In view of the approximations made in the assumptions and the (slight) observational errors both methods agree in showing no certain variation of the modulus for periods between 4 sec. and 28 sec.

IV. CHECK ON CALCULATIONS OF MOMENTS OF INERTIA

If we assume that this result is established by method (2) we may of course reverse method (1) to give a valuable check on the correctness of the calculations of the moments of inertia of the inertia system S_3 and the bar which forms a part of it. Thus, for each suspension, if in the experiments there is no appreciable change of modulus with frequency or tension, we should have

$$K_B/K_A=(l_A/l_B)(T_B/T_A)^2,$$

where K_B and K_A are the moments of inertia in cases B and A, *viz.*, 19.65×10^3 g cm^2 and 2.341×10^3 g cm^2. (The [negligible] moment of inertia, *ca.* 0.33, g cm^2, of the holder is included.) The ratio $K_B/K_A=8.395$; while the ratios $l_A/l_B(T_B/T_A)^2$ for the three suspensions are 8.413, 8.395, and 8.377, with the mean 8.395, exactly equal to K_B/K_A.

This work has been done in the Norman Bridge Laboratory of the California Institute with facilities provided by the University of California, the Institute, the Carnegie Institution of Washington, and the National Research Council.

We have desired to make further observations on German silver, with wires of different diameters and in the frequency range between our higher and lower values, as well as precise observations on other substances; but the pressure of other work has hitherto prevented this.

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A Note on Weinstein's Variational Method

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Weinstein's modification of the Ritz principle is used to derive (1) a lower bound for the n-th energy-level of a quantum mechanical system if a lower bound for the $(n+1)$-st level is known; and (2) an upper bound for the n-th level if an upper bound for the $(n-1)$-st level is known.

1. INTRODUCTION

By applying the Ritz variational principle to the equation

$$(H-\lambda)^2\psi=W\psi \tag{1}$$

Weinstein[1] was able to obtain both lower and upper bounds for the energy levels of the Schroedinger equation

$$H\psi=E\psi. \tag{2}$$

The chief theoretical weakness of this method is that it gives no hint as to which one of the energy levels the bounds obtained refer to.

Stevenson and Crawford[2,3] have made use of Weinstein's method in an improved form to establish a theoretical lower bound for the ground-level of the helium atom. In their calculations both the lower and upper bounds obtained lie well below the experimental value of the second energy level and therefore, of necessity, refer to the ground state.

In section 2 of the present note the method of Stevenson and Crawford is generalized to give a lower bound for E_n if a lower bound of E_{n+1} is known. Since no general theoretical method is available for determining the latter, its value may

[1] D. H. Weinstein, Proc. Nat. Acad. of Sci. **20**, 529 (1934).

[2] A. F. Stevenson, Phys. Rev. **53**, 199 (1938).

[3] A. F. Stevenson and M. F. Crawford, Phys. Rev. **54**, 374 (1938).

have to be taken from experimental data. The process can be repeated and lower bounds for E_{n-1}, E_{n-2}, $\cdots E_1$ obtained in succession.

In section 3 an analogous procedure leads to an upper bound for E_n (and by iteration for E_{n+1}, E_{n+2}, $\cdots$) if an upper bound of E_{n-1} is known.

2. LOWER BOUND

If we use the notation

$$A_{\mathrm{Av}} \equiv \int \psi^* A \psi dx,$$

where the integral is extended over the whole configuration space, we can express Weinstein's basic result by the statement that some energy level, E, will be found in any one of the intervals

$$\lambda - [(H^2)_{\mathrm{Av}} - 2\lambda(H)_{\mathrm{Av}} + \lambda^2]^{\frac{1}{2}} \leqslant E \leqslant \lambda + [(H^2)_{\mathrm{Av}} - 2\lambda H_{\mathrm{Av}} + \lambda^2]^{\frac{1}{2}}, \quad (3)$$

where λ can be given an arbitrary real value and H_{Av}, $(H^2)_{\mathrm{Av}}$ are formed with an arbitrary, normalized ψ.

Suppose that E_{n+1}^l is a lower bound of E_{n+1}. Then, if we choose λ so that

$$\lambda + [(H^2)_{\mathrm{Av}} - 2\lambda H_{\mathrm{Av}} + \lambda^2]^{\frac{1}{2}} = E_{n+1}^l \quad (4)$$

it is clear from (3) that

$$E_n \geqslant \lambda - [(H^2)_{\mathrm{Av}} - 2\lambda H_{\mathrm{Av}} + \lambda^2]^{\frac{1}{2}} \quad (5)$$

since otherwise no level would fall into the range (3).[4] Evaluating λ from (4) and substituting into (5) we find

$$E_n \geqslant H_{\mathrm{Av}} - \frac{(H^2)_{\mathrm{Av}} - (H_{\mathrm{Av}})^2}{E_{n+1}^l - H_{\mathrm{Av}}},$$

or

$$E_n^l = H_{\mathrm{Av}} - \frac{(H^2)_{\mathrm{Av}} - (H_{\mathrm{Av}})^2}{E_{n+1}^l - H_{\mathrm{Av}}}. \quad (6)$$

We can now use E_n^l as a lower bound for E_n and repeat the procedure to obtain an E_{n-1}^l, etc.

