FIG. 2. $K$-shell ejected electron spectrum in the $\beta$ decay of Pr. The shown curves do not include shape factor corrections, and they are both normalized to the data point at the second peak.

As can be seen, the ODFS result does not deviate much from the Dirac wave function case for large momenta. The larger deviation at smaller momenta is significant, as the ODFS curve gives a larger $P_K$. Inclusion of the shape factor has a tendency to raise the tail of the distribution and lower the higher momenta peak. At lower momenta the shape factor has a much smaller effect. In the case of $^{143}$Pr, we show the curves without shape factors. From previous results we expect that the shape factor has a much smaller effect on the shape of the spectrum. The fit of the ODFS result is better than the Dirac wave function case.

As is also very evident from Table II, there is disagreement in the $\beta^+$ decay case of $^{64}$Cu. Both experiments produced an averaged $K$-shell shakeoff probability of $(13.23\pm0.65)\times10^{-4}$, while the theoretical results are from $(5.8$ to $8.5)\times10^{-4}$. This large discrepancy cannot as yet be blamed on other processes, since they seem to have been estimated to be less than 3% of the shakeoff value.

## V. THE SHAKEUP AND OTHER PROCESSES

The $K$-shakeup process corresponds to the final state having a $K$ vacancy with one electron promoted to a high bound state and the other in the continuum state. The expressions to calculate this process have been given in LC and will not be rewritten here. Basically, we need an initial $K$-shell wave function overlap with the final $ns$ bound state wave functions. The same problem, in terms of rearrangement effects, occurs here as in the shakeoff case. In solving for the shakeup state, we simply ran the ODFS program with one $K$-shell electron promoted to some of the lowest allowed unoccupied level. The overlaps between the initial parent $K$-shell wave function and these higher states are obtained and the shakeup contribution (neither correcting for phase space nor $\beta$ particle

TABLE III. Shakeup contributions in In beta decay.

| | ODFS | Dirac w.f. |
|---|---|---|
| $\langle 1s \mid 6s' \rangle$ | 0.000 338 7 | 0.001 677 2 |
| $\langle 1s \mid 7s' \rangle$ | 0.000 222 1 | 0.001 315 2 |
| $\langle 1s \mid 8s' \rangle$ | 0.000 157 0 | 0.001 068 0 |
| $\langle 1s \mid 9s' \rangle$ | 0.000 116 1 | 0.000 890 0 |
| $\langle 1s \mid 10s' \rangle$ | 0.000 090 1 | 0.000 756 8 |
| $\sum_{n=6}^{10} \mid \langle 1s \mid ns' \rangle \mid^2$ | $21.03\times10^{-8}$ | $704.82\times10^{-8}$ |
| $\sum_{n=6}^{\infty} \mid \langle 1s \mid ns' \rangle \mid^2$ | | $940.95\times10^{-8}$ |

and shakeup electron exchange) is calculated.

Table III shows a comparison of these overlap integrals in In $\beta^-$ decay case with the corresponding Dirac wave function overlaps. The results show a drastic reduction in the shakeup contribution between the ODFS and Dirac wave function contributions. For example, the Dirac wave function shakeup value is $0.188\times10^{-4}$, where the 2 $K$-shell initial occupancy is now accounted for, while the ODFS value [extrapolated by taking $(\sum_{n=6}^{10})_{\text{ODFS}}\times0.188\times10^{-4}/(\sum_{n=6}^{10})_{\text{Dirac}}$] is $0.0056\times10^{-4}$. Thus, this will at most affect the third significant figure of the shakeoff contribution. A similar result in Cu $\beta^-$ decay also bears this out, $0.993\times10^{-4}$ using Dirac wave functions versus $0.098\times10^{-4}$ using ODFS. Thus, after correction for phase space, one would ascribe shakeup as at most a 1% contribution. Owing to this we have not included shakeup values in Table II.

