drally coordinated crystals, on the other hand, the optical spectra are now well understood in terms of quantum-mechanical one-electron energy-band models. In these spectra there is no evidence for the existence of an appreciable fraction ($\frac{1}{2}$, in the case of II-VI crystals) of nonbonding electrons as postulated by the classical resonating-bond theory.

In conclusion I hope that my confusion over the nomenclature of resonating bonds will not obscure the remarkable correlation[4] of cohesive energies of tetrahedrally coordinated crystals with dielectrically defined ionic character, a correlation that is accurate to about 1% for horizontal sequences. The spectroscopic ionicities have also been demonstrated[6] to be accurate to about 1% in predicting fourfold or sixfold coordination of $A^N B^{8-N}$ crystals. Such success should not be considered surprising in view of the quantum-mechanical basis of the spectroscopic approach.[7]

[1]L. Pauling, preceding Letter [Phys. Rev. Letters 23, 480 (1969)].
[2]J. C. Phillips, Solid State Phys. 18, 55 (1966).
[3]H. R. Philipp and H. Ehrenreich, Phys. Rev. 129, 1550 (1963).
[4]J. C. Phillips, Phys. Rev. Letters 22, 645 (1969).
[5]A. W. Streitwieser, Jr., Molecular Orbital Theory (John Wiley & Sons, New York, 1961), Chap. 9.
[6]J. C. Phillips, Chem. Phys. Letters 3, 286 (1969).
[7]The reader may feel that success is too strong a word to use in view of the discrepancies for GaP and InAs listed in Table II. However, in those cases the A and B cores are not isoelectronic, as they are for GaAs and BN, where (3) is so accurate. From Fig. 1 of Ref. 4 one can show that for an R_1-R_2 sequence ($R_1 \neq R_2$) the deviations from linearity always correspond to a shift in the cohesive energy closer to the linear relation which holds for the row to which the anion belongs. For GaSb and InAs this shift amounts to ±6 kcal/mole, respectively, so that core corrections, although present, do not seriously affect the validity of the linear relation (3).

COULOMB ENERGIES AND THE EXCESS NEUTRON DISTRIBUTION FROM THE STUDY OF ISOBARIC ANALOG RESONANCES†

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The effects determining the energies of isobaric analog resonances are studied. In particular, the compound and continuum shifts, nuclear two-body correlations, isospin-nonconserving nuclear forces, and isospin impurity are discussed. These effects are important in deriving the excess neutron density from analog-resonance experiments.

The displacement energy ΔE_d (Fig. 1) deduced from isobaric-analog-resonance (IAR) experiments is becoming a very useful tool for studying the distribution of the (N-Z) excess neutrons in nuclei.[1,2] The bulk of the displacement energy arises from the Coulomb matrix element between

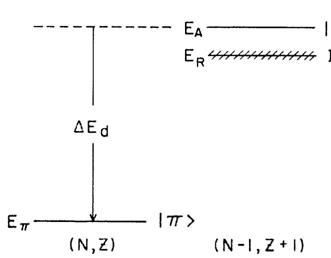

FIG. 1. The relation between the parent state $|\pi\rangle$, the analog state $|A\rangle$, and the IAR. The difference $E_A - E_\pi$ is termed displacement energy. E_R differs from E_A by the continuum and compound shift.

the densities of the protons and the excess neutrons. In order to extract precise information from the experimentally determined positions of the IAR, the small remainder of ΔE_d has to be studied in detail. In this Letter we investigate various quantities that contribute to the displacement energies and calculate several new terms. These include the continuum and compound mixing,[3] nuclear two-body correlations, the isospin-nonconserving parts of the nuclear force, and the isospin impurity in the parent state. The inclusion of these terms significantly modifies the value of ΔE_d as well as its isotopic dependence.

