the end-point energy of 5.3±0.8 MeV and a possible component with 2 MeV higher end point, the latter had much lower intensity and was discarded because of the danger of the summing of the coincident gamma rays to the main beta component. The subtraction of the higher energy component did not change the end-point energy of the 5.3-MeV component, therefore the value is believed to be free from gamma contribution.

The coincidence gamma spectrum taken with the beta crystal biased integrally at 1.3 MeV, established the feeding of the 0.99- and 1.13-MeV gammas by strong beta rays. This experiment shows that the new nuclide is beta active, with the beta-decay energy more than 3 MeV.

The gamma-gamma coincidences were studied with sum-peak spectrometry. A double sum-peak was observed at 2.19±0.03 MeV, clearly showing the coincidence of the 1.13- and 0.99-MeV gammas. The energy difference between the sum peak and the arithmetic sum of the gamma-ray energies is in agreement with the nonlinearity of NaI(Tl) detectors.[4] On the basis of the absence of a sum peak with an energy of ~2.3 MeV, it is concluded that more than 70% of the 1.13-MeV peak is due to a single gamma, therefore, the multiplicity of the first excitation energy observed in the decay of the other high-spin In isomers, is less than 30% of the 1.13-MeV peak in the decay of In^{124}. The possible coincidence of 3.21-MeV gamma between 0.99- and 1.13-MeV gammas was not conclusively established partly because of the strongly interfering gammas from N^{16}, and partly because of the large escape probability of one or both annihilation quanta from the 3.21-MeV gamma. This produces secondary sum peaks which remain poorly resolved.

The observed feeding of 2.12-MeV level by strong beta rays rules out all other reaction products of Sn^{124} except $In^{124}(n,p)$ and $Cd^{121}(n,\alpha)$. Yamada and Matumoto[5] predict the beta disintegration energy of 7.4 MeV for In^{124} and 4.6 MeV for Cd^{121}. If the 5.3-MeV beta component would feed the level at 2.12 MeV, the total beta-disintegration energy would coincide with the predicted value for In^{124}. This feeding, although likely, could not be conclusively shown. Therefore, the assignment of the 3.6-sec activity to In^{124} is based on the energy fit between the observed gamma-ray energy of 1.13 MeV and the known first excitation energy of Sn^{124}. Furthermore, there are pronounced similarities in the decay of the odd-odd indium isomers.[1] The same systematic features are evident also in the decay of the 3.6-sec activity.

I wish to express my thanks to Professor A. Fry and Professor P. K. Kuroda for valuable support and I am also indebted to the accelerator team for technical assistance.

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Shell-Model Calculation of the Even-Parity States of Ne^{20}†

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The nuclear shell model has been applied to calculate the positive-parity energy levels of Ne^{20}. The problem of four interacting particles in the $2s$-$1d$ shell has been solved for low-lying states using a technique which is particularly suited to automatic computation. The resulting energy levels are in quite good agreement with the experimental results for a reasonable internucleon potential.

I. INTRODUCTION

THE nuclear shell model has met with considerable success in describing the properties of nuclei which are close in the periodic table to closed-shell nuclei. An extensive theory, initiated by the work of Racah, has been developed for the purpose of classifying and computing nuclear states in the shell model. Despite the generality of these methods, calculations for systems of more than three nucleons have rarely been attempted, particularly in the full intermediate coupling scheme. The reason for this is that it is necessary to compute and diagonalize very large matrices since the number of possible configurations increases rapidly with increasing particle number.

In view of the increasing importance of large scale automatic computation it is desirable to develop techniques which are readily adaptable to machine calculation even though they may be less efficient. It is the purpose of this paper to describe one such method and its application to the positive-parity states of the Ne^{20} nucleus.

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II. METHOD OF CALCULATION

The conventional intermediate coupling method[1] is to exploit the fact that the angular momentum commutes with the Hamiltonian to reduce the vector space of the system. The calculation of the Hamiltonian matrix elements between angular momentum eigenvectors is rather involved, however, requiring extensive use of recoupling coefficients.

The model assumed for the Ne^{20} nucleus is two protons and two neutrons in the $2s-1d$ shell outside an O^{16} core. There is a large number of possible configurations; Table I shows N_J and N_M, the number of states of particular J^2 and J_z, respectively. It is seen that the conventional method would require computing and diagonalizing matrices of dimension greater than 100.

