Analysis of Muonic-Atom Isomer Shifts in ²⁰⁹Bi and ²⁰⁷Pb[†]

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The observed muonic-atom isomer shifts in 209 Bi and 207 Pb are analyzed in terms of a single particle or hole coupled to collective vibrations of the nuclear core by means of the weakcoupling Hamiltonian of Bohr. The isomer shift is a delicate effect which is sensitive to certain details of nuclear structure. Although the data for these two nuclei are limited, they strongly suggest two conclusions: (1) that vibrational excitation is not strictly volume conserving, but results in a slight increase of nuclear volume; and (2) that the proton core reacts significantly to changes in state of the valence particle, in a way which is not accounted for by the present model. This reaction is found to be stronger in the case of a valence neutron than in the case of a valence proton. In addition, the Ford-Wills radial-moment analysis is found to be adequate for the analysis of isomer shifts, though the refined method of Barrett is superior. As a byproduct of this work, nuclear wave functions are obtained which may be useful for other applications.

I. INTRODUCTION

When muonic atoms are formed, processes sometimes occur which result in the muon reaching its ground state at a time when the nucleus is in an excited state. Subsequent deexcitation of the nucleus generally occurs before the muon decays or is captured, and thus the nuclear transition is perturbed by the presence of the muon. The change in transition energy from its normal value is called the muonic isomer shift.¹

Isomer shifts for four transitions in ²⁰⁹Bi have been measured by two different groups,^{2,3} and isomer shifts for three transitions in ²⁰⁷Pb have been measured by a third group.⁴ Their results are listed in Table I. The known energy levels5-7of ²⁰⁹Bi and ²⁰⁷Pb which are relevant to our discussion are shown in Fig. 1. The uncertainties in ΔE_{exp} are all nearly 1 keV in ²⁰⁹Bi, due to the fact that the reference energies are obtained by Coulomb excitation and thus are not especially well known. In ²⁰⁷Pb, however, the unperturbed levels may be seen through the decay of ²⁰⁷Bi, and so the experimental uncertainties are less. The correction $\Delta E_{\rm hfs}$, due to the magnetic hyperfine splitting of the nuclear levels, will be discussed later. It is probably sufficient to note here that this correction is not well known, and though small, may contribute as much as 1 keV to the uncertainty in ΔE_{is} . The values for ΔE_{hfs} in Table I are those which have been calculated by the experimental groups. It appears that 1 keV is a reasonable estimate for the total uncertainty in ΔE_{is} , though it could be larger. A consistency check on the isomer shifts for ²⁰⁹Bi may be made by observing that the last two lines in the isomer-shift column should sum to give the entry in the first line.

Since $\Delta E_{\rm hfs}$ should not exhibit this quality (a point which will be evident later), the fact that $\Delta E_{\rm exp}$ nearly does so provides experimental evidence that $\Delta E_{\rm hfs}$ is small.

In what follows, we compare these values for $\Delta E_{\rm is}$ with predictions based on various applications of the weak-coupling model of Bohr.⁸

II. CONTRIBUTIONS TO THE ISOMER SHIFT

We may write the Hamiltonian of the muonnucleus system as

$$H = H_N + T_\mu - e\Phi_{\mu}^{(i)} + H_b^{(i)} + H_M + H';$$

 H_N is the nuclear Hamiltonian, T_{μ} is the muon kinetic energy, $\Phi_{\mu}^{(i)}$ is the electrostatic potential generated by the average charge distribution of the nucleus when it is in state *i*, $H_p^{(i)}$ is the nuclear-polarization Hamiltonian for the same state *i*, H_M is the magnetic interaction between the muon and the nucleus, and H' represents everything else, including radiative corrections and any sofar unknown effects. Though the third and fourth terms each depend explicitly on the nuclear state under consideration, their sum does not, since

$$-e\Phi_{\mu}^{(i)} = \langle i | V_{C} | i \rangle$$

and

$$H_{h}^{(i)} = V_{C} + e \Phi_{\mu}^{(i)}$$
,

where $V_{\rm C}$ is the Coulomb interaction between the muon and the protons in the nucleus. It is customary to treat the last three terms in H as perturbations, in which case the unperturbed states of the system are direct products of muon and nuclear eigenstates. This procedure is evidently justified, as studies of ordinary muonic atoms (where the

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FIG. 1. Energy levels of ²⁰⁹Bi and ²⁰⁷Pb. Arrows represent those transitions in which isomer shifts have been measured.

nucleus remains in the ground state, allowing one to ignore H_N) based on the second and third terms are found to reproduce the measured muon energy levels to within 1% or less. In these studies, $\Phi_{\mu}^{(ground)}$ is computed from a phenomenological charge distribution. The splitting of V_C into two terms is convenient, as it separates the difficult problem of computing the dynamical response of the nucleus to the muon from the much easier problem of finding the muon eigenstates in a static potential.

The energy of a nuclear transition from state j to state i when a muon is present in the ground state is thus

$$\begin{split} E(j) - E(i) &= E_N^{(j)} - E_N^{(i)} - e\langle \mathbf{1}S | \Phi_{\mu}^{(j)} - \Phi_{\mu}^{(i)} | \mathbf{1}S \rangle \\ &+ \Delta \langle H_{\mu} \rangle + \Delta \langle H_{M} \rangle + \Delta \langle H' \rangle , \end{split}$$

where the muon state $|1S\rangle$ is defined by

$$[T_{\mu} - e\Phi_{\mu}^{(0)}]|1S\rangle = E_{\mu}^{(1S)}|1S\rangle,$$

and $\Phi_{\mu}^{(0)}$ is the electrostatic potential generated by a charge distribution which closely resembles that of the nucleus in any of the states under consideration. Though we are specifying first-order perturbation theory for the change in the Coulomb binding energy of the muon due to the change in the nuclear charge distribution, we must use more elaborate methods if we wish to calculate some of the other contributions. The difference $E_N^{(j)} - E_N^{(i)}$ is the transition energy observed when a muon is not present. Thus the uncorrected isomer shift is

$$\Delta E = -e \langle \mathbf{1S} | \Phi_{\mu}^{(j)} - \Phi_{\mu}^{(i)} | \mathbf{1S} \rangle + \Delta \langle H_{p} \rangle + \Delta \langle H_{M} \rangle + \Delta \langle H' \rangle .$$
(1)

We examine the contributions in order of increasing importance.

Effects Other Than Change of Coulomb Binding Energy

The contribution of H' to the muon binding energy in the 1S state is typically about 1%, amounting to about 70 keV in the lead region. Almost all of this is known to come from the radiative corrections, which depend on the nuclear state only through its average charge distribution and thus contribute an

| ²⁰⁹ Bi | Darr | nstadt (Re | ef. 2) | | Columbia (Ref. 3 | 3) |
|---|-----------------------------------|---------------------|---------------------------|---------------------------|---------------------|-----------------|
| Transition | ΔE_{\exp} | $\Delta E_{ m hfs}$ | ΔE_{is} | ΔE_{exp} | $\Delta E_{ m hfs}$ | ΔE_{is} |
| $\frac{15}{2} + - \frac{9}{2}$ | 6.3 ± 0.6 | 0.4 | 6.7 | 5.7 ± 0.5 | 0.8 | 6.5 |
| $\frac{9+}{2} - \frac{9-}{2}$ | 7.0 ± 1.1 | 0.0 | 7.0 | 7.5 ± 1.0 | -0.4 | 7.1 |
| $\frac{13}{2}^{+a} - \frac{9}{2}^{-}$ | 2.3 ± 0.7 | 0.9 | 3.2 | 2.5 ± 0.5 | 0.9 | 3.4 |
| $\frac{15}{2}$ - $\frac{13}{2}$ - $\frac{1}{2}$ | 2.7 ± 0.8 | -0.2 | 2.5 | 3.3 ± 1.0 | -0.3 | 3.0 |
| | ²⁰⁷ Pb | | Virg | inia (Ref. 4) | | |
| | Transition | | ΔE_{exp} | $\Delta E_{ m hfs}$ | ΔE_{is} | |
| | $\frac{3}{2}^{-}-\frac{1}{2}^{-}$ | | 1.49 ± 0.3 | 0.4 | 1.9 | |
| | $\frac{5}{2} - \frac{1}{2}$ | | 0.06 ± 0.3 | 0.3 | 0.4 | |
| · · · · · · · · · · · · · · · · · · · | $\frac{7}{2}^{-}-\frac{5}{2}^{-}$ | | 6.14 ± 0.4 | 0.4 | 6.5 | |

TABLE I. Experimental isomer shifts. All energies in keV.