If the parent state $|\pi\rangle$ is an eigenstate of the Hamiltonian H with N neutrons and Z protons, the analog state is defined by[3]

$$|A\rangle = T_- |\pi\rangle \langle \pi | T_+ T_- | \pi\rangle^{-1/2} \quad (1)$$

and the displacement energy by

$$\Delta E_d = E_A - E_\pi = \langle A|H|A\rangle - \langle\pi|H|\pi\rangle = \frac{\langle\pi|T_+[H,T_-]|\pi\rangle}{\langle\pi|T_+T_-|\pi\rangle}. \tag{2}$$

Although ΔE_d is not observable directly, it is the main part of the energy difference $E_R - E_\pi$, where E_R is the position of IAR. Because of the commutator in Eq. (2), the displacement energy ΔE_d depends only on the isospin-nonconserving parts of the Hamiltonian.

The difference $E_R - E_A$, which is also proportional to $[H, T_-]$, is determined by the compound mixing (or "internal mixing") and the continuum mixing ("external mixing" or "Thomas-Ehrmann Shift").[3,4] Saturating the interaction of $|A\rangle$ with the compound states by the antianalog state acting as a kind of doorway state, the compound mixing is estimated as a few keV. The continuum shift is computed for all channels (open and closed) which strongly couple to the analog state. This shift is of the order of the total width of the IAR and can be significant.

Returning to the calculation of ΔE_d, we list the various contributions from $[H, T_-]$:

(1) The proton-neutron mass difference Δm in the kinetic energies leads to a dynamic p-n mass effect of the order of $\epsilon_F \Delta m/m$, where ϵ_F is the Fermi energy ($\simeq$30 MeV).

(2) The electromagnetic spin-orbit force in $[H, T_-]$ contains the magnetic interaction and the spin precession in the Coulomb field and contributes significantly to the state dependence of ΔE_d.

(3) The contribution of the charge dependence of nuclear forces can be calculated[5] from the difference in the n-n and n-p interactions since

$$[V^{\text{nucl}}(1,2), T_-] = [V_{pn}^{\text{nucl}}(1,2) - V_{nn}^{\text{nucl}}(1,2)][\tau_z(1)\tau_-(2) + \tau_z(2)\tau_-(1)] \times 14. \tag{3}$$

One finds from the analysis of low-energy nucleon-nucleon scattering that V_{np} is 4% more attractive[6] than V_{pp} (which we assume to be equal[6] to V_{nn}). Therefore we have the rough estimate

$$\Delta E_d^{\text{c.d.}} \simeq -0.04[(2T-1)/A]\, V, \tag{4}$$

where V is an averaged ($T=1$) field strength in nuclei ($V \simeq 30$ MeV). Note that this term is linear in $2T(\equiv N-Z)$ and therefore will contribute to the isotopic dependence[7] of ΔE_d. We have also calculated $\Delta E_d^{\text{c.d.}}$ for several nuclei from a phenomenological force[8] which separately fits p-p and n-p scattering. Strong spin dependence is found and the average seems somewhat smaller than the estimate of Eq. (4). However, more work has to be done to assess the accuracy of the values for $\Delta E_d^{\text{c.d.}}$.

(4) The Coulomb energy

$$\Delta E_d^{\text{Coul}} = \left\{\int d\vec{x}\, d\vec{y} [\rho_n(\vec{y}) - \rho_p(\vec{y})] \frac{e^2}{|\vec{x}-\vec{y}|}\rho_p(\vec{x}) - (\text{exchange terms})\right\} / 2T \tag{5}$$

contains the interaction of the excess neutron density $\rho_n - \rho_p$ with the proton distribution ρ_p. Equation (5) is derived using a single-particle model for the parent state $|\pi\rangle$ and assuming good isospin for this state. Configuration mixing may lead to correction terms of either sign.[9] The exchange term may be estimated by using the infinite-matter Pauli correlation function between an average particle and one at the top of the Fermi sea. We get

$$\Delta E_d^{\text{ex}} = -\frac{g}{4}\frac{Z}{A}\frac{1}{(k_F r_0)^2}\frac{e^2}{r_0}\left(1 - \frac{1}{2A^{2/3}}\frac{1}{(k_F r_0)^2}\right)\left(1 - \frac{N-Z}{12Z}\right) \tag{6}$$

with $r_0 = 1.2$ fm and $k_F = 1.4\ \text{fm}^{-1}$.

