Relation between the Isotope or Isomer Shift and the Nuclear-Charge Distribution*

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It is shown, for a model in which the nuclear-charge distribution is that of a uniformly charged sphere of radius R, that the isotope or isomer shift is proportional to R^k where $k=1+(1-\alpha^2Z^2)^{1/2}$.

The isotope and the isomer shift measure the change in the interaction energy between nuclear charge and electrons because of finite nuclear size.[1,2] If the electronic charge distribution sees a nuclear Coulomb potential V_f from a finite nucleus and V_p from a point nucleus, then first-order perturbation theory gives the shift as

$$\Delta E=\int \Delta V|\psi(r)|^2 d^3r/\int|\psi(r)|^2 d^3r \quad , \tag{1}$$

where $\psi(r)$ is the electronic wave function obtained for the zero-order (point nucleus) potential, and $\Delta V=V_f-V_p$. For a model in which the nucleus is a uniformly charged sphere of radius R, the perturbation potential is

$$\Delta V=-\frac{Ze^2}{R}\left[\frac{3}{2}-\frac{1}{2}\left(\frac{r}{R}\right)^2\right]+\frac{Ze^2}{r} \quad , \quad r<R$$

$$=0, \qquad r>R \quad . \tag{2}$$

If $\psi(r)$ is constant over the nuclear volume, as is true for light atoms, Eq. (1) then gives

$$\Delta E=\tfrac{2}{5}\pi Ze^2R^2|\psi(0)|^2 . \tag{3}$$

Thus with these various approximations, the isotope or isomer shift measures the square of the nuclear radius. For more general nuclear-charge distributions, one can show[2] that the mean-square nuclear-charge radius $\langle r^2\rangle$ (i.e., the second moment of the nuclear-charge distribution) is measured, and Eq. (3) is valid if we take $\langle r^2\rangle=\frac{3}{5}R^2$.

The assumption of constant $\psi(r)$ is valid only in the nonrelativistic limit. For high Z atoms, we must obtain the wave functions by a solution of the Dirac equation. This gives $|\psi(r)|^2_{\rm rel}=|f(r)|^2+|g(r)|^2$, where the large and small parts of the radial wave function, $f(r)$ and $g(r)$, are not constant over the nuclear volume. For s electrons in the field of a point nucleus, both f and g vary near the origin as[3]

$$f(r),\ g(r)=Nr^{\sigma-1} \quad , \tag{4}$$

where N is a normalization constant, $\sigma=(1-\alpha^2Z^2)^{1/2}$ and α is the fine-structure constant. Integration of Eq. (1) then gives[4]

$$\Delta E=CR^k \quad , \tag{5}$$

where C is a function of σ and the nonrelativistic value $|\psi(0)|^2$, and

$$k=2(1-\alpha^2Z^2)^{1/2} \quad . \tag{6}$$

Thus when relativistic effects are considered, it would appear that the shift measures a moment of the nuclear-charge distribution which gives substantial deviation from the nonrelativistic value of $k=2$ for high Z (see Fig. 1).

It has been previously recognized[5,6] that this result is not correct. Since one always has $\sigma<1$, the wave functions in Eq. (4) are singular at the origin, and thus are not suitable for use in a perturbation-theory calculation. Wu and Wilets[6] have used an expansion of $|\psi(r)|^2_{\rm rel}$ to order of $\alpha^2Z^2r^2$ to show that an expression of the form of Eq. (5) is correct if we take

$$k\approx 2-0.354\alpha^2Z^2 \quad . \tag{7}$$

As seen in Fig. 1, this gives a departure from the nonrelativistic value of $k=2$ which is considerably less than that of the relativistic first-order perturbation-theory result. However, no attempt has been made to assess the validity of the various approximations involved in the Wu–Wilets calculation. It is the purpose of the present paper to show that a straightforward calculation which does not suffer from the inconsistency of the perturbation-theory approach or the approximate form of the Wu–Wilets result can show explicitly what moment of the nuclear-charge distribution is measured by the isotope or isomer shift.

In an important paper, Broch[7] has shown the following result: The energy shift ΔE due to a change of potential $\Delta V=V_1-V_2$ is given by

$$\Delta E=\int_0^\infty \Delta V(u_1u_2+v_1v_2)dr/\int_0^\infty(u_1u_2+v_1v_2)dr \quad , \tag{8}$$

where $u=rf$, $v=rg$, and the subscripts 1 and 2 denote the wave functions obtained by solutions of the Dirac equation for the potentials V_1 and V_2, respectively. This is an exact result, obtained by combining the Dirac equations for the two potentials and doing a single integration. It thus does not suffer from the shortcomings of perturbation theory, and in fact has been used several times[7-10] to discuss corrections to the perturbation-theory calculation of the absolute value of

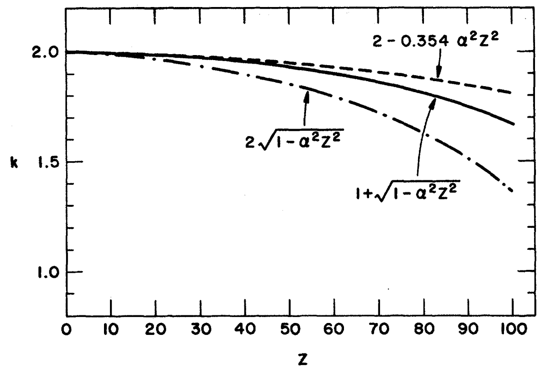

FIG. 1. Variation of k and Z as obtained from first-order perturbation theory (dot-dashed line), the approximation of Wu and Wilets (dashed line), and the present result (solid line).

the isotope shift. Since $\Delta V = 0$ for $r > R$ in the isotope-shift problem, Broch points out that one makes only a very small error by taking

$$\int_0^\infty (u_1 u_2 + v_1 v_2)\, dr \approx \int_0^\infty (u_1^2 + v_1^2)\, dr = 1 \quad . \tag{9}$$

Thus for this problem we have

$$\Delta E = \int_0^R \Delta V (u_1 u_2 + v_1 v_2)\, dr \quad , \tag{10}$$

where ΔV is given by Eq. (2). The wave functions in the presence of a point nucleus, u_1 and v_1, can be obtained from Eq. (4). For the wave functions, when one has a finite nucleus, u_2 and v_2, we again consider a uniformly charged sphere. Near the origin, one may take a power series for both u_2 and v_2,[5,11]

$$u_2(r),\ v_2(r) = \sum_n a_n \frac{r^{n+1}}{R^n} \quad , \tag{11}$$

where the expansion coefficients a_n show no explicit dependence on R. Rose has shown[11] that such a series converges for this potential, so solutions to any desired degree of accuracy may be obtained. With these results, integration of Eq. (10) then gives

$$\Delta E = F R^k \quad , \tag{12}$$

with

$$k = 1 + (1 - \alpha^2 Z^2)^{1/2} \quad . \tag{13}$$

The factor F contains numerical constants, including a sum over the a_n, but no dependence on R. Equations (12) and (13) are valid to all orders of the expansion of Eq. (11), and hence constitute an essentially exact result. One notes that for small Z, this gives the proper R^2 behavior. Equation (13) is compared with the perturbation-theory result and the Wu–Wilets expression in Fig. 1. The latter is seen to underestimate the decrease from $k = 2$ for heavy atoms, however, the dependence of Eq. (13) on Z is still rather weak. In the vicinity of $Z = 90$ one sees that the isotope or isomer shift measures the $k = 1.7$ moment of the nuclear-charge distribution.

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