The method to be described uses a standard technique for finding the eigenvalues and eigenvectors of a Hermitian matrix H of dimension N. The method is to commence with an arbitrary vector $\mathbf{u}_0$ and to multiply it repeatedly by H. It is convenient to normalize the result at each stage, defining the sequence

$$\mathbf{u}_{n+1}=H\mathbf{u}_n/|H\mathbf{u}_n|\,.$$

The eigenvectors and eigenvalues of H will be denoted by $\mathbf{v}_i$ and λ_i and we will suppose that $|\lambda_1|>|\lambda_2|>\cdots>|\lambda_n|$. If $\mathbf{u}_0$ is expressed as $\sum a_i\mathbf{v}_i$ one can see that

$$\mathbf{u}_n=\sum a_i\lambda_i{}^n\mathbf{v}_i/[\sum a_i{}^2\lambda_i{}^{2n}]^{1/2}.$$

It is evident from this that

$$\lim_{n\to\infty}\mathbf{u}_n=\mathbf{v}_1.$$

Convergence to the ground state can be ensured by subtracting some sufficiently large constant from the matrix. If $\mathbf{v}_1, \mathbf{v}_2,\cdots,\mathbf{v}_r$ have been found, $\mathbf{v}_{r+1}$ is determined by considering vectors orthogonal to those already found. Although this method is less favored than the Jacobi method for complete diagonalization, it may be more suitable to the shell model since only a few low-lying states can be considered physically significant. This method has been discussed in detail by Wilkinson.[2]

The calculation is carried out in the representation in which the j^2 and j_z of each particle are diagonal and protons and neutrons are regarded as distinguishable; that is, the states are products of two Slater determinants. To compute the eigenvectors of a particular spin, say $J(J+1)$, we consider all those states whose total J_z is J. The vector space is now unnecessarily large. On the other hand, the matrix H can transform a given state into only a limited number of other states (perhaps $\frac{1}{10}$ the total number) since if the interaction is a two-particle operator it can change the state of only two particles at a time.

[1] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic Press, Inc., New York, 1963), pp. 261–282.
[2] J. H. Wilkinson, Proc. Cambridge Phil. Soc. **50**, 536 (1954).

TABLE I. Number of states of particular J^2, (N_J) and particular J_z, (N_M).

J or M	0	1	2	3	4	5	6	7	8
N_J	46	97	143	129	109	64	36	12	4
N_M	640	594	497	354	225	116	52	16	4

The matrix multiplication is carried out by considering successively each state, choosing a pair of particles, p-p, n-n, or p-n, in each of the six possible ways, determining the new states which may be obtained by changing the quantum numbers of the pair and whether the new state is allowed by the exclusion principle, and then finding the matrix element connecting the initial and final states. The conservation of J_z in the two-particle matrix elements reduces the number of possible transitions considerably. If a p-p or n-n pair is picked the exchange term is included in the matrix element. If a p-n pair is picked the quantum numbers of the final state may be a permutation of the standard ordering. It is necessary to include a factor of (±1) depending on the parity of the permutation.

The error at any stage can be estimated from the quantity

$$e_n=(|H\mathbf{u}_n|^2/(\mathbf{u}_n,H\mathbf{u}_n)^2)-1\,,$$

which is zero if $\mathbf{u}_n$ is an eigenvector of H. If $e_n<\epsilon^2$, the error in λ can be shown to be less than $\epsilon^2\lambda^2/|\lambda-\lambda_j|$ and the norm of the error in $\mathbf{v}$ is less than $|\epsilon\lambda/(\lambda-\lambda_j)|$, where λ_j is the eigenvalue which occurs closest to λ (see the Appendix). It is seen that if two states are nearly degenerate the results may be seriously in error, but this is a characteristic of any method.

The presence of a nearly degenerate state is serious in another way in that it causes the convergence to be very slow. After several iterations the principle error in $\mathbf{v}_i$ is produced by $\mathbf{v}_{i+1}$, the next excited state. One has then $\mathbf{u}_n\approx\mathbf{v}_i+\epsilon\mathbf{v}_{i+1}$, $\mathbf{u}_{n+1}\approx\mathbf{v}_i+\rho\epsilon\mathbf{v}_{i+1}$, where $\rho=\lambda_{i+1}/\lambda_i$. If ρ is close to unity, the convergence is very slow. To avoid this difficulty, the correction $\mathbf{u}_{n+1}-\mathbf{u}_n$ at each stage was increased by a factor $(1-\rho_a)^{-1}$, where ρ_a is an approximation to ρ given by e_{n+1}/e_n. In this way the rate of convergence was improved to the extent that only 17 iterations were required in a case in which ρ was 0.97. The method causes instability, however, so that the normal correction of $\mathbf{u}_{n+1}-\mathbf{u}_n$ was used if $e_{n+1}>e_n$. It also appears to be necessary that all the eigenvalues be negative. To ensure this, an upper bound A on the largest eigenvalue was subtracted from the matrix. The bound used was