(5) The finite-size correction due to the proton charge distribution is calculated as the first term of a series in the ratio of the proton size to the nuclear radius. Including the exchange term we get

$$\Delta E^{\text{f.s.}} = -\frac{4\pi e^2}{2T}\frac{\langle r_p^2\rangle}{3}\int d\vec{x} [\rho_n(\vec{x}) - \rho_p(\vec{x})]\ \rho_p(\vec{x})[1 - \tfrac{1}{2} + (2/25)k_F^2\langle r_p^2\rangle] \tag{7}$$

with $\langle r_p^2\rangle = 0.64\ \text{fm}^2$. We have used a flat-top model for the charge distribution of the proton in order to estimate the small correction in $k_F^2\langle r_p^2\rangle$ to the exchange term. We find $\Delta E_d^{\text{f.s.}}$ to be roughly constant and of the order of -0.1 MeV.

(6) The effect of short-range correlations between protons and excess neutrons may be estimated by writing the density for a pair of nucleons as $\rho_{np}(\vec{x},\vec{y}) = \rho_n(\vec{x})\rho_p(\vec{y})[1 + f_c(|\vec{x}-\vec{y}|)]$, where $f_c(r)$ modifies

the behavior of two nucleons at small distances. We obtain for the correlation correction to the Coulomb energy

$$\Delta E_d^{\text{corr}} = \frac{4\pi e^2}{2T}\left(\frac{\pm|\langle r_c^2\rangle|}{6}\right)\int d\vec{x}\,[\rho_n(\vec{x})-\rho_p(\vec{x})]\,\rho_p(\vec{x}), \tag{8}$$

$$\pm|\langle r_c^2\rangle| = 6\int dr\,[r f_c(r)]\,[1+f_{\text{P}}(r)]\,[1+f_{\text{f.s.}}(r)]. \tag{9}$$

The second factor in Eq. (9) describes the influence of the Pauli correlations with $f_{\text{P}}(0) = -\frac{1}{2}$ and the third term contains the effect of the finite proton size on ΔE_d^{corr}. For attractive nucleon-nucleon correlations, which are expected to prevail in nuclei, the positive sign holds in Eq. (8). We have taken the crude value $\Delta E_d^{\text{corr}} \sim 0.1$ MeV, which corresponds to a correlation length $\langle r_c^2\rangle^{1/2} = 0.9$ fm. The correlation correction is probably the most sensitive point in our calculations, and more work must be done to fix the effect of the nuclear correlations on the displacement energy.

(7) We estimate the effect of the isospin impurity in the parent state $|\pi\rangle$ on the Coulomb energy by writing the parent state as a combination of states with isospins T and $T+1$: $|\pi\rangle = (1-\epsilon^2)^{1/2}T\rangle + \epsilon|T+1\rangle$. Then

$$\Delta E_d^{T\text{-imp}} = -\epsilon^2\frac{2T-1}{2T+1}|\Delta E|, \tag{10}$$

where ΔE is the separation energy between the states $|T\rangle$ and $|T+1\rangle$.[10] A collective model for the

Table I. The different contributions to the resonance energies of isobaric analog resonances. The half-radius $c = c_0 A^{1/3}$ and skin thickness t of the charge distribution are values extrapolated from those given in Ref. 12. The rms radius R_{rms} for protons is calculated from the charge distribution and is corrected for the proton finite size. The only adjustable parameter in the calculation is the half-radius of the neutron potential $R = r_0 A^{1/3}$. It influences most strongly the direct term of ΔE_d^{Coul} and is varied until theoretical and experimental values for $E_r - E_\pi$ agree. R_{rms} for all neutrons is the weighted average of the values for the protons and excess neutrons. All energies are given in MeV.

