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Abstract

An accurate and efficient numerical method of solving the radial Schroedinger equation for diatomic molecule has been employed in two tests relating to approximate potential functions. First, quantitative estimates have been made of the errors in the approximate eigenvalue equation derived by Pekeris for the rotating Morse oscillator. Secondly, as an example of testing a potential function for which no analytic solution is known, the eigenvalues of the Clinton potential have been compared with those of the Morse and with experiment.

Introduction

The worth of a function used for representing the potential energy of a diatomic molecule must be judged principally by the agreement between the eigenvalues it predicts and the spectroscopically-observed term values. The profusion of such functions in the literature is due in part to the difficulty of making this comparison. Exact analytic solutions for the eigenvalues and eigenfunctions have been obtained for relatively few potential models.

Varshni¹ has used an approximate method to compare the class of three-parameter potential functions which can be specified by the dissociation energy, D_e , the fundamental frequency, ω_e , and the equilibrium internuclear distance, r_e . It is based on two approximate formulae, derived by Dunham,² which give the spectroscopic constants $\omega_e x_e$ and α_e in terms of derivatives of the potential function evaluated at r_e . Dunham² used a W.K.B. method and a potential expressed as a power series in the internuclear displacement. Since the constants D_e , ω_e , B_e (or, equivalently, r_e), $\omega_e x_e$ and α_e give the most important contributions to the eigenvalues, this method certainly gives a valid and useful comparison. Still, it is applicable to only a restricted class of functions, and the neglect of higher-order terms in the eigenvalue equation could in some cases alter the comparison significantly.

Varshni¹ noted another possible method for making the comparison with experiment, but it is less attractive. When sufficient experimental data are available the Rydberg-Klein-Rees method (see Jarman³ for a recent formulation of this procedure) can be used to build up a potential curve by computing classical turning points for each vibrational eigenstate.

Such a curve could then be compared with any postulated potential function but the information gained is less than satisfactory. One could safely assume that a potential function which disagreed considerably with the RKR curve over its whole range would give poorer results than a function which agreed very well with the RKR curve. However, it would be difficult to choose between two functions whose departures from the RKR were approximately equal in magnitude but in different regions of the curves. In any case, no quantitative estimate of the difference between theoretical and observed eigenvalues is obtained by this procedure.

A direct and unambiguous comparison between theory and experiment is possible for any assumed potential curve through the use of numerical methods. Such methods have been applied to central field problems for many years but the computational labor they entail is very considerable when high accuracy is desired. It is only through the recent advances in computer technology that the widespread use of these methods has become practicable.

The present paper deals with two applications of numerical methods in problems relating to diatomic potential functions. Following some remarks on the method itself, it is shown how it can be used to give quantitative estimates to the accuracy of an approximate analytic solution. The example chosen is widely-used eigenvalue formula derived by Pekeris⁴ for a rotating Morse oscillator. The second application is one in which are found the properties of a potential for which no analytic solution has yet been given. This is a potential function recently proposed by Clinton,⁵ and it is compared with the Morse⁶ potential and with experiment.

The Numerical Method

Cooley⁷ has recently described a numerical method for solving the Schrodinger radial equation. It employs the Numerov⁸ method of integration together with an eigenvalue predictor-corrector formula which is based on a second-order iteration-variation procedure due to Löwdin.⁹ The form in which the equation is solved is

$$d^2\psi/dr^2 + [E - U(r)]\psi(r) = 0 \quad (1)$$

where ψ is the radial equation multiplied by r , and $U(r)$ is the effective potential energy,