$$A=\max_i[H_{ii}+(\textstyle\sum_{j\neq i}H_{ij}{}^2)^{1/2}].$$

Low-lying states of spin higher than those sought can decrease the rate of convergence or appear instead of the desired state if they are of lower energy. To avoid this difficulty these states were projected out initially

by multiplying $\mathbf{u}_0$ by

$$P_J=\prod_{L>J}^{8}[J^2-L(L+1)].$$

This is readily done since J^2 can be expressed as a two-particle operator. Another approach, which is probably preferable, is to compute the eigenvectors in order of decreasing J and use the lowering operator J^- to decrease J_z. The initial state $\mathbf{u}_0$ can then be chosen orthogonal to the eigenvectors of higher spin.

The initial vector $\mathbf{u}_0$ was chosen to be the single configuration for which $(\mathbf{u}_0,H\mathbf{u}_0)$ is minimum. Since the principal error in $\mathbf{v}_r$ is $\mathbf{v}_{r+1}$, the difference $\mathbf{u}_n-\mathbf{u}_{n-1}$ at the last iteration is a good initial vector for the calculation of $\mathbf{v}_{r+1}$.

III. RESULTS

Since the nature of the internucleon force within the nucleus is rather uncertain the calculation was performed for four different sets of force parameters. The four cases will be labeled A, B, C, and D.

In case A the potential is of the Rosenfeld form:

$$V(r)=V_0(-0.13+0.93P^r+0.46P^\sigma-0.26P^rP^\sigma)\times e^{-r/a}/(r/a),$$

with $V_0=-45$ MeV and $a=1.37$ F. The single-particle energies for protons and neutrons were assumed to be the same and were taken from the data for O^{17}: $E_p(\frac{5}{2})=E_n(\frac{5}{2})=0$, $E_p(\frac{1}{2})=E_n(\frac{1}{2})=0.88$ MeV, and $E_p(\frac{3}{2})=E_n(\frac{3}{2})=5.08$ MeV. The resulting energy levels, relative to the ground state are shown in Fig. 1. The wavy lines show the experimental observations as tabulated by Pearson *et al.*,[3] together with two further levels observed by Kuehner and Almqvist.[4] The energy of the ground state is -22.5 MeV, corresponding to a binding energy relative to O^{16} of 32.0 MeV if it is assumed that the $d_{5/2}$ protons and neutrons are bound to O^{16} with energies of 0.60 and 4.14 MeV, respectively. The range b of the harmonic-oscillator wave functions was assumed to be 1.64 F in each of cases A, B, and C.

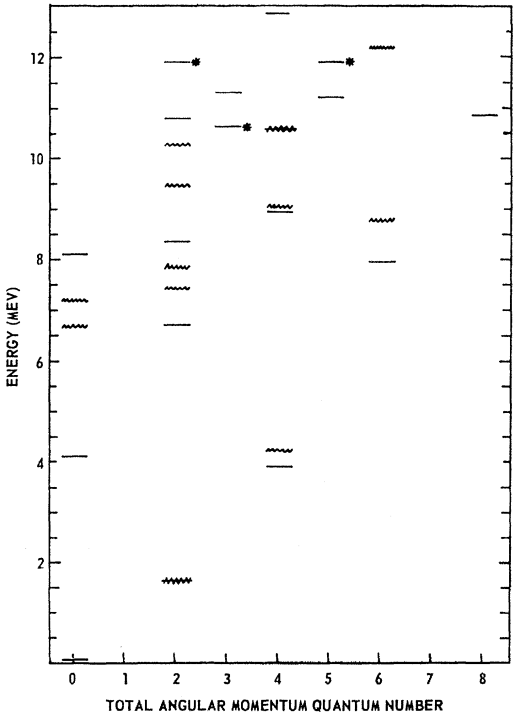

FIG. 1. Positive-parity energy levels of Ne^{20} computed in case A. The observed levels are shown by wavy lines. An asterisk indicates that the level is $T=1$.