^a This is the state at 1.608 MeV.

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insignificant amount to the isomer shift when compared with the change in the Coulomb binding energy. The other known corrections in H' are even smaller and can all be shown to contribute negligible amounts to the isomer shift.

After all known corrections are applied, however, there remains a possible discrepancy of as much as 5 keV between experimental and theoretical values for the binding energy of the 1S muon in lead.9, 10 This apparent discrepancy (whose existence is not absolutely certain) has been attributed to an underestimate of the nuclear-polarization effect in present theoretical calculations.9,10 Another possible source is a so far undiscovered anomalous muon-nucleon interaction (which we have implicitly included in H'). If this hypothetical interaction were due to a central force, it is clear that it would be too weak to have any appreciable effect on the isomer shift. If it were to depend on the relative angular momenta involved, its main effect would be similar to that due to the magnetic interaction between the muon and the nucleus, and we will discuss this possibility when we discuss H_M.

The contribution of the nuclear-polarization Hamiltonian H_b to the isomer shift is difficult to calculate explicitly, but we may make the following observation about its probable magnitude, based on the calculations of Chen¹¹ and Skardham ar^{12} (each of whom independently predicts about a 6-keV increase in the 1S muon binding in ²⁰⁸Pb due to H_{h}). Nuclear polarization does not contribute to the muon binding energy in first-order perturbation theory, and in second-order the effect comes primarily from virtual excitations of the nucleus to highly collective states. For this reason, changes in the nuclear polarization due to changes in the state of the valence particle are probably negligible. Also, the total angular momentum of the nuclear state is evidently unimportant, since the $\frac{15^+}{2}$ and $\frac{9^+}{2}$ states in ²⁰⁹Bi show approximately the same isomer shift. It should be recalled that these states are both almost entirely a $1h_{9/2}$ proton coupled to a 3⁻ core vibration. The energy denominators for virtual multiple transitions with $l \ge 2$ are large enough and their total contributions small enough that they contribute negligibly to the isomer shift. It is not possible at present to reach as firm a conclusion about the contributions of l=0and l=1 excitations. A definite conclusion must await further calculations, though it would be surprising if they contributed as much as 1 keV to the isomer shifts. In what follows, we assume $\Delta \langle H_{\bullet} \rangle = 0$. This assumption is subject to greatest doubt for the collective states around 2.6 MeV. The nuclear-polarization effect should be greater for these states than for the ground state, causing

 $\Delta \langle H_p \rangle$ to be negative. The reason for this is that the spectrum of excited states available by l=0 or l=1 transitions from the 3⁻ state contains more members of lower energy than the spectrum available from the ground state.

The effect of the magnetic interaction Hamiltonian H_{M} on the isomer shift has been studied by Gal, Grodzins, and Hüfner.¹³ The main effect is to split each nuclear state into an unresolved doublet, so that to obtain ΔE_{exp} one must average Eq. (1) in the correct way over the members of the relevant doublets. It is known that the initial populations of the upper pair of levels are not statistical. In addition, there is usually a fast interdoublet magnetic dipole transition between the higher pair of states, which produces a preferential population of the lower member of the doublet for decay to lower states. The splitting depends in an important way on the distribution of magnetic moment within the nucleus, and at present there is no direct experimental evidence nor reliable theoretical prediction of what this should be.¹⁴ Calculations indicate corrections in ²⁰⁷Pb and ²⁰⁹Bi of the order of 0.5 to 1 keV. We should note that since these corrections rest heavily on theoretical calculations of the hyperfine splitting of the nuclear levels, an anomalous spin-spin muon-nucleon interaction which is small enough not to have been seen so far could make a substantial difference in $\Delta E_{\rm hfs}$.

Effect of Change of Coulomb Binding Energy Radial-Moment Interpretation

Thus we are left with the first term in Eq. (1) as the dominant term in the isomer shift. In the coordinate representation we write

$$\Delta E_{is} = -e \int d^{3}r [\Phi_{\mu}^{(j)} - \Phi_{\mu}^{(i)}] \psi_{1S}^{\dagger} \psi_{1S}$$
$$= \int r^{2} dr \phi^{(1S)}(r) \int d\Omega [\rho^{(j)}(\vec{\mathbf{r}}) - \rho^{(i)}(\vec{\mathbf{r}})], \qquad (2)$$

where we have used Green's theorem in the second step. The spherically symmetric quantity $\phi^{(1S)}(r)$ is the potential generated by the muon charge density, and it satisfies

$$\frac{d}{dr}\left[r^2\frac{d}{dr}\phi^{(\mathrm{ls})}(r)\right] = 4\pi e r^2\psi^\dagger_{\mathrm{ls}}(r)\psi_{\mathrm{ls}}(r) \ .$$

The quantity $\rho^{(j)}(\vec{\mathbf{r}})$ represents the average charge density of the nucleus in state j, normalized to Ze. For our calculations we use the relativistic muon wave function and calculate $\phi^{(1S)}$ numerically, though there are useful approximations that one may make for $\phi^{(1S)}$ which lead to simple physical interpretations of the isomer shift. We discuss these next.

Ford and Wills found by a semiempirical method¹⁵ that a particular transition in a given muonic atom is sensitive to a specific and generally nonintegral moment of the nuclear charge density. In particular, they found that small changes in the 1S binding energy in Pb were proportional to changes in the radial moment $\langle r^{1.03} \rangle$. Following Ford,¹⁶ we notice that Eq. (2) tells us that if we can write to a good approximation,

$$\phi^{(1S)}(r) = A + Br^k, \qquad (3a)$$

in the regions where $r^2 \int [\rho^{(i)}(\vec{\mathbf{r}}) - \rho^{(i)}(\vec{\mathbf{r}})] d\Omega$ is appreciably large, then we have

$$\Delta E = ZeB\Delta \langle r^k \rangle$$
.

Barrett¹⁷ pointed out that fits of the form

$$\phi(r) = A + Br^k e^{-\alpha r} , \qquad (3b)$$

which lead to

$$\Delta E = ZeB\Delta \langle r^{k}e^{-\alpha r} \rangle$$

can increase the accuracy of analysis for many transitions.¹⁸ It turns out that this additional accuracy is not needed at present in analyzing the isomer shift, a point which we will demonstrate in Sec. IX. We will content ourselves for the time being with asserting that to sufficient accuracy, one can interpret the isomer shifts in lead and bismuth by means of the formula

$$\Delta R_{h} = C \Delta E_{is}$$
,

with k = 1.1 and C = 1.25 fm/MeV. The quantity R_k is the Ford-Wills equivalent radius, defined by

$$R_{k} = \left[\frac{1}{3}(k+3)\langle \gamma^{k} \rangle\right]^{1/k}$$

With accuracy that is good enough for qualitative considerations, we may make a further approximation and set k=1 and C=1.2 fm/MeV. Though this integral moment is somewhat more convenient to deal with, the results thereby obtained can be used only as a rough guide, a point which will be demonstrated in Sec. IX. We should note in addition that since C is near 1 fm/MeV, the measured isomer shifts indicate changes in nuclear radius of a few thousandths of a fermi.

III. NUCLEAR MODEL, METHOD OF CALCULATION OF ISOMER SHIFTS

Throughout this paper, the nucleus under consideration is assumed to consist of a single particle or hole coupled to core vibrations by means of the coupling Hamiltonian¹⁹

$$H_{c} = k(r) \sum_{\lambda \mu} \beta_{\lambda \mu} Y_{\lambda \mu}(\theta, \phi), \qquad (4)$$

where the form of k(r) depends on the parametrization used in describing the average single-particle potential. If we write

$$V(\mathbf{\vec{r}}) = V(\boldsymbol{r} - R(\theta, \phi), A_0),$$

where A_0 is a surface-thickness parameter and R is a radial parameter which contains all the angular dependence of V and is written

$$R = R_{0} \gamma \left[1 + \sum_{\lambda \mu} \beta_{\lambda \mu} Y_{\lambda \mu}(\theta, \phi) \right], \qquad (5)$$

we get

$$k(r) = -R_0 \frac{dV}{dr} \, .$$

The factor γ is a function of the deformation parameters $\beta_{\lambda\mu}$ and is inserted to conserve volume, if necessary. Since the Hamiltonian H_c includes only the first-order terms in $\beta_{\lambda\mu}$, which conserve volume automatically, we may set $\gamma = 1$. We should note that in most treatments the factor R_0 in k(r) is replaced by r, due to a different parametrization of the deformed single-particle potential. However, we have found that the differences thus obtained are unimportant.