$$U(r) = [J(J+1) - \Lambda^2]/r^2 + Z_a Z_b / r + E_{el}(r). \quad (2)$$

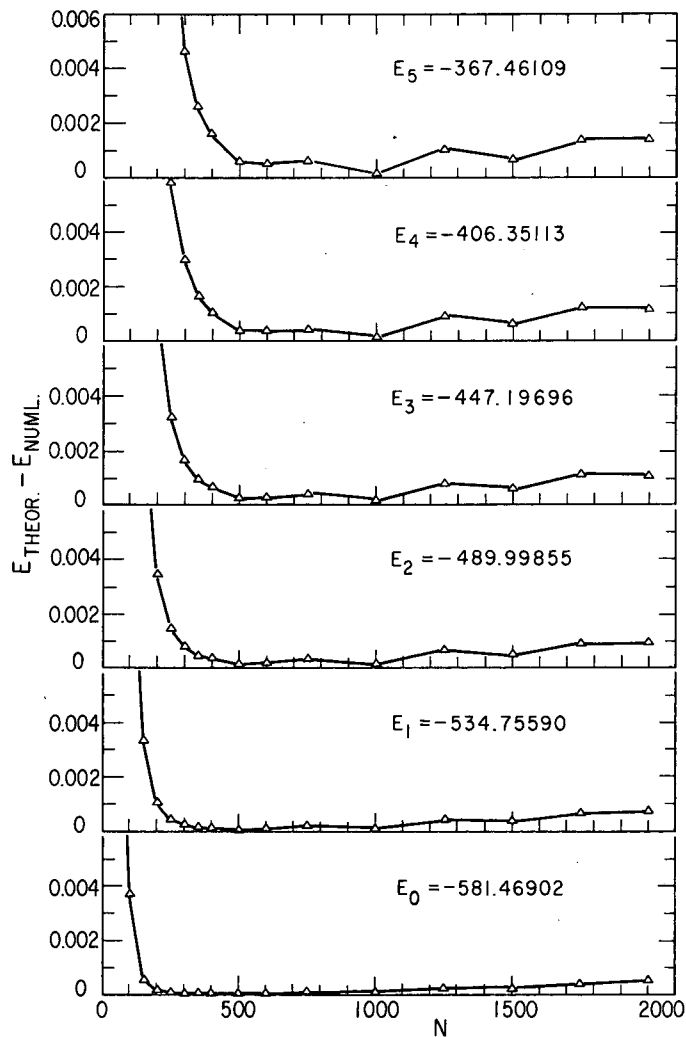
J and Λ are the quantum numbers for rotation and for the z -component of electronic angular momentum, the second term is the Coulomb repulsion energy of the nuclei, and $E_{el}(r)$ is the electronic energy obtained by solving the electronic wave equation for each fixed internuclear distance r .

In using Eq. (1) it is necessary to employ dimensionless units of energy and length. When length is measured in Bohr radii, $a_0 = 0.529172 \text{ \AA}$, the unit of energy is equivalent to $hN_0/8\pi^2 c a_0^2 \mu_A$ wave numbers, where N_0 is Avagadro's number (physical scale) and μ_A is the reduced mass in Aston units. The numerical value of this factor is $60.2198/\mu_A$. Hence, to convert the eigenvalues and spectroscopic constants for HCl from the values tabulated below to the more familiar units of cm^{-1} , multiply by 61.4557.

Cooley has made available a Fortran SHARE program* embodying

* A minor modification is required in order to make his 704 program compatible with the 7090. The author is indebted to Mr. R. N. Zare for this information. It is anticipated that a detailed description of this modification, together with other useful ones, will soon be available as a UCRL report by Mr. Zare and the author.

his procedure and has reported tests of its accuracy when up to 200 intervals are used in the integration. In the present application higher accuracy was obtained by increasing N, the number of intervals used. One cannot ensure a continuous improvement in accuracy by increasing N indefinitely, quite apart from storage and time considerations. As N increases, the build-up of truncation error will eventually offset the simultaneous reduction in the error which arises from replacing the differential equation by a finite-difference equation. If the latter source of error is reduced to a virtual zero before the former becomes appreciable a plot of eigenvalue versus N should vary rapidly at low N values, approach a near-constant value and then break away from it gradually as truncation error builds with increasing N. This appears to be true of Cooley's program when it is used on an IBM 7090 (which carries just over 8 significant decimal figures). Figure 1 shows the variation with N of the six lowest eigenvalues for HCl fitted to a Morse potential. It will be noted that the higher the eigenvalue (i.e., the more rapidly the eigenfunction varies with r), the greater is the value of N at which the nearly constant portion of the curve is reached. On the other hand the breaking away from this



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Fig. 1. Rate of convergence of numerical eigenvalues with N , the number of intervals used in the numerical integration. The theoretical values of E_v are computed from Eq. (4), using the spectroscopic constants for HCl given by Rank et al.¹³

region at higher N is much less a function of eigenvalue. Further, the somewhat erratic behavior in this portion of the curve is essentially the same for every eigenvalue. Both these observations are consistent with the interpretation that the errors above $N=1000$ are principally truncation errors.

All the calculations reported in the following sections of this paper were made using 1000 intervals of 0.007 atomic units each. The criterion for choosing the range of integration is that the values of the normalized eigenfunction should be essentially zero at both extremes. On the IBM 7090 numbers smaller in magnitude than 10^{-39} produce a machine zero. For a Morse potential virtually all diatomic molecules will fulfill this condition at a lower bound of $r_e - 2$ atomic units and an upper bound of $r_e + 5$. The higher the ratio of $\omega_e/\omega_e x_e$, the more this range can be reduced.