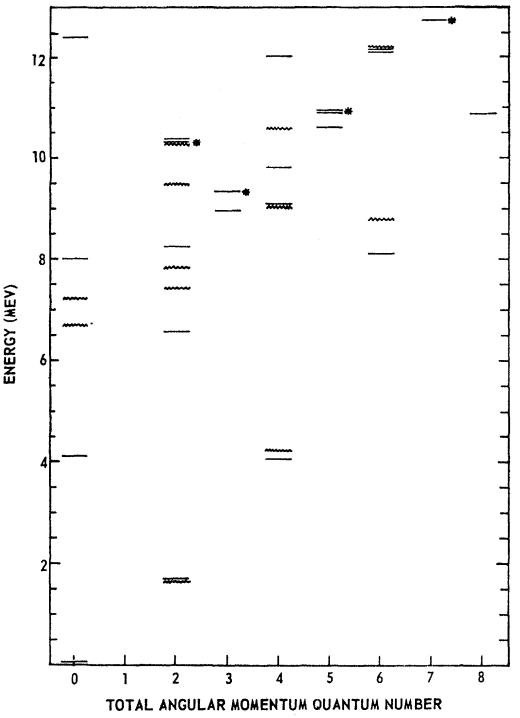

FIG. 2. Positive-parity energy levels of Ne^{20} computed in case B.

In case B the potential was taken to be

$$V(r)=\tfrac{1}{12}V_0(5+5P^r+P^\sigma+P^rP^\sigma)e^{-r/a}/(r/a),$$

with $V_0=-45$ MeV, $a=1.37$ F. This has the same radial dependence as the potential in case A, but the exchange mixture may be more realistic. The single-particle energies were taken from O^{17} and F^{17}; they are $E_p(\frac{5}{2})=E_n(\frac{5}{2})=0$, $E_p(\frac{1}{2})=0.50$, $E_n(\frac{1}{2})=0.88$, $E_p(\frac{3}{2})=5.82$, $E_n(\frac{3}{2})=5.08$. The Coulomb repulsion between protons was also included. The results are shown in Fig. 2. The energy of the ground state is -23.5 MeV, corresponding to a binding energy relative to O^{16} of 33.0 MeV.

Case C differs from B only in the values of a and V_0.

[3] J. D. Pearson, E. Almqvist, and J. A. Kuehner, Can. J. Phys. 42, 489 (1964).

[4] J. A. Kuehner and E. Almqvist, Bull. Am. Phys. Soc. 9, 430 (1964).

The range a was chosen to be 1.0 F and V_0 was -84.5 MeV; the value of V_0a^2 is the same as in case B. The results are shown in Fig. 3. The binding energy relative to O^{16} is in this case 32.6 MeV.

The approach in case D was quite different from that in the other three. The nuclear internucleon potential enters the calculation via the moments defined by

$$J_n=\left(\frac{\pi}{2}\right)^{1/2}\int_0^\infty x^{2n}e^{-x^2/2}V(bx)x^2dx.$$

In this case, the moments were chosen arbitrarily to be $J_0=-6.91$, $J_1=-5.00$, $J_2=-3.06$, $J_3=-95.2$, and $J_4=-3084$ MeV. The exchange mixture and single-particle energies of case B were again used. These values of J_n give, in the singlet even potential, the parameters deduced by Pandya[5] in a study of the oxygen isotopes. The results are shown in Fig. 4. The binding energy relative to O^{16} is 38.4 MeV.

It is observed that case B gives the best agreement with experimental observations, all of the levels except the first excited spin-zero level falling within 1 MeV of the observed levels. The ground-state energies in cases A, B, and C all agree well with the observed binding energy relative to O^{16} of 33.0 MeV.

It should be remarked that the figures show all the levels which have been computed below 13 MeV. In some cases, particularly for $J=2$, there may be other

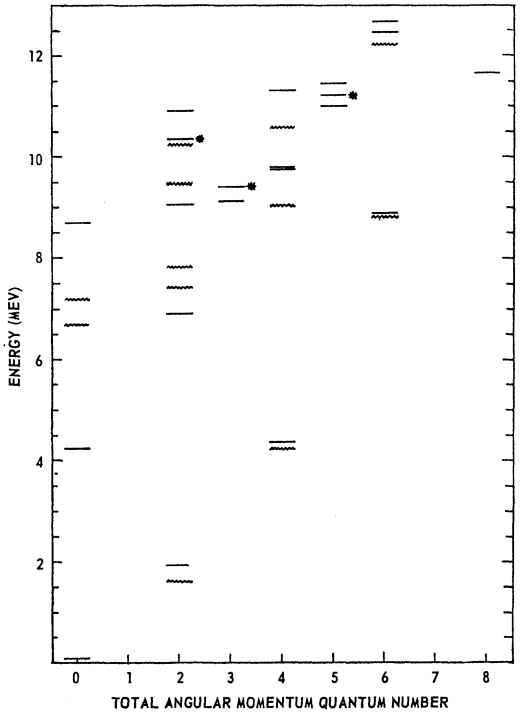

FIG. 3. Positive-parity energy levels of Ne^{20} computed in case C.