	$\|\pi\rangle$ Parent State	Ca^{49}	Sr^{89}	Ba^{139}	Pb^{209}
E_R-E_A	Contin.-Comp. Mixing	-0.06	-0.10	-0.17	-0.48
	Dyn. p-n Mass Effect	0.04	0.04	0.04	0.04
	El.Magn. Spin Orbit	-0.07	-0.08	-0.01	-0.02
$\Delta E_d^{C.D.}$	Estimate Eq. (5)	-0.20	-0.16	-0.23	-0.25
	Phenomen. Force	-0.02	-0.16	—	—
ΔE_d^{Coul}	Direct Term	7.60	12.10	15.46	19.95
	Exchange Term	-0.31	-0.35	-0.35	-0.35
$\Delta E_d^{F.S.}$	Finite Proton Size	-0.10	-0.11	-0.11	-0.11
ΔE_d^{CORR}	Short Range Correlat.	~0.1	~0.1	~0.1	~0.1
ΔE_d^{T-IMP}	Collective Model	-0.01	-0.04	-0.06	-0.09
E_R-E_π	Theory	7.08±.20	11.40±.25	14.67±.25	18.79±.25
	Experiment	7.083±.015 [a]	11.40±.02 [a]	14.67±.02 [a]	18.790±.013 [b]
c_o [fm]	Charge Distribution	1.03	1.08	1.09	1.12
t [fm]	Charge Distribution	2.3	2.3	2.3	2.2
r_o [fm]	Neutron Potential	1.06±.08	1.10±.05	1.11±.05	1.12±.04
R_{rms} [fm]	Excess Neutrons	3.71±.18	4.36±.15	4.99±.15	5.63±.15
	Protons	3.42	4.10	4.75	5.42
	All Neutrons	3.51±.04	4.17±.05	4.83±.05	5.50±.05

[a] M. Harchol, A. A. Jaffe, J. Miron, I. Unna, and J. Zioni, Nucl. Phys. A90, 459 (1967).
[b] W. R. Wharton, P. von Brentano, W. K. Dawson, and P. Richard, Phys. Rev. 176, 1424 (1968).

state $|T+1\rangle$ yields[11]

$$\epsilon^2 = 5.5\times10^{-7}Z^{8/3}/(T+1),$$
$$|\Delta E| = 170A^{-1/3}\ \text{MeV}. \tag{11}$$

A single-particle model will lead to considerably larger values[11] for the isospin impurity ϵ^2 and may increase the estimate for $\Delta E_d^{T\text{-imp}}$ by a factor of 2 to 4. Because of the strong isospin dependence of ϵ^2, $\Delta E_d^{T\text{-imp}}$ will significantly influence the isotopic dependence of the displacement energy.

In Table I, we present an analysis of the effects which determine the resonance energy E_R. The proton density appearing in the direct term of Eq. (5) has been replaced by a distribution of Fermi type with parameters extrapolated from those given in Hofstadter and Collard[12] and corrected for the proton's finite size. The exchange term has been calculated using single-particle proton wave functions. The density $\rho_n-\rho_p$ of the excess neutrons is calculated from single-particle wave functions generated in a Saxon-Woods potential well with a diffuseness of 0.65 fm. The well depth is adjusted in order to reproduce the experimental binding energies. The radius of the well is varied until calculated and experimental resonance energies agree.

Except for the dynamic p-n mass effect and probably the short-range correlations, all corrections discussed in this Letter are negative. Thus, in order to compensate these corrections and reach agreement with the experimental value of E_R, the Coulomb energy has to be increased, which is done by decreasing the radius of the potential well. The mean square radius of the distribution of the excess neutrons is given in Table I. The uncertainties assigned to the values reflect mainly the estimated uncertainties in the contributions $\Delta E_d^{\text{c.d.}}$, ΔE_d^{corr}, and $\Delta E_d^{T\text{-imp}}$. The poor knowledge of the thresholds and strengths of the inelastic decays of IAR'S introduces an uncertainty of several tens of keV in the evaluation of the continuum shift.

The displacement energy depends on the distribution of the excess neutrons ρ_n-ρ_p. Since the proton distribution is known, the rms radius R_{rms} for all neutrons can be calculated as the weighted average of the R_{rms} for the protons and excess neutrons. We find the radius for the distributions of all neutrons and all protons to be rather similar. (For example, see Fig. 2) The same conclusions have been reached by Nolen and Schiffer,[13] although they do not treat several of the new effects discussed here.