Numerical integrations of the eigenfunctions to obtain expectation values of r^{-2} were made by repeated application of Simpson's rule, sometimes called the parabolic rule (cf., Hildebrand¹⁰).

Values of the spectroscopic constants were obtained from the eigenvalues by the differencing procedures usually applied in the analysis of spectra. (This whole procedure can be regarded as taking the spectrum of a molecular model with a computer.) In order to minimize the errors caused by the neglect of higher-order differences, the fourth differences $\Delta^4 G_2$ and $\Delta^4 B_2$ were set equal to $24\omega_e z_e$ and $24\epsilon_e$, respectively, the differences $\Delta^4 G_3$ and $\Delta^4 B_3$ being used only as an indication of the validity of the assumption of constant fourth differences. All lower-order differences contributing to $\Delta^4 f_2$ were

then solved the remaining constants, and unweighted averages of these were tabulated. The relevant difference equations may be found in Herzberg.¹¹

The entire numerical procedure is very economical in terms of computer time. Cooley's program requires about 0.4 seconds to compute the eigenfunction at 1000 points and to correct the trial eigenvalue for the next iteration. Since the predictor-corrector formula is based on a second-order procedure relatively few iterations are necessary in order to obtain eight-figure constancy in the eigenvalue, even for an initial trial value which is several percent in error. All the calculations reported below, including 12 eigenvalue determinations, required about one-half minute of computing time on the IBM 7090.

Accuracy of the Pekeris Eigenvalue Equation for
the Rotating Morse Oscillator

Pekeris'⁴ approximate solution to the radial equation for a Morse⁶ potential is inexact for two reasons. First, the rotational contribution to the potential is approximated using an expansion for $1/r^2$ in which only the first three terms are retained. By treating the terms neglected as a perturbation Pekeris showed that their effect on the eigenvalues should be very slight. In view of the widespread use of his approximate solution, a more quantitative estimate of the error is useful. Secondly, in his development the lower limit of an integration over r is taken as $-\infty$ instead of zero. This has been discussed by ter Haar,¹² who concluded that the error should have

negligible effects for systems involving nuclear or larger masses. Again, it is of interest to set an upper bound to this error through an exact numerical solution.

The Morse⁶ potential for a rotationless state is given by

$$U(r) = D_e [1 - e^{-\beta(r-r_e)}]^2 - D_e \quad (3)$$

where D_e is the dissociation energy, r_e the equilibrium internuclear distance and β a disposable parameter, the energy being measured from a zero at the dissociation limit. In the following calculations the values assigned to D_e and r_e were 605.559 and 2.40873, corresponding very closely to the experimental values¹³ for HCl, and β was set equal to 0.988879. If the Pekeris solution were exact, this value of β would imply a value of ω_e matching that for HCl [see Eq. (4a) below].

The eigenvalue equation derived by Pekeris may be written

$$\begin{aligned} E_{v,J} = & -D_e + \omega_e(v + 1/2) - \omega_e x_e(v + 1/2)^2 \\ & + J(J+1)[B_e - \alpha_e(v + 1/2) + \gamma_e(v + 1/2)^2 + \dots] \\ & + D_e J^2(J+1)^2 + \dots \end{aligned} \quad (4)$$

where

$$\omega_e = 2\beta \sqrt{D_e} \quad (4a)$$

$$\omega_e x_e = \beta^2 \quad (4b)$$

$$B_e = r_e^{-2} \quad (4c)$$

$$\alpha_e = \frac{3}{\beta e^3 \sqrt{D_e}} \left[\beta - \frac{1}{r_e} \right] \quad (4d)$$

$$r_e = \frac{3}{2\beta^2 r_e^6 D_e} [5 - 10r_e \beta + \frac{23}{4} r_e^2 \beta^2 - \frac{7}{6} r_e^3 \beta^3] \quad (4e)$$

$$D_e(\text{rot.}) = \frac{1}{\beta^2 r_e^6 D_e} \quad (4f)$$

Note that the rotationless states do not involve terms in $(v + 1/2)$ higher than the second power. Therefore, non-zero third differences in the eigenvalues for these states will indicate an error due to the second cause cited above.

The calculated and numerical eigenvalues for the $J=0$ states of the first six vibrational levels of HCl are given in Table I, together with first, second and third differences for the latter. Within machine limits the third differences are zero and the values of ω_e and $\omega_e x_e$ derived from the first and second differences agree exactly with Eqs. (4a) and (4b). Hence, the incorrect limit of integration introduces an error of less than one part in 10^7 in ω_e .