We expand the nuclear wave function in the direct product basis of core and single-particle states, with the amplitudes of admixture being determined by H_c and the uncoupled eigenvalues. In order to calculate isomer shifts for the coupled wave functions, it is necessary to obtain charge densities and calculate isomer shifts for the single-particle states and core states separately. We calculate the single-particle wave functions in a modified, energy-dependent Woods-Saxon well with spinorbit coupling, with the unbound states being handled by a method which is described in the next section. The proton core is assumed to be approximately describable by the volume-conserving density function

$$\rho(r-c(\theta,\phi),a)$$

$$\approx \rho(r-c_{0},a) + c_{0} \frac{\partial \rho}{\partial c} \bigg|_{\beta=0} \sum_{\lambda\mu} \beta_{\lambda\mu} Y_{\lambda\mu}$$

$$+ \frac{1}{2} c_{0}^{2} \sum_{\lambda\mu} |\beta_{\lambda\mu}|^{2} \left\{ |Y_{\lambda\mu}|^{2} \frac{\partial^{2} \rho}{\partial c^{2}} \bigg|_{\beta=0} - \frac{a_{2}}{4\pi a_{1}} \frac{\partial \rho}{\partial c} \bigg|_{\beta=0} \right\},$$
(6)

where $a_1 = \int \partial \rho /\partial c |_{\beta=0} r^2 dr$ and $a_2 = \int \partial^2 \rho /\partial c^2 |_{\beta=0} r^2 dr$, and we have used the same approach as in parametrizing the single-particle potential. That is, $c(\theta, \phi) = c_0 \gamma [1 + \sum_{\lambda \mu} \beta_{\lambda \mu} Y_{\lambda \mu}(\theta, \phi)]$, and *a* is a surface-thickness parameter. The second term in braces appears by virtue of the assumption that .

volume is conserved. We have neglected the second-order terms $\beta_{\lambda\mu}{}^2 Y_{\lambda\mu}{}^2$ because they contribute nothing.

We note that odd powers of $\beta_{\lambda \mu}$ have expectation value zero, and that

$$\left\langle \sum_{\mu} \left| \beta_{\lambda \mu} \right|^2 \right\rangle = \frac{\hbar \omega_{\lambda}}{2c_{\lambda}} \sum_{\mu} (2n_{\lambda \mu} + 1) ,$$

where $\sum_{\mu} n_{\lambda \mu}$ is the number of phonons present of mode λ , $\hbar \omega_{\lambda}$ is their energy, and c_{λ} is the nuclear stiffness parameter for mode λ . If we integrate Eq. (6) over angles, this allows us to write for the purpose of computing the isomer shift due to the core, with third-order accuracy in the vibrational parameters,

$$\left\langle \int d\Omega \rho (r - c(\theta, \phi), a) \right\rangle$$

= $4\pi\rho (r - c_0, a) + \frac{1}{2} c_0^2 \sum_{\lambda} \frac{\hbar\omega_{\lambda}}{2c_{\lambda}} \sum_{\mu} (2n_{\lambda\mu} + 1)$
 $\times \left\{ \frac{\partial^2 \rho}{\partial c^2} \Big|_{\dot{\beta}=0} - \frac{a_2}{a_1} \frac{\partial \rho}{\partial c} \Big|_{\beta=0} \right\}.$

This gives us

$$\int d\Omega \left[\rho(\sum_{\mu} n_{\lambda \mu} = 1) - \rho(\sum_{\mu} n_{\lambda \mu} = 0) \right]$$
$$= c_0^2 \frac{\hbar \omega_{\lambda}}{2c_{\lambda}} \left\{ \frac{\partial^2 \rho}{\partial c^2} \Big|_{\beta=0} - \frac{a_2}{a_1} \left. \frac{\partial \rho}{\partial c} \right|_{\beta=0} \right\}.$$

This is the quantity which is to be inserted into Eq. (2), which then represents the isomer shift in a core transition from a state with one phonon of mode λ to the ground state, assuming that the vibration is volume-conserving. The quantity $(\hbar \omega_{\lambda}/2c_{\lambda})^{1/2}$, which we call the amplitude of vibration, may be extracted from observed collective transition rates. The amplitudes which we use throughout this paper were so obtained^{5, 20, 21} and are listed in Table II, along with the experimental vibrational energies.

We have chosen one of the simpler ways of describing a volume-conserving vibration. More complicated ways appropriate for large deformations can be shown to lead to negligible (and probably physically meaningless) differences here.

TABLE II. Vibrational parameters.

| λ^{π} | $(\hbar\omega_{\lambda}/2c_{\lambda})^{1/2}$ | ħω _λ (MeV) |
|-----------------|--|--------------------------|
| 2+ | 0.025 | 4.07 |
| 3- | 0.042 | 2.615 |
| 4+ | 0.024 | 4.30 |
| 5 | 0.028 | 3.20 |

Our volume-conservation requirement defines the volume of the nucleus as

$$V=\frac{1}{\rho(0)}\int\rho(r)d^3r\,,$$

and requires it to be independent of all $\beta_{\lambda\mu}$. For our calculations we used a Fermi function for the spherical charge distribution, with parameters $c_0 = 6.6$ fm and a = 0.53 fm. Of the variety of effects which may result from using different chargedensity functions and parametrizations, probably the largest comes from the fact that the derivatives are inversely proportional to powers of *a*, and that the skin thickness for any smooth distribution is known to only 5 or 10%.²² Due to cancellations, however, the errors therby induced in the isomer shift are only about 1 or 2%.

IV. CALCULATION OF ISOMER SHIFTS IN ²⁰⁹Bi IMPLIED BY THE MINNESOTA WAVE FUNCTIONS

Calculations of ²⁰⁹Bi wave functions perturbed to first order by H_c have been made by Broglia²³ using as a basis 11 of the lowest single-proton states along with the set of core states which consists of the ground state and excited states with one phonon of mode $\lambda = 1$, 2, or 3. He used $k(\mathbf{r}) = -rdV/dr$.

As a preliminary exercise, we calculated isomer shifts for his admixtures, using the vibrational parameters which he reported (and which coincide with ours for $\lambda = 2$ and 3) and a set of single-particle wave functions which we had calculated with no serious attempt to fit the observed single-particle energies. The results are listed in Table III, normalized to zero for the $\frac{9}{2}$ ground state.

The agreement between these calculations and the experimental numbers is poor, but we may make the following observations about the results.

TABLE III. Isomer shifts relative to the ground state in 209 Bi obtained from Minnesota wave functions. All energies in keV.

| Contributions from | E _{is} (Theory) | E _{is} (Exp) |
|-----------------------|---|---|
| Core | 2.6 | |
| Single particle | -0.2 | |
| Total | 2.4 | 6.5 ± 1.0 |
| Core | 2.5 | |
| Single particle | -0.4 | |
| Total | 2.1 | 7.1 ± 1.0 |
| Core | 0.5 | |
| Single particle | 4.9 | |
| Total | 5.4 | 3.4 ± 1.0 |
| | Contributions from Core Single particle Total Core Single particle Total Core Single particle Total | $\begin{array}{c c} \hline Contributions \\ from \\ \hline (Theory) \\ \hline \\ \hline \\ Core \\ Total \\ \hline \\ Core \\ 2.6 \\ 1.4 \\ \hline \\ Core \\ 2.5 \\ Single particle \\ -0.4 \\ \hline \\ Total \\ \hline \\ Core \\ 0.5 \\ \hline \\ Single particle \\ 4.9 \\ \hline \\ Total \\ \hline \\ 5.4 \\ \hline \end{array}$ |

The $\frac{9}{7}$ and $\frac{13}{7}$ states are known to be of nearly pure single-particle character, and the $\frac{15}{2}$ and $\frac{9}{2}$ are essentially octupole core vibrations coupled to the $1h_{g/2}$ single-particle state. The latter fact shows up well in the near equality of the predicted isomer shifts for these two states, as well as in the experimental numbers. It appears that an increase in the contribution from the core by a factor of about 2.5 and a decrease in the contribution from the $1i_{13/2}$ single-particle state by a factor of about 0.5 is needed to obtain agreement with experiment.