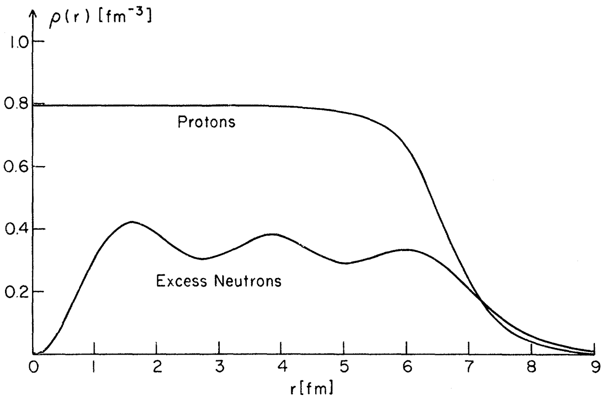

FIG. 2. The distributions of the protons and excess neutrons for Pb^{209}. The proton distribution is the empirical charge distribution of Fermi type corrected for the finite proton size. The excess neutron distribution is computed from the Saxon-Wood potential whose radius is adjusted so that the correct Coulomb energy is obtained.

We wish to acknowledge discussions with J. Schiffer and J. Nolen about the Coulomb energy and with B. Mottelson, I. Talmi, and D. Kurath about isospin nonconservation in the parent state.

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[1]J. P. Schiffer, in Proceedings of the International Conference on Nuclear Isospin, Asilomar, California, 1969 (to be published).

[2]H. A. Bethe and P. J. Siemens, Phys. Letters 27B, 549 (1968); J. Atkinson and S. D. Bloom, in Proceedings of the International Conference on Nuclear Isospin, Asilomar, California, 1969 (to be published).

[3]A. K. Kerman, in Proceedings of the International Conference on Nuclear Isospin, Asilomar, California, 1969 (to be published).

[4]D. Robson, Phys. Rev. 137, B535 (1965); H. A. Weidenmüller, Nucl. Phys. 99, 269 (1967); A. Mekjian and W. M. MacDonald, Nucl. Phys. A121, 385 (1968).

[5]The compound mixing due to the charge-dependent nuclear forces has been estimated by A. Z. Mekjian, Phys. Rev. (to be published).

[6]E. M. Henley, in Isobaric Spin in Nuclear Physics, edited by J. D. Fox and D. Robson (Academic Press, Inc., New York, 1966), p. 3.

[7]R. Sherr, Phys. Letters 24B, 321 (1967).

[8]B. Rouben, thesis, Massachusetts Institute of Technology, 1969 (unpublished).

[9]As an example, we assumed the ground state of Sr^{89} to have the particle-plus-core configuration $|\pi\rangle = \alpha|d_{5/2}0^+\rangle + \beta|s_{1/2}2^+\rangle$, where $|0^+\rangle$ and $|2^+\rangle$ are states

in Sr^{88}. Then

$$\Delta E_d=\{\alpha^2\langle d_{5/2}0^+|T_+[H,T_-]|d_{5/2}0^+\rangle +\beta^2\langle s_{1/2}2^+|T_+[H,T_-]|s_{1/2}2^+\rangle +2\alpha\beta\langle d_{5/2}0^+|T_+[H,T_-]|s_{1/2}2^+\rangle\}/2T.$$

The nondiagonal element is evaluated to be 4 keV by using the experimentally known $B(E2)$ value for the transition $2^+\rightarrow 0^+$. The difference between the two diagonal elements in ΔE_d cannot be calculated without further assumptions concerning the structure of the 0^+ and 2^+ states.

[10]A contribution $-\epsilon^2|\Delta E|/T(2T+1)$ arising from the compound mixing of the analog state with the state $T_-|T+1\rangle$ has been added to Eq. (10).

[11]A. Bohr, J. Damgård, and B. R. Mottelson, in Nuclear Structure, edited by A. Hossain, Harun-ar-Rashid, and M. Islam (North-Holland Publishing Company, Amsterdam, The Netherlands, 1967), p. 1.