Two procedures are available for testing Eqs. (4c,d, and e). The values of B_v can be obtained either from the relation

$$B_v = \left[\frac{1}{r^2} \right] = \int \psi_v r^{-2} \psi_v dr \quad (5)$$

or by obtaining a series of rotational eigenvalues for each vibrational state. Standard differencing procedures can then be used to solve for the constants in the equation

$$B_v = B_e - \alpha_e (v+1/2) + \gamma_e (v+1/2)^2 + \delta_e (v+1/2)^3 + \epsilon_e (v+1/2)^4. \quad (6)$$

Both methods were used but only the set of B_v 's obtained from Eq. (5)

Table I. Eigenvalues $G(v)(=E_{v,0})$ for the rotationless states of HCl, assuming a Morse potential. Since $\Delta^3 G=0$, $\Delta^2 G_{v+1} = -2\omega_e x_e$ and $\Delta^1 G_{v+1/2} = \omega_e + 2v\omega_e x_e$.

v	$G(v), \text{Eq. (4)}$	$G(v), \text{Numl.}$	$\Delta^1 G$	$\Delta^2 G$	$\Delta^3 G$
0	-581.46902	-581.46913	46.71311		
1	-534.75590	-534.75602	44.75734	-1.95577	+0.00001
2	-489.99855	-489.99868	42.80158	-1.95576	.00000
3	-447.19696	-447.19710	40.84582	-1.95576	-0.00001
4	-406.35113	-406.3512	38.89005	-1.95577	
5	-367.46107	-367.46123			

was used to obtain the constants α_e , etc. The value of B_v given by Eq. (5) is unambiguous whereas forcing the eigenvalues to fit the equation

$$E_{v,J} - E_{v,0} = B_v J(J+1) - D_v J^2(J+1)^2 \quad (7)$$

results in a B_v value that depends upon which eigenvalues are used. The values given in Table II are the results of a least-squares fit of the four eigenvalues for states $J=7$ through 10, the lowest four for which the left-hand side of Eq. (7) retains six significant figures.

The same states were used to determine the constants D_v , which could be expressed by the relation

$$D_v = D_e + \beta_e (v + 1/2). \quad (8)$$

Table II gives the results for B_v . The good agreement between columns three and four attests to the consistency of the eigenfunctions and eigenvalues obtained in this procedure. The very small differences between columns two and four at low v increasing markedly as v increases indicates again that the principal error in Eq. (4) is the neglect of higher-order terms. To better illustrate the magnitude of the error, Fig. 2 shows the differences between calculated and numerical eigenvalues for levels $J=0$ to 20 of $v=0$. Note that the first several states are all low by the same amount. Hence the rotational spacing predicted by Eq. (4) for these states is exact to within the limits of this calculation.

Table II. Rotational constants B_v from the Pekeris solution, from the numerical eigenvalues and from the numerical eigenfunctions.

v	B_v , calc. Eqs. (4c,d,e)	B_v , numl., from $E_{v,J}$	B_v , numl., from Eq. (5)	Δ^1_B	Δ^2_B	Δ^3_B	Δ^4_B
0	0.16981808	0.169812	0.16981818				
				-.00511297			
1	0.16470616	0.164698	0.16470521		-.00005383		
				-.00516680		-.00000223	
2	0.15954333	0.159532	0.15953840		-.00005606		-.00000032
				-.00522286		-.00000255	
3	0.15432959	0.154309	0.15431554		-.00005861		-.00000052
				-.00528147		-.00000307	
4	0.14906495	0.149029	0.14903407		-.00006168		
				-.00534315			
5	0.14374940	0.143687	0.14369093				