[5] S. P. Pandya, Nucl. Phys. 43, 636 (1963).

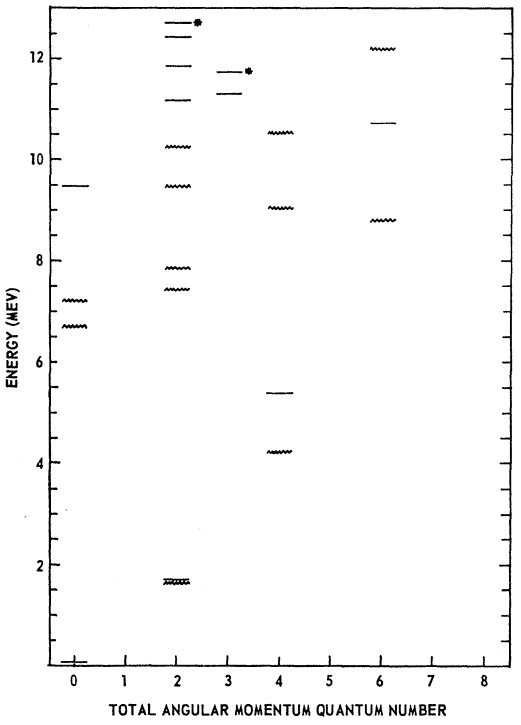

FIG. 4. Positive-parity energy levels of Ne^{20} computed in case D.

levels above those computed but below 13 MeV. It is also observed that there are no states of $J=1$. These were not found because round-off error, or the inexact commutativity of J^2 and H, caused convergence to the lowest $J=2$ state. It is estimated, however, that the lowest $J=1$ state is at 13.4 MeV in case A and 14.5 MeV in case B.

The convergence criterion, ϵ^2, for calculating λ_n and ν_n was chosen to be $0.5\times10^{-5}\times2^n$. From this we can say that the energies below 10 MeV should be accurate to about 0.1 MeV. Above 10 MeV the errors may be greater, particularly in the cases in which two levels are almost degenerate. We believe, however, that none of the levels should be in error by more than 0.5 MeV. On the other hand, the eigenvectors for these higher levels are probably seriously in error.

While no use has been made in the calculation of the isotopic spin formalism, it is possible to assign an isotopic spin quantum number to the various states. The states computed are all of $T=0$ or 1. The states of $T=1$ are marked in the figures with an asterisk. The excited state with $J=2$, $T=1$ in case B agrees reasonably well with the value of 11.1 MeV obtained by averaging the ground-state energies of the analog nuclei F^{20} and Na^{20}.

The electric quadrupole transition moments have been computed for all pairs of states. Unfortunately, only the two $E2$ transitions for the first two excited levels are observed. The computed lifetimes of the 1.63- and 2.62-MeV transitions are respectively 4.3×10^{-11}

TABLE II. Values of $B(E2)/e^2$ for various pairs of states. The higher excited states of a particular spin are denoted by one or two asterisks.

Pair of states	$B(E2)/e^2$ (F^4)
0–2	1.65
0–2*	3.90
0–2**	0.43
2–2**	4.04
2–4	1.75
2*–4	2.42
4–4*	5.13
4–6	0.76

and 3.7×10^{-12} sec. These are greater than the observed values[6] by a factor of about fifty indicating that the shell model does not adequately describe these properties. In Table II we list the values of $B(E2)/e^2$ for certain transitions where

$$B(E2)/e^2=\left(\frac{2J'+1}{2J+1}\right)\left[\frac{\langle J'M|Q_0^2|JM\rangle}{\langle JM20|J2J'M\rangle}\right]^2,$$

and

$$Q_0^2=\sum_i r_i^2 Y_{2,0}(\theta_i,\varphi_i),$$

the sum being over the two protons.