Two remarks must be made here. It is easily verified that for fixed H_{Av}, $(H^2)_{\mathrm{Av}}$ the left-hand side of (4) is an increasing function of λ. Therefore its minimum value is reached when $\lambda = -\infty$ and equals H_{Av}. Its maximum value is $+\infty$. It follows that a real solution, λ, of (4) exists if and only if $H_{\mathrm{Av}} \leqslant E_{n+1}^l$. (This has been tacitly assumed in deriving (6).) The trial-function ψ, which we use in the computation of H_{Av} and $(H^2)_{\mathrm{Av}}$ in (6), is therefore not entirely arbitrary, but subject to the condition

$$H_{\mathrm{Av}} \leqslant E_{n+1}^l. \quad (7)$$

This inequality will be satisfied whenever E_{n+1}^l is a fair approximation to E_{n+1}, and ψ is a reasonable trial-function for the n-th (or indeed any lower) state.

Secondly, we might have taken λ to satisfy

$$\lambda + [(H^2)_{\mathrm{Av}} - 2\lambda H_{\mathrm{Av}} + \lambda^2]^{\frac{1}{2}} = A < E_{n+1}^l \quad (8)$$

instead of (4) and, by an analogous argument, would have found that

$$E_n \geqslant H_{\mathrm{Av}} - \frac{(H^2)_{\mathrm{Av}} - (H_{\mathrm{Av}})^2}{A - H_{\mathrm{Av}}}, \quad (9)$$

provided that

$$H_{\mathrm{Av}} \leqslant A. \quad (10)$$

But we observe that (6) is a better estimate for E_n than (9) and that (7) is less restrictive on ψ than (10). Therefore (6) represents the best result obtainable by this method.

3. UPPER BOUND

In a precisely similar manner we can show that if E_{n-1}^u is an upper bound of E_{n-1}, then

$$E_n \leqslant H_{\mathrm{Av}} + \frac{(H^2)_{\mathrm{Av}} - (H_{\mathrm{Av}})^2}{H_{\mathrm{Av}} - E_{n-1}^u}, \quad (11)$$

as long as ψ is normalized and satisfies the condition

$$H_{\mathrm{Av}} \geqslant E_{n-1}^u. \quad (12)$$

It is clear that if only $E_{n-1}^u < 0$, we can always satisfy (12) by taking a ψ of sufficiently oscillatory nature.

The inequality (11) allows of two types of application:

(1) If by any method one has obtained an upper bound of E_{n-1} he can, by the use of a single trial-function, determine an upper bound of E_n. This process may be continued.

[4] Strictly speaking, if $E_{n+1}^l = E_{n+1}$, then a level, namely, E_{n+1}, would fall into the interval (4), even if (5) were not satisfied. However, by a simple limiting process, one can easily verify that (5) must hold even in this case.

(2) One can determine an upper bound for E_1 by the usual Ritz method and then construct successively upper bounds of $E_2, E_3, \cdots, E_k, \cdots$. At each stage a single trial-function, ψ_k, is used, and three integrals, $N=\int\psi_k^*\psi_k dx$, $H_{Av}=\int\psi_k^* H\psi_k dx$, $(H^2)_{Av}=\int\psi_k^* H^2\psi_k dx$ must be evaluated. It is important that successive ψ's need not be orthogonal. For energy levels of high order this procedure would seem to be a simplification over the conventional method, due to Hylleraas and Undheim,[5] and an alternative method suggested by the author.[6] For these methods require that the successive ψ's must be normal and orthogonal and that at each stage the integrals $\int\psi_i^* H\psi_k dx$ $(i=1, 2, \cdots k)$ be evaluated. This means that at the k-th stage a total of $2k$ integrals must be found. Furthermore, in the procedure of Hylleraas and Undheim, a determinantal equation of order k must finally be solved. One must keep in mind, however, that the integrals for $(H^2)_{Av}$ which occur in our method, are in general quite difficult to evaluate.

[5] E. A. Hylleraas and R. Undheim, Zeits. f. Physik, p. 759 (1930).
[6] W. Kohn, Phys. Rev. **71**, 635 (1947).

For convenience we combine the inequalities (6) and (11) and the conditions (7) and (12) for the case when both $E_{n+1}{}^l$ and $E_{n-1}{}^u$ are known:

$$H_{Av}-\frac{(H^2)_{Av}-(H_{Av})^2}{E_{n+1}{}^l-H_{Av}}\leqslant E_n\leqslant H_{Av}+\frac{(H^2)_{Av}-(H_{Av})^2}{H_{Av}-E_{n-1}{}^u} \quad (13)$$

for any normalized trial-function ψ satisfying

$$E_{n-1}{}^u\leqslant\int\psi^* H\psi dx\leqslant E_{n+1}{}^l. \quad (14)$$

Let us note that all the results derived above retain their validity in the case of degeneracy (non-degeneracy was nowhere assumed) as long as the levels are ordered according to non-decreasing magnitude.

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