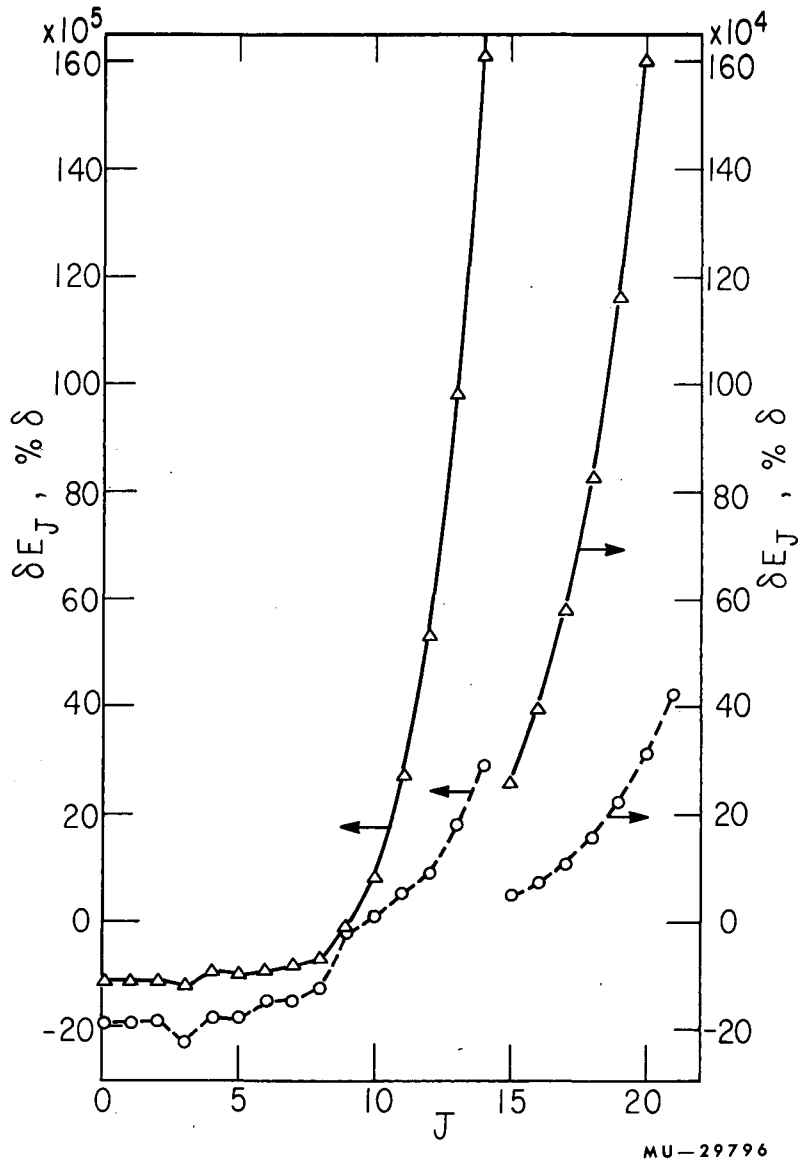


Fig. 2. Comparison of numerically-obtained rotational eigenvalues with those calculated from the Pekeris equation, Eq. (4). Triangles with solid guide lines indicate $\delta E_j \equiv$ calculated-numerical; circles with broken guide line show $\% \delta \equiv (1 - \text{calc}/\text{numl.}) \times 100$.

The final results of this comparison are summarized in Table III.

Table III. Spectroscopic parameters for HCl fitted to a Morse curve. Values calculated from Pekeris' solution compared with numerically obtained values.

Parameter	Calculated from Eqs. (4)	Numerical Solution
ω_e	48.66888	48.66888
$\omega_e x_e$	0.977882	0.977882
B_e	0.17235495	0.17235457
α_e	5.0610×10^{-3}	5.06038×10^{-3}
γ_e	-2.545×10^{-5}	-2.565×10^{-5}
δ_e	---	-2.66×10^{-7}
ϵ_e	---	-1.3×10^{-8}
$D_e(\text{rot})$	8.646×10^{-6}	8.6×10^{-6}
β_e	---	-3×10^{-8}

The excellent agreement gives grounds for considerable confidence in the accuracy of the numerical procedure. Also, the calculation shows that Eq. (2), without higher terms in $J(J+1)$, represents the Morse eigenvalues to an accuracy that is sufficient for most purposes. The neglect of the higher terms introduced an error of one part in 60,000 for the separation of level $J=20$ from $J=0$. The error introduced by the false integration limit is too small to be evident in eight-figure calculations (safely, less than one part in 10^7).

The Clinton Potential Compared with the Morse
and with Experiment

Clinton⁵ recently has suggested a potential function

$$U(r) = -D_e (r_e/r)^\sigma [1 - \ln(r_e/r)^\sigma] \quad (9)$$

where the dimensionless quantity σ can be expressed in terms of the same three parameters used to specify the Morse potential. They are related by the equation

$$\sigma = \sqrt{2} \beta r_e . \quad (10)$$

No analytic solutions for the eigenfunctions or eigenvalues of the Clinton potential have been derived as yet. The chief merit of this potential function is that it predicts more accurately than does the Morse the finite value of r at which the potential is zero, r_c . This has been established experimentally only for the case of H_2^+ but Clinton⁵