V. METHOD OF CALCULATION OF NUCLEAR WAVE FUNCTIONS

In order to find the dependence of the results on the parameters and approximations used, we recalculated the amplitudes of admixed states by diagonalizing the Hamiltonian

$$H_{N} = H^{(S)} + H^{(P)} + H_{c}$$

to all orders in a variety of direct product bases. $H^{(s)}$ is Bohr's surface Hamiltonian, and $H^{(P)}$ is the Hamiltonian for the valence particle in the appropriate spherically symmetric potential. We took $k(r) = -R_0 dV/dr.$

The single-particle wave functions were obtained by numerical integration using Hamming's method,²⁴ whose accuracy was carefully investigated and found to be substantially superior to the usual Runge-Kutta method. We expect numerical errors in our eigenvalues to be less than 0.2 keV. with corresponding accuracy in the wave functions. The potential used in $H^{(P)}$ was

$$V = V_s(r) + V_{so}(r) + V_{co}(r) ,$$

where for $r \ge 1$ fm,

$$V_{s}(r) = -V_{0}(E)/(1 + e^{(r-R_{0})/A_{0}}),$$

$$V_{so}(r) = -\lambda_{so} \left(\frac{\hbar}{mc}\right)^{2} \frac{\vec{1} \cdot \vec{s}}{2r} \frac{d}{dr} V_{s}(r).$$

For r < 1, the above expressions were set equal to their value at r = 1 so that a power series solution about the origin could be obtained, in order

to avoid integrating numerically through the angular momentum barrier. The Coulomb potential V_{co} was taken to be that due to a uniform charge distribution of radius $R_c = 6.6$ fm, a number taken from muonic-atom data. The parameters R_0 , A_0 , and λ_{so} were taken to be adjustable.

We allowed the strength of the potential to be velocity-dependent in the following way: We set

$$V_0(E) = V_0(0) + C_E E$$
,

where $V_0(0)$ and C_E are adjustable parameters for a given nucleus, and $V_0(E)$ is the potential well depth for a state of energy E. Final values of Eand $V_0(E)$ were obtained by an interative procedure. We were unable to get reasonable fits to the observed levels in ²⁰⁹Bi with $C_E = 0$, since the known energy differences $2f_{5/2}-2f_{7/2}$ and $1i_{13/2}-1h_{9/2}$ are in that case nearly independent of everything except λ_{so} , and a single value of λ_{so} could not be found to fit both differences. We were able to get good fits, however, with $C_E \neq 0$. The parameters used for two different sets of wave functions are listed in Table IV, and the corresponding singleparticle energies and isomer shifts (measured from the $1h_{9/2}$ state) are shown in Table V. Set 1 represents a good fit as it is to the observed energy levels, and Set 2 represents a good fit when the perturbations due to the core are taken into account with a particular choice of basis (to be discussed later).

Even with $C_E \neq 0$, it was not possible to obtain a good fit to the observed levels of ²⁰⁷Pb. We attribute this to the inadequacy of the simple diagonal pairing interaction which we assumed.²⁵ The parameters of our best fit are shown in Table IV. and the corresponding single-particle energies with pairing corrections included are listed in Table VI. We have also included in Table VI the isomer shifts which would exist if the neutron had charge e. This was done so that we could investigate the possibility that an "effective charge" of the neutron might describe the response of the core to its motion.

We represented the unbound proton states by the resonances which were found by applying the arti-

| TABLE IV. Potential parameters. | | | | | | | | |
|---------------------------------|-----------------------------|------------------------|------------------------|-----------------|-------------------------------|----------------|---|--|
| | V ₀ (0) (MeV) | R ₀ (fm) | A ₀ (fm) | λ _{so} | <i>R</i> _c (fm) | C _E | Binding of lowest single- particle state (MeV) | |
| ²⁰⁹ Bi Set 1 | 63.0 | 7.4 | 0.74 | 25.0 | 6.6 | 0.40 | $-3.536(1h_{9/2})$ | |
| ²⁰⁹ Bi Set 2 | 62.0 | 7.4 | 0.71 | 22.4 | 6.6 | 0.30 | $-3.599(1h_{9/2})$ | |
| ²⁰⁷ Pb | 46.5 | 7,31 | 0.657 | 32.5 | | 0.16 | $-6.887(3p_{1/2})^{a}$ | |

^a Includes pairing energy.

ficial boundary condition that the wave functions have zero derivative at the outermost turning point, a condition which insures that the state thus obtained represents maximum probability that the proton will be found within the nucleus. Normalization was a problem only for the highest states considered, due to the small amount of tunneling through the Coulomb barrier for most of these wave functions.

VI. CALCULATION OF ADMIXED WAVE FUNCTIONS

We obtained admixed nuclear wave functions, energies, and corresponding isomer shifts by diagonalizing H_N numerically under various assumptions. We used several different sets of single-particle wave functions, two of which appear in Table V for ²⁰⁹Bi and one of which appears in Table VI for ²⁰⁷Pb. We used various combinations of the four known one-phonon, isospin-independent core states, and for a few runs added hypothetical onephonon 6^+ , 7⁻, 8^+ , and 9⁻ vibrations in order to get an idea of the effect of more degrees of freedom for the core. For all of these hypothetical states we took $(\hbar\omega_{\lambda}/2c_{\lambda})^{1/2} = 0.028$ and $\hbar\omega_{\lambda} = 3.5$ MeV.²⁶ Since none of them become admixed by more than a few percent, the exact values of their parameters are unimportant.

Incorporation of the giant dipole resonance presented serious problems. When we used the phenomenological coupling strength given in Ref. 5, we found that the nearly pure single-particle levels were lowered by almost 2 MeV with respect to the nearly pure core oscillations. If this described the physical situation correctly, it would mean that the 2.615-MeV 3^- vibration in ²⁰⁸Pb should ap-

pear at over 4 MeV in ²⁰⁹Bi, which is clearly not the case. In addition, the results of Ref. 5 require us to believe that the magnitude of H_c for this isospin-dependent vibration is 5 times as large as it is for the isospin-independent vibrations, and this does not seem very reasonable. In view of the above difficulties, we left the giant-dipole state out of our final calculations, though the calculations which we did make with it indicate that it is unimportant in isomer shifts of the low-lying levels.

Since we did not consider single-particle excitations of more than one particle or hole, we decided that the most appropriate place to truncate our single-particle basis was at the minimum energy required for a combined particle-hole excitation. This occurs at about 5 MeV in ²⁰⁹Bi and about 4 MeV in ²⁰⁷Pb. The resulting wave functions for these bases mixed with the four core states of Table II are listed in Tables VII and VIII. The singleparticle wave functions and energies used are those of Tables V and VI, with Set 2 being used for ²⁰⁹Bi. We made use of the fact that in ²⁰⁷Pb, the highest occupied level $(3p_{1/2})$ contains one particle and one hole, so that excitations of the particle to higher levels, as well as excitations of the hole could be treated within the framework of our model. The energies obtained for ²⁰⁹Bi represent a good fit to the experimental spectrum, while those for ²⁰⁷Pb are substantially worse but still reasonable.

It should be noted that a predominantly collective state is mixed with other collective states by H_c only through its pure single-particle components, as H_c connects only those states which differ by one vibrational quantum. Thus, for example, all the amplitudes except for two in the higher $\frac{13}{2}$

TABLE V. Single-particle energies and isomer shifts for ²⁰⁹Bi.

| | Set | t 1 | Set 2 | | |
|-------------------|------------|--------------------------|-------------------|--------------------------|--|
| State | E (MeV) | E _{is} (keV) | <i>E</i> (MeV) | E _{is} (keV) | |
| $1h_{9/2}$ | 0.0 | 0.0 | 0.0 | 0.0 | |
| $2f_{7/2}$ | 0.916 | -3.12 | 1.435 | -3.54 | |
| $1i_{13/2}$ | 1,615 | 6.38 | 2.175 | 6.08 | |
| $2f_{5/2}$ | 2.847 | -3.87 | 3.264 | -4.18 | |
| 3p _{3/2} | 3,105 | -5.72 | 3.747 | -6.09 | |
| $3p_{1/2}$ | 3.884 | -5.59 | 4.480 | -5.94 | |
| $2g_{9/2}$ | 6.283 | 2.22 | 7,174 | 2.01 | |
| $1i_{11/2}$ | 6.327 | 2.82 | 6,630 | 2.89 | |
| $1j_{15/2}$ | 7.073 | 9.22 | 8.036 | 8.98 | |
| $3d_{5/2}$ | 8.657 | 2.65 | 9,632 | 3.38 | |
| $2g_{7/2}$ | 9.065 | 1.94 | 9.787 | 1.95 | |
| $4s_{1/2}$ | 9.720 | 6.29 | 10.645 | 9.72 | |
| $3d_{3/2}$ | 9.997 | 4.60 | 10.862 | 6.28 | |