The calculations were performed on an IBM 7040 computer. The calculations for case A took approximately 5 h, and those of cases B, C, and D took about 90 min apiece. When eigenvectors for one potential have been found, they can be used as a starting point for other calculations, thereby decreasing the time markedly.

IV. CONCLUSIONS

With two or three exceptions the positive-parity energy levels of Ne^{20} are described quite well by the shell model. One of the exceptions is the first excited $J=0$ state which is in error by about 2.5 MeV. One characteristic of this level has been noticed; it has a very large (0.67) amplitude for the $(s_{1/2})^4$ state. The energy is therefore quite sensitive to the $s_{1/2}$ single-particle energies and to one particular Slater integral. The other discrepancy is the presence of relatively low-lying states of $J=3$ which are not observed. In fact, these results imply that the ground state of F^{20} should be of spin 3 rather than the observed spin 2. A much greater discrepancy exists in the electromagnetic-transition moments. The shell model is apparently quite incapable of describing these properties.

The method of calculation described may be quite useful in extending the shell model to problems of several particles. While we have described the method for the nuclear shell model, there is no reason why it should not be applicable to problems of atomic structure and it could conceivably be applied to simple axially symmetric problems of molecular structure.

One disadvantage of the method is that the resulting eigenvectors are in a form which is quite uninstructive. It might be said, however, that if more than 100 configurations are involved in a wave function, the amplitude of a particular one may not be of great interest. We can say at least that configuration mixing seems to be very important. In case B the probability of finding the $(d_{5/2})^4$ state in the ground state is only 0.11, while the probability of finding the $(s_{1/2})^4$ state is 0.16.

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APPENDIX

The results of this Appendix should be standard. We have, however, been unable to find them in the numerical analysis literature, so that they are included for completeness.

If $e<\epsilon^2$, we can write

$$(H\mathbf{u},H\mathbf{u})-(\mathbf{u},H\mathbf{u})^2<\epsilon^2(\mathbf{u},H\mathbf{u})^2,$$

where $\mathbf{u}$ is an approximation to $\mathbf{v}$, an exact eigenvector. If we write $\mathbf{u}=(1-|\mathbf{w}|^2)^{1/2}\mathbf{v}+\mathbf{w}$, where $(\mathbf{v},\mathbf{w})=0$, $\mathbf{w}$ being the error in $\mathbf{u}$, we obtain

$$(H\mathbf{u},H\mathbf{u})=\lambda^2-\lambda^2|\mathbf{w}|^2+|H\mathbf{w}|^2,$$
$$(\mathbf{u},H\mathbf{u})=\lambda-\lambda|\mathbf{w}|^2+(\mathbf{w},H\mathbf{w}).$$

If these are substituted into the inequality and only terms of lowest order in $|\mathbf{w}|^2$ retained the result is

$$(H\mathbf{w},H\mathbf{w})-2\lambda(\mathbf{w},H\mathbf{w})+\lambda^2|\mathbf{w}|^2<\epsilon^2\lambda^2,$$

or $|H\mathbf{w}-\lambda\mathbf{w}|<|\epsilon\lambda|$. If $(\mathbf{u},H\mathbf{u})$ is used to estimate λ, it is seen that the magnitude of the error is

$$|\lambda|\mathbf{w}|^2-(\mathbf{w},H\mathbf{w})|$$
$$=|(\mathbf{w},\lambda\mathbf{w}-H\mathbf{w})|\leq|\mathbf{w}|\,|H\mathbf{w}-\lambda\mathbf{w}|<|\epsilon\lambda|\,|\mathbf{w}|.$$

To estimate $|\mathbf{w}|$, we expand $\mathbf{w}$ in eigenvectors of H. Then

$$|H\mathbf{w}-\lambda\mathbf{w}|^2=\sum(\lambda_k-\lambda)^2b_k^2<\epsilon^2\lambda^2.$$

If λ_i is the eigenvalue closest to λ we can write

$$(\lambda_i-\lambda)^2\sum b_k^2<\epsilon^2\lambda^2,$$

or, since $\sum b_k^2=|\mathbf{w}|^2$,

$$|\mathbf{w}|<\epsilon|\lambda/(\lambda-\lambda_i)|.$$

[6] M. A. Clark, H. E. Gove, and A. E. Litherland, Can. J. Phys. 39, 1241 (1961); D. K. Alkhazov, A. P. Grinberg, I. K. Lemberg, and V. V. Rozhdestvenksii, Zh. Eksperim. i Teor. Fiz. 36, 322 (1959) [English transl.: Soviet Phys.—JETP 9, 222 (1959)].