[12]R. Hofstadter and H. R. Collard, Landolt-Börnstein Nuclear Physics and Technology (Springer-Verlag, Heidelberg, Germany, 1967), Group I, Vol. 2, p. 21.

[13]J. A. Nolen and J. P. Schiffer, Phys. Letters 29B, 396 (1969).

COULOMB EXCITATION OF THE COLLECTIVE SEPTUPLET AT 2.6 MeV IN ^{209}Bi†

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Beams of 18-MeV α particles and 70-MeV ^{16}O were used for $E3$ Coulomb excitation of the weak-coupling $3^-|h_{9/2}\rangle$ septuplet $J^\pi=\frac{3}{2}^+$, $\cdots$, $15/2^+$ at 2.6 MeV in ^{209}Bi. A complete decay scheme was obtained and short lifetimes were determined from observed Doppler effects. We deduce several absolute transition probabilities for both excitation and decay involving the multiplet and low-lying single-particle states.

The ^{209}Bi septuplet originating from the weak coupling of the $1h_{9/2}$ proton to the octupole vibration in ^{208}Pb has been studied by many authors[1,2] by means of inelastic particle scattering. Hafele and Woods[2] were the first to resolve all states but two of this multiplet, and in this way were able to assign spins by exploiting the $(2J+1)$ dependence of the cross section. The details of the weak-coupling model for this multiplet and admixtures therein were discussed by Mottelson,[3] Broglia, Damgård, and Molinari,[4] and Hamamoto.[5]

The gamma rays following Coulomb excitation of this multiplet by 18-MeV α particles and 70-MeV oxygen ions were the subject of the present experiment. The target consisted of a thick piece of zone-purified ^{209}Bi which was machined, degreased, and mounted shortly before the evacuation of the target chamber; in this way impurity lines could be reduced to a great extent. Oxygen was the principal contaminant. Figure 1 shows relevant sections of the 4096-channel gamma spectra observed with an Oak Ridge Technical Electronics Corporation 32-cm^3 Ge(Li) detector at 90°. The energy resolution was 4.5 keV. A level diagram is shown in Fig. 2. Errors are ±0.5 keV for the 896.5-, 1608.9-, and 2741.4-keV states and ±1 keV for the others.

With alpha particles, spectra were obtained in five steps from 0° to 90°. The angular distributions were isotropic within the experimental error of ~15%. Intensities were obtained from the alpha-particle spectra, although the ^{16}O-induced yield at 90° gives virtually the same results.

Lifetimes for the $\frac{3}{2}^+$, $\frac{5}{2}^+$, and $\frac{15}{2}^+$ members of the multiplet were determined from a combination of Coulomb-excitation yields and branching ratios; those for the $\frac{7}{2}^+$, $\frac{9}{2}^+$, $\frac{11}{2}^+$, and $\frac{13}{2}^+$ members were determined from the Doppler broadening observed in the ^{16}O-induced spectra, and partially from the Doppler shifts seen in the α-induced spectra.[6] The rather large errors reflect the necessity of a decomposition of the overlapping Doppler broadening (shifted) lines in the ^{16}O case (see Fig. 1) in order to extract widths (average shifts). Such a decomposition was feasible because of the good energy and intensity information extracted from the α-induced spectra where all the lines were well separated. The 992-keV transition from the $\frac{11}{2}^+$-$\frac{13}{2}^+$ doublet to the 1609-keV $i_{13/2}$ state in the ^{16}O-induced spectrum could be decomposed into two lines with a (2 ± 1)-keV separation because of the appreciable Doppler shift observed in the presumed $\frac{11}{2}^+$ member of the doublet. A $(15\pm5)\%$ $\frac{11}{2}^+\rightarrow i_{13/2}$ $M1$ branch was observed, which has to be considered as tentative, since it could also originate from a small background peak located at the same position. The $\frac{13}{2}^+$ level decays almost entirely to the $i_{13/2}$ state, but a 1% branch to the ground state is required in order to agree with the lifetime extracted from the $E3$ Coulomb-excitation yield.

The absolute value of the $B\!\uparrow\!(E3)$ to the multi-