TABLE VI. Single-particle energies and isomer shifts for ²⁰⁷Pb.

| | 101 FD. | |
|------------------|----------------|--------------|
| | E ^a | E_{is}^{b} |
| State | (MeV) | (keV) |
| $1h_{9/2}^{-1}$ | 3.429 | -2.11 |
| $2f_{7/2}^{-1}$ | 3,137 | -0.20 |
| $1i_{13/2}^{-1}$ | 1.629 | -9.41 |
| $3p_{3/2}^{-1}$ | 1.080 | 0.58 |
| $2f_{5/2}^{-1}$ | 0.751 | 0.11 |
| $3p_{1/2}^{-1}$ | 0.0 | 0.0 |
| $2g_{9/2}$ | 3.422 | 7.32 |
| $1i_{11/2}$ | 4.505 | 5,78 |
| $3d_{5/2}$ | 5.180 | 14.04 |
| $1j_{15/2}$ | 5.205 | 12,95 |
| $4s_{1/2}$ | 5.749 | 24.76 |
| $3d_{3/2}$ | 6.436 | 22,98 |
| $2g_{7/2}$ | 6.512 | 10.09 |

^a Hole energies include pairing energy.

^b Calculated as if the neutron had charge +e.

state in ²⁰⁹Bi are essentially second-order in the vibrational parameters. The net effect of this is that although the addition of more degrees of freedom for the core lowers the single-particle energies substantially, it has little effect on the vibrational states. This must be viewed as a defect in the present scheme, since the experimental fact that the 2.615-MeV 3⁻ level in ²⁰⁸Pb appears at nearly the same energy in ²⁰⁹Bi and ²⁰⁷Pb indicates that the degrees of freedom which perturb the single-particle energies have either a negligible effect on them or have nearly the same effect on the energies of the collective states. Since the effect was found to be nonneglibible in all our calculations, we must conclude that the picture of noninteracting core vibrations is incomplete.

The wave functions listed in Tables VII and VIII probably represent the most reasonable compromise within the framework of our model, though the values given for the smallest components should probably not be taken too seriously.

VII. CALCULATION OF ISOMER SHIFTS

The isomer shifts in Table III indicate that for the states under consideration the mixing caused by H_c has little effect on the isomer shift. We found this to be true with only a few exceptions in all of the calculations which we did. For this reason, the problem of fitting the observed isomer shifts in ²⁰⁹Bi has two nearly independent aspects: fitting the vibrational shifts, and fitting the singleparticle shifts.

In attempting to fit the vibrational shifts exhibited strongly in the $\frac{15^+}{2^+}$ and $\frac{9}{2^+}$ states, we may assume either that the 3⁻ vibrational amplitude in Table II is wrong, that Eq. (6) does not adequately describe the vibrating charge density, or both. If we

TABLE VII. Energies and amplitudes of the admixed wave functions for ²⁰⁹Bi calculated using the core states of Table II and the six lowest proton states of Set 2. All energies in MeV.

| nlj, <i>\</i> | <u>9</u> (0 .0) | $\frac{7}{2}$ - (0.903) | 13+ 2 (1.586) | $\frac{5}{2}^{-}$ (2.808) | $\frac{3}{2}^{-}$ (3.078) | $\frac{1}{2}^{-}$ (3.646) | 13+ (2.867) | Other septuplet states (2.832) |
|--------------------------------|--|----------------------------|---------------------|---------------------------|---------------------------|---------------------------|----------------|---|
| $1h_{9/2}$ | 0.980 | 0.026 | | | | | | |
| $\frac{2J_{7/2}}{1}$ | | 0.926 | 0 883 | | | | 0 196 | |
| $2f_{E/2}$ | | | 0.000 | 0.872 | | | -0.130 | |
| $3p_{3/2}$ | | | • | 0.011 | 0.869 | | . , | |
| 3p _{1/2} | | | | | | 0.751 | | |
| $1h_{9/2}, 2$ | 0.117 | 0.033 | | 0.354 | | | | |
| $2f_{7/2}, 2$ | -0.019 | 0.097 | | -0.060 | 0.229 | | | |
| $1i_{13/2}, 2$ | | | 0.124 | | | | -0.026 | |
| $2f_{5/2}, 2$ | 0.060 | 0.024 | | 0.091 | 0.054 | 0.144 | | |
| 3p _{3/2} , 2 | | 0.064 | | -0.038 | 0.077 | -0.107 | | |
| $3p_{1/2}, 2$ | | | | 0.063 | 0.067 | | | |
| $1h_{9/2}, 3$ | | | 0.179 | | | | 0.982 | 1.000 |
| $2f_{7/2}, 3$ | | | 0.333 | | | | -0.098 | 2.000 |
| $1i_{13/2}, 3$ | 0.059 | -0.302 | | | | | | |
| $2f_{5/2}$, 3 | | | | | | | | |
| 3p _{3/2} , 3 | | | | | | | | |
| 3p _{1/2} , 3 | | | | | | | | |
| $h_{9/2}, 4$ | -0.103 | -0.058 | | -0.238 | -0.163 | -0.572 | | · · · · · |
| $2f_{7/2}, 4$ | 0.033 | -0.084 | | 0.109 | -0.151 | 0.277 | | |
| $1i_{13/2}, 4$ | | | -0.112 | | | | 0.023 | |
| 2 f _{5/2} , 4 | -0.046 | -0.046 | | -0.073 | -0.121 | | | |
| $3p_{3/2}, 4$ | 0.020 | -0.044 | | 0.085 | | | | |
| $3p_{1/2}, 4$ | -0.032 | -0.049 | | | | | | |
| $1h_{9/2}, 5$ | | | -0.140 | | | | 0.072 | . : |
| $2f_{7/2}$, 5 | | | -0.144 | | | | 0.037 | |
| 1 <i>i</i> _{13/2} , 5 | -0.060 | 0.140 | | -0.126 | 0.340 | | | |
| 2 f _{5/2} , 5 | | | -0.046 | | | | 0.009 | |
| 3p _{3/2} , 5 | | | -0.083 | | | | 0.017 | |
| 3p _{1/2} , 5 | ************************************** | | | | | | | |

assume that Eq. (6) is adequate, we must multiply the 3⁻ vibrational amplitude in Table II by about 1.5 in order to reproduce the experimental result. There are two objections to this, however. One is that the collective transition rates are fairly well known,⁵ and they imply the values listed in Table II. The second is that the over-all energy splitting of the $|3^-, 1h_{9/2}\rangle$ septuplet is essentially proportional to the square of the 3⁻ vibrational amplitude, and with a suitable choice of basis, the present model predicts over-all splittings which are always at least as large as the experimentally observed value of 0.25 MeV (though the level ordering is not correct).

For these reasons, we were led to question the form of Eq. (6). Since it seems highly unlikely that a different volume-conserving parametrization or a different method of requiring volume conservation can make up the really enormous difference between experiment and theory, we decided to try dropping volume conservation. This is of no consequence for the energy levels, since the changes of core radius being considered are only a few thousandths of a fermi, and the associated compressional energy changes may be estimated²⁷ to be less than 1 keV. In addition, any physical

| TABLE VIII. | Energies and amplitudes | of the admixed way | e functions for ²⁰⁷ J | Pb calculated | using the core states of |
|-------------|----------------------------|----------------------|----------------------------------|---------------|--------------------------|
| TAB | LE II and the eight lowest | single-particle or l | iole states of Table | e VI. All ene | rgies are in MeV. |