We have not calculated fully the direct-collision process. This corresponds in our model to reintroducing the two continuum-electron interactions. The estimates of Intemann using Dirac wave functions, however, bear out the earliest estimates of Feinberg. A partial inclusion of the direct-collision process can be taken into account as follows (again using Cu $\beta^-$ decay as an example). We place both of the continuum electrons into bound orbits and calculate the ODFS central potential and use it for solving the continuum wave function, i.e., do ODFS for the configuration

$$\{\,[\mathrm{Ar}]1s^{-1}3d^{10}4s^{2}5s\,\}_{30}\,.$$

The extracted potential for the continuum state would then include some of the mutual continuum-electron interactions as well as interactions with the other electrons in the bound state. Our results show that in the case of In and Cu $\beta^-$ decay, the direct-collision contribution as included above is not more than 0.5% of the shakeoff values. However, this does not detract from the other estimates where a more direct calculation of the mutual interaction in continuum state is performed.

## VI. DISCUSSION AND CONCLUSIONS

The experimental numbers in Table II have been brought up to date from the LC (Ref. 14) table by including newer data from subsequent experiments.[21,22,34–44] These numbers have been produced by taking weighted averages of the data. We have also corrected the electron-spectrometer data to reflect the fact that our new theory produces negligible shakeup. For example, in the case of $^{89}$Sr, the result quoted by Beery[43] is $(7.3\pm1.5)\times10^{-4}$. This was obtained by correcting his raw data by a factor of $[I(SO)+I(SU)]/[2I(SO)+I(SU)]$, where the intensities $I$ for shakeoff and shakeup were obtained from the table of theoretical numbers in LC. In the LC table the values of $I(SU)$ were not negligible as they were produced using Dirac wave functions, whereas with ODFS wave functions, they are. We thus correct the $^{89}$Sr value to $(7.12\pm1.45)\times10^{-4}$ and used a weighted average between this value and that of Hansen and Parthasaradhi,[44] namely $(8.6\pm0.7)\times10^{-4}$. This procedure was similarly applied to Pr, Sm, and Bi.

Our results for the total shakeoff probability $P_K$ agree reasonably well with the data, when we use

the SCF potential that emerges from the Lindgren and Rosén ODFS procedure. As we have argued, this potential may not be the actual potential felt by the continuum electron, if it was produced in the Slater sense. However, by the numerical optimization used by Lindgren and Rosén, some of the effects due to the electron being in the continuum may have been included in an average way. This may be why the difference between the results $P$(ODFS) and $P$(LDA) is not very great. One would still suggest that the correct potential is somewhere in between these two limits.

The results from the spectrum fits to the ejected electron in coincidence with $K$ x rays give further credence to the model. Thus, as far as $\beta^-$ decay shakeoff is concerned, the LC/IMS model is now in agreement with the data, except for the case of Cl, where the data give a value which is about a factor of 2 lower than predicted. Whether this is a real discrepancy or not remains to be seen. If it is real then the ODFS model used would seem to break down at low $Z$. However, we feel that this may be unrealistic as the experiment involved in Cl $\beta$ decay shakeoff is a difficult one. There may be some leeway for direct-collision contributions if they are less than 15%.

The problem as it stands seems to be with $\beta^+$ decay shakeoff. In the two measured values available, both on Cu, the experimental numbers are almost a factor of 2 larger than $P$(LDA). In fact the ratio of $P_K(\beta^+)/P_K(\beta^-)$ ranges from 0.41 to 0.69, which differs drastically from the experimental ratio of $1.11\pm0.1$. If we took the final configuration as has been done in previous calculations, i.e., with both $K$ electrons remaining, and use the SCF potential to solve for the continuum state (i.e., frozen orbital limit), the results in Table I indicate the ratio $P_K(\beta^+)/P_K(\beta^-)=1.25$. This result suggests that the final-state configuration in $\beta^+$ decay may be more complicated than for the case of $\beta^-$ decay. For $\beta^+$ decay, there is no Pauli exchange effect. The Pauli effect may thus produce a major difference, in terms of rearrangement relaxation of the final electron cloud when $\beta^+$ decay shakeoff occurs in contrast to the case of $\beta^-$ decay. If this is so, further $\beta^+$ decay data should exhibit similar discrepancies. If not, then Cu $\beta^+$ decay may by coincidence be the only case where the discrepancy may exist. There are experiments in progress to determine $\beta^+$ decay shakeoff in Co. We hope that the results would throw further light on the discrepancy encountered in Cu. In order to facilitate comparison, we have included in the table the values for $\beta^+$ shakeoff in Co. We do not know the solution to this discrepancy. However, we find that the model seems to produce good agreement with data in the sister process of electron-capture-decay shakeoff where the final state has two $K$ vacancies.[45]

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