| nlj,λ | $\frac{1}{2}^{-}$ (0.0) | 5 ⁻ (0.692) | 3- (0.856) | $\frac{13}{2}$ + (1.577) | 7- (2.475) | 9- (3.326) | $\frac{5}{2}^+$, $\frac{7}{2}^+$ (3.006) |
|-------------------------------------|-------------------------|---------------------------|---------------|--------------------------|---------------|---------------|--|
| $3p_{1/2}^{-1}$ | 0.972 | | | | | | |
| $2f_{5/2}^{-1}$ | | 0.964 | | | | | |
| $3p_{3/2}^{-1}$ | | | 0.945 | · | | | |
| $1i_{13/2}^{-1}$ | | | | 0.953 | | | |
| $2f_{7/2}^{-1}$ | | | | | 0.845 | 0.014 | |
| $2 \sigma_{0,1}$ | | | | | | 0,914 | |
| $1i_{11/2}$ | | | | | | | |
| $3p_{1/2}^{-1}, 2$ | | 0.086 | 0.089 | | | | |
| $2f_{5/2}^{-1}, 2$ | 0.109 | 0.083 | 0.047 | | 0.042 | 0.177 | |
| $3p_{3/2}^{-1}$, 2 | -0.084 | -0.035 | 0.068 | | 0.105 | | |
| $1i_{13/2}^{-1}, 2$ | | | | 0.113 | | | |
| $2f_{7/2}^{-1}, 2$ | | -0.022 | 0.076 | | 0.065 | -0.018 | |
| $1h_{9/2}^{-1}, 2$ | | 0.063 | | 0.005 | 0.015 | 0.076 | |
| $2g_{9/2}, 2$ | | | | 0.065 | | | |
| ± <i>v</i> _{11/2} , 2 | | | | 0.012 | | | |
| $3p_{1/2}^{-1}, 3$ | | | | | | | |
| $2f_{5/2}^{-1}, 3$ | | | | | | | |
| $3p_{3/2}$, 3 | | | | | a 400 | | |
| $1_{13/2}^{-1}, 3$ | | | | 0.100 | -0.420 | 0.159 | |
| $4J_{7/2}$, 3 12 -1 9 | | | | 0.109 | | | 1 000 |
| $2 \sigma_{10} 3$ | | 0.055 | -0 186 | 0.030 | -0 151 | 0.050 | 1.000 |
| $1_{i_{11}}$, 3 | | -0.145 | 0.100 | | -0.039 | -0.162 | |
| 1 4 | | | | | 0.100 | | |
| $3p_{1/2}^{-1}, 4$ | | -0.066 | -0.105 | | -0.126 | -0.157 | |
| $\frac{2}{5/2}, \frac{4}{1}$ | | 0.079 | -0.105 | | -0.075 | -0.122 | |
| $1_{i_{10}}^{j_{3/2}}, \frac{1}{4}$ | | 0.010 | | -0.102 | 0.010 | 0.000 | |
| $2f_{7/2}^{-1}, 4$ | 0.082 | 0.041 | -0.052 | | -0.056 | 0.032 | |
| $1h_{9/2}^{-1}, 4$ | -0.063 | -0.047 | -0.028 | | -0.026 | -0.067 | |
| $2g_{9/2}, 4$ | | | | -0.051 | | | |
| $1i_{11/2}, 4$ | | | | -0.021 | | | |
| $3p_{1/2}^{-1}, 5$ | | | | | | | |
| $2f_{5/2}^{-1}, 5$ | | | | -0.073 | | | |
| $3p_{3/2}^{-1}, 5$ | | | | -0.132 | | | |
| $1i_{13/2}^{-1}$, 5 | | -0.069 | 0.173 | | 0.175 | -0.126 | |
| $2f_{7/2}$, 5 | | | | -0.079 | | | |
| $1h_{9/2}^{-1}, 5$ | 0 195 | 0.061 | 0.070 | -0.039 | 0.001 | 0.040 | |
| $2g_{9/2}, 5$ | -0.125 | -0.061 | 0.079 | | 0.081 | -0.046 | |
| 11 _{11/2} , 5 | 0.095 | 0.008 | 0.044 | | 0.041 | 0.090 | |

| | | Set | t 2. | | |
|-----------------------|--------------------------|--------------------------|--------------------------|--------------------------|---------------------------------|
| Number of | single- | | | · , | |
| in basis: | tates 6 E | 9 E | 11 E | 13 E | Experimen values <i>E</i> |
| State | (MeV) | (MeV) | (MeV) | (MeV) | (MeV) |
| <u>9-</u> 2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| | (-0.217) | (-0.365) | (-0.411) | (-0.428) | , |
| $\frac{7}{2}^{-}$ | 0.903 | 0.858 | 0.836 | 0.804 | 0.897 |
| <u>13</u> + 2 | 1.586 | 1.497 | 1,533 | 1.550 | 1.608 |
| $\frac{5}{2}$ | 2.808 | 2.675 | 2.588 | 2.565 | 2.822 |
| $\frac{3}{2}^{-}$ | 3.078 | 2.937 | 2.836 | 2.788 | 3.108 |
| $\frac{1}{2}^{-}$ | 3.646 | 3.584 | 3.342 | 3.359 | 3.624 |
| $\frac{3+}{2}$ | 2,832 | 2.980 | 3.026 | 2.976 | 2.491 |
| 5+ 2 | 2.832 | 2.980 | 3.020 | 3.037 | 2.615 |
| $\frac{7}{2}$ | 2.832 | 2.980 | 2,939 | 2,956 | 2.581 |
| 9+ 2 | 2.832 | 2.962 | 3.008 | 3.025 | 2.563 |
| <u>11</u> + 2 | 2.832 | 2.737 | 2.780 | 2.797 | 2.598 |
| $\frac{13}{2}$ + | 2.867 | 3.010 | 3.055 | 3.072 | 2.600 |
| <u>15</u> + 2 | 2.832 | 2.980 | 3.026 | 3.043 | 2.740 |
| State | E _{is} (keV) | E _{is} (keV) | E _{is} (keV) | E _{is} (keV) | $E_{ m is}$ (keV) |
| <u>9-</u> | 0.0 | 0.0 | 0.0 | 0.0 | |
| $\frac{7}{2}$ | -1.85 | -1.91 | -1.92 | -1.91 | |
| <u>13</u> + | 5.46 | 5.57 | 5.55 | 5.54 | 3.4 ± 1.0 |
| 5 | -2.82 | -2.80 | -2.81 | -2.79 | |
| $\frac{3}{2}$ | -3.76 | -3.80 | -3.83 | -3.82 | |
| $\frac{1}{2}$ | -2,93 | -3.45 | -3.67 | -3.68 | |
| $\frac{3}{2}$ | 6.65 | 6.53 | 6.51 | 6.46 | |
| 5+ 2 | 6.65 | 6.53 | 6.50 | 6.49 | |
| $\frac{7}{2}$ + | 6.65 | 6.53 | 6.39 | 6.38 | |
| 9+ 2 | 6.65 | 6.48 | 6.46 | 6.45 | 7.1 ± 1.0 |
| <u>11</u> + 2 | 6.65 | 6.12 | 6.09 | 6.07 | |
| - <u>13</u> + 2 | 6.57 | 6.48 | 6.46 | 6.44 | |
| - | | | | a | |

TABLE IX. Energies and isomer shifts in ²⁰⁹Bi calculated using the core states of Table II and proton states from

process (such as a transition rate) which is sensitive to the first-order terms in an expansion in powers of $\beta_{\lambda\mu}$ is not capable of providing information on the matter, since these terms conserve volume automatically.

ond term in braces to have adjustable magnitude. Charge must still be conserved, however, and to do so we multiply the right side of Eq. (6) by a factor $(1 - \epsilon)$, where ϵ is second order in $\beta_{\lambda\mu}$. This is equivalent through second order to adding a term inside the braces proportional to $\rho(\mathbf{\tilde{r}})|_{\beta=0}$ and of magnitude such that the integral over all

We may generalize Eq. (6) to describe a nonvolume-conserving vibration by allowing the secspace of what is in the braces is zero. The re-sult is

$$\begin{split} \rho(r-c(\theta,\phi),a) &\approx \rho|_{\beta=0} + c_0 \frac{\partial \rho}{\partial c} \bigg|_{\beta=0} \sum_{\lambda\mu} \beta_{\lambda\mu} Y_{\lambda\mu} \\ &+ \frac{c_0^2}{2} \sum_{\lambda\mu} |\beta_{\lambda\mu}|^2 \left\{ |Y_{\lambda\mu}|^2 \frac{\partial^2 \rho}{\partial c^2} \right|_{\beta=0} \\ &- (1-\alpha) \frac{a_2}{4\pi a_1} \frac{\partial \rho}{\partial c} \bigg|_{\beta=0} - \alpha \frac{a_2}{Ze} \rho|_{\beta=0} \left\}, \end{split}$$

where α provides a measure of the change of volume. The case $\alpha = 0$ corresponds to volume conservation, while $\alpha = 1$ corresponds to setting $\gamma = 1$ in the charge-density version of Eq. (5). We obtained reasonable fits to the observed vibrational isomer shifts only with α in the vicinity of 3, which corresponds to an average value of c in the vibrational state which is larger than c_0 . Thus we conclude that the vibrations result in an increase in the volume of the nucleus. All results in the remainder of this paper reflect the choice $\alpha = 3$.

We should note in addition that if the nuclear polarization by the muon contributes a negative shift for these transitions, which we concluded was likely in Sec. II, the need to increase the isomer shift contribution from the vibrating core is even greater.

Energies and isomer shifts for ²⁰⁹Bi calculated under various assumptions are shown in Tables IX and X. Table IX shows the effect of changing the number of single-particle states in the basis. Single-particle energies and wave functions from Set 2 were used, with the lowest 6, 9, 11, and 13 states forming the basis along with the four core states of Table II. The numbers in parentheses in the first line of the energy columns represent the shift in energy of the ground state due to the admixtures of other states. It should be noted that the energy splitting of the $|3^-, 1h_{9/2}\rangle$ septuplet is about 0.27 MeV in all cases except the first, lending support to the contention that the 3^- vibrational amplitude used is not too small.

Table X shows the effect of varying the core states in the basis. We have used all 13 proton energies and wave functions of Set 1 (so that to see the effect of changing from Set 1 to Set 2 we may compare column 2 of Table X with column 4 of Table IX). The splitting of the septulet increases slightly when the number of core states is increased, but in all cases it is >0.25 MeV.

A qualitative feature of all our calculations, which is exhibited in Tables IX and X, is that the isomer shifts are generally slowly varying functions of the variables involved. The only exception which we found to this rule occurs when a near degeneracy occurs in two admixed wave functions of the same spin and parity. In this case, the amplitudes of admixture become rapidly varying functions of the variables and the resulting isomer shifts are sensitive in an unphysical way to the parameters used. The only example of this effect of interest which we found involves the $\frac{9}{2}$ tate in ²⁰⁹Bi, and the result may be seen in the unusually low value of the $\frac{9}{2}^+$ isomer shift in column 3 of Table X. The low value of the $\frac{11^+}{2}$ isomer shift in the same column is probably due to the same effect but in a less marked way. When this occurs, of course, it is necessary to determine whether the near degeneracy really exists or is merely an unfortunate result of a particular choice of variables. It is worth noting that the nearly pure single-particle states are generally too low in energy to encounter nearly degenerate admixed states of the same spin and parity.

Though the experimental isomer shifts for the $\frac{9+}{2}$ and $\frac{15+}{2}$ states are well reproduced for all cases except one in Tables IX and X, none of the calculations which we did came very close to the experimental value for $\frac{13+}{2}$ state. Evidently the core readjusts to partially compensate for the change in the single-particle state. Table X shows that adding more degrees of freedom for the core produces a small effect in this direction, but it is not nearly enough.²⁸

Energies and isomer shifts calculated for ²⁰⁷Pb under various assumptions are shown in Table XI. Except for the last column, we have used the single-particle energies and wave functions listed in Table VI, and the number of core states and singleparticle states used appears at the head of each column. Column 5 shows the results of using the same wave functions to calculate the matrix elements of H_c but adjusting the single-particle energies so that the energies of the admixed states are close to the experimental energies. In all the calculations, the $\frac{7}{2}$ isomer shift is much larger than the other nearly pure single-particle shifts, in qualitative agreement with the experimental results. However, neither it nor the $\frac{3}{2}$ - shift is nearly large enough. It appears again that the proton core is responding strongly to the single-particle motion in a way which is not accounted for by the present model. It also seems fairly clear that the proton core responds more strongly to a valence neutron than a valence proton, since the discrepancies in ²⁰⁷Pb are substantially larger than the one in ²⁰⁹Bi.

VIII. MONOPOLE CORE READJUSTMENT

The weak-coupling model takes into account changes in shape of the core in response to singleparticle motion, but it has nothing to say about over-all changes in size of the self-consistent po-

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| | Core states used: 3 ⁻ | 2+3-4+5- T | 2+3-4+5- 6+7-8+9- | Experimental values |
|--------------------|-------------------------------------|--------------------------|--------------------------|--------------------------|
| State | (MeV) | (MeV) | (MeV) | (MeV) |
| <u>9</u> - 2 | 0.0 | 0.0 | 0.0 | 0.0 |
| | (-0.184) | (-0.442) | (-0.953) | |
| $\frac{7}{2}$ | 0.454 | 0.294 | 0.198 | 0.897 |
| $\frac{13}{2}$ + | 1,175 | 1.021 | 0.810 | 1.608 |
| $\frac{5}{2}^{-}$ | 2,575 | 2.196 | 1.864 | 2.822 |
| $\frac{3}{2}$ | 2.747 | 2.177 | 2.216 | 3.108 |
| $\frac{1}{2}^{-}$ | 3.565 | 2.856 | 2.824 | 3.624 |
| $\frac{3+}{2}$ | 2.728 | 2.976 | 3.476 | 2.491 |
| <u>5</u> + 2 | 2.792 | 3.049 | 3.559 | 2.615 |
| $\frac{7}{2}$ + | 2.712 | 2.955 | 3.434 | 2.581 |
| 9+ 2 | 2.778 | 3.025 | 3.426 | 2.563 |
| $\frac{11}{2}$ + | 2.574 | 2.783 | 3.155 | 2.598 |
| $\frac{13}{2}$ + | 2,826 | 3.077 | 3.580 | 2.600 |
| <u>15</u> + 2 | 2.799 | 3.057 | 3,568 | 2.740 |
| | | | | |
| State | E _{is} (keV) | E _{is} (keV) | E _{is} (keV) | E _{is} (keV) |
| $\frac{9}{2}$ | 0.0 | 0.0 | 0.0 | |
| $\frac{7}{2}^{-}$ | -1.49 | -1.54 | -1.61 | |
| <u>13</u> + 2 | 6.00 | 5.85 | 5.49 | 3.4 ± 1.0 |
| $\frac{5}{2}^{-}$ | -3.30 | -2.71 | -1.94 | |
| $\frac{3}{2}^{-}$ | -4.89 | -3.59 | -3.22 | |
| $\frac{1}{2}^{-}$ | -4.96 | -3,86 | -2.86 | |
| <u>3</u> + 2 | 6.51 | 6,37 | 6.10 | |
| <u>5</u> + 2 | 6.54 | 6.45 | 6.18 | |
| <u>7</u> + 2 | 6.46 | 6.29 | 5.87 | |
| <u>9</u> + 2 | 6.49 | 6.29 | 4.23 | 7.1 ± 1.0 |
| $\frac{11}{2}$ + | 6.29 | 5.95 | 5.03 | |
| $\frac{13}{2}$ + | 6.51 | 6.43 | 6.18 | |
| <u>1 ö</u> + 2 | 6.55 | 6.46 | 6.20 | 6.5 ± 1.0 |

TABLE X. Energies and isomer shifts in ²⁰⁹Bi calculated using the 13 proton states of Set 1 and varying numbers of core states.

tential caused by changes in state of the valenceparticle, potential changes which in turn produce changes in the size of the nuclear core. A quantitative treatment of this effect requires knowledge of the realistic nucleon-nucleon interaction and the ability to calculate second- and higher-order effects, since these are probably substantial. However, we may look at the first-order effect in the following semiquantitative way.

If we approximate the nucleon-nucleon potential by means of a δ function, we may write for the total potential seen by a proton in the nucleus,

$$V_{b}(\mathbf{\tilde{r}}) = C_{L}\rho_{b}(\mathbf{\tilde{r}}) + C_{U}\rho_{n}(\mathbf{\tilde{r}}), \qquad (7)$$

where we have assumed that the nn and pp interactions have average strength C_L and the np in

| Number of core states: | 4 | | 4 | 8 | 4 | · · · · · · · · · · · · · · · · · · · |
|------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|---------------------------------------|
| particle states: | 8 | 8 | 13 | 13 | 8 | Experimenta values |
| State | E (MeV) | E (MeV) | E (MeV) | E (MeV) | E ^a (MeV) | E (MeV) |
| $\frac{1}{2}^{-}$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| | (-0.391) | (-0.557) | (-0.617) | (-0.908) | (-0.384) | |
| <u>5</u> - 2 | 0.692 | 0.453 | 0.792 | 0.636 | 0.587 | 0.570 |
| $\frac{3}{2}$ | 0.856 | 0.877 | 0.929 | 0.947 | 0.897 | 0.897 |
| $\frac{13}{2}$ + | 1.577 | 1.254 | 1.607 | 1.323 | 1.620 | 1.633 |
| $\frac{7}{2}$ | 2.475 | 2.252 | 2,561 | 2.359 | 2.389 | 2.339 |
| $\frac{9}{2}$ | 3.326 | 3.026 | 3.489 | 3.276 | 3.422 | 3.43 |
| <u>5</u> + 2 | 3.006 | 3.172 | 3.110 | 3.384 | 2.999 | 2.610 |
| <u>7</u> + 2 | 3.006 | 3.172 | 3.104 | 3.361 | 2.999 | 2.655 |
| State | E _{is} (keV) |
| $\frac{1}{2}$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | , |
| $\frac{5}{2}$ | 0.14 | 0.21 | 0.05 | 0.11 | 0.11 | 0.4 ± 0.6 |
| $\frac{3}{2}$ | 0.28 | 0.25 | 0.20 | 0.17 | 0.27 | 1.9 ± 0.6 |
| $\frac{13}{2}$ + | 0.22 | 0.36 | 0.19 | 0.28 | 0.24 | |
| $\frac{7}{2}$ | 1.42 | 1.20 | 1.21 | 0.96 | 1.30 | 6.4 ± 0.6 |
| <u>9</u> - 2 | 0.49 | 0.57 | 0.36 | 0.43 | 0.50 | |
| <u>5+</u> 2 | 6.57 | 6.49 | 6.00 | 5.79 | 6.57 | |
| $\frac{7}{2}$ + | 6.57 | 6.49 | 6.11 | 5.84 | 6.57 | |
| | | | | | | |

TABLE XI. Energies and isomer shifts in ²⁰⁷Pb calculated using varying numbers of core states and single-particle states.

^a Single-particle energies fixed so that the resulting mixed states have energies which are nearly correct.

tion has strength C_U . The densities $\rho_p(\mathbf{\tilde{r}})$ and $\rho_n(\mathbf{\tilde{r}})$ are those for the protons and neutrons, respectively, and their normalizations determine the scale for C_L and C_U . A change in proton or neutron density gives for the fractional change in potential

$$\frac{\Delta V_{p}(\vec{\mathbf{r}})}{V_{p}(\vec{\mathbf{r}})} = \frac{C_{L} \Delta \rho_{p}(\vec{\mathbf{r}}) + C_{U} \Delta \rho_{n}(\vec{\mathbf{r}})}{(ZC_{L} + NC_{U})\rho_{0}(\vec{\mathbf{r}})}$$

where $\rho_0(\mathbf{\dot{r}})$ is assumed to describe the radial dependence of the total proton or neutron densities but is normalized to represent one particle. If we assume that the protons in the core respond to local changes in potential like a degenerate Fermi gas, we have

$$\frac{\Delta \rho_c(\vec{\mathbf{r}})}{\rho_c(\vec{\mathbf{r}})} = \frac{3}{2\rho_0(\vec{\mathbf{r}})} \frac{\Delta \rho_p(\vec{\mathbf{r}}) + (C_U/C_L)\Delta \rho_n(\vec{\mathbf{r}})}{\left[Z + (C_U/C_L)N\right]},$$

where $\rho_{c}(\mathbf{\tilde{r}})$ represents the density of protons in the

core and is equal to $Z\rho_0(\mathbf{\tilde{r}})$. Thus if $\Delta\rho_p(\mathbf{\tilde{r}})$ and $\Delta\rho_n(\mathbf{\tilde{r}})$ represent changes in state of a valence proton or neutron, the above result gives these particles a total effective charge of

$$e_n = e \frac{C_U}{C_L} \frac{3/2}{\left[1 + (C_U/C_L)(N/Z)\right]}$$
(8a)

for the neutron, and

$$e_{p} = e \left\{ 1 + \frac{3/2}{\left[1 + (C_{U}/C_{L})(N/Z) \right]} \right\}$$
(8b)

for the proton.

The idea of using C_U and C_L as adjustable parameters in calculations of nuclear properties was apparently originated by Seyler and Blanchard.²⁹ Since then others have used similar approaches with varying results, as C_U and C_L depend on the form of the interaction assumed (not generally a δ function) and the data being fit. If we use Eq. (7)

| $k:$ $B:$ $\alpha:$ | Ford- Wills 1.00 1.10×10 ⁻² | Ford- Wills 1.10 8.28×10 ⁻³ | Barrett 2.315 1.570×10 ⁻³ 0.134 | Exact |
|---------------------|---|---|---|----------|
| State | Eis | E_{is} | E_{is} | E_{is} |
| <u>9</u> - 2 | 0.0 | 0.0 | 0.0 | 0.0 |
| $\frac{7}{2}^{-}$ | -2.23 | -1.91 | -1.85 | -1.85 |
| $\frac{13}{2}$ + | 5.44 | 5.43 | 5.46 | 5.46 |
| $\frac{5}{2}$ | -3.23 | -2.91 | -2.82 | -2.82 |
| $\frac{3}{2}^{-}$ | -5.28 | -4.58 | -3.77 | -3.76 |
| $\frac{1}{2}^{-}$ | -4.07 | -3.53 | -2.93 | -2.93 |
| <u>9</u> + 2 | 6.82 | 6.75 | 6.65 | 6.65 |

TABLE XII. Isomer shifts in 209 Bi calculated with the Ford-Wills and Barrett approximations, using the wave functions of Table VII. All energies are in keV.

to reproduce the potential well strengths in Table IV, we get $C_U/C_L \approx 5$. From Eq. (8a) we see that e_n/e varies between 0 and 1 as a function of C_U/C_L for the nuclei under consideration, since $Z/N \approx \frac{2}{3}$, and Eq. (8b) tells us that e_p/e varies from $\frac{5}{2}$ to 1. For C_U appreciably greater than C_L , both the proton and neutron have effective charges of about e, with magnitudes which are fairly insensitive to the actual value of C_U/C_L .

If incorporation of an effective charge is to reproduce the isomer shift of the $\frac{13^4}{2}$ state in 209 Bi, however, it must be less than *e* for the proton. Thus we must make the hypothesis that there is a second-order effect, larger than and in the opposite direction from the first-order effect, which produces an effective charge of the proton of about 0.5*e*. This is not unreasonable, but it is certainly beyond the scope of the present discussion.

We made several isomer shift calculations for 207 Pb in which we allowed the effective charge of the neutron to be nonzero. Typical results are exhibited in Fig. 2, where we have plotted the isomer shifts relative to the ground state vs e_n/e for the three measured excited states. The basis used was that of column 1 of Table XI. The cross-hatched areas represent the experimental shifts, and it is quite obvious that no single value of e_n can reproduce these numbers. Thus it appears that an effective charge approach is not adequate.



FIG. 2. Predicted isomer shifts in ²⁰⁷Pb relative to the ground state as a function of neutron effective charge. Cross-hatched areas represent the experimental isomer shifts.

IX. COMPARISON OF EXACT CALCULATIONS WITH THE FORD-WILLS AND BARRETT APPROXIMATIONS

All of the above calculations are exact from the point of view of the muon, since the exact muongenerated potential was used in Eq. (2). Results obtained by using the approximations (3a) and (3b) for various values of the parameters involved are shown in Table XII, using the ²⁰⁹Bi wave functions of Table VII. The first column of isomer shifts contains the result of a Ford-Wills fit where kwas forced to be 1, and the next two columns contain results from best fits over appropriate regions for the two approximating forms. The exact result is shown in the last column. The accuracy of the Barrett fit is remarkable. However, the simpler Ford-Wills form produces errors which are smaller than the present uncertainties in ΔE_{exp} and ΔE_{hfs} , and thus we see semiempirical evidence that the equivalent radius interpretation discussed in Sec. II is justified. It is also clear from the first column that interpretation of isomer shifts in bismuth and lead in terms of changes in the first radial moment of the nuclear charge distribution is only qualitatively justified.

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*Present address.

¹We use the term "isomer shift" loosely here, as it has come to be reserved for what is left after magnetic hyperfine effects have been accounted for. We will adhere to convention in the remainder of this paper and use the term "uncorrected isomer shift" to mean the total change in energy of a given nuclear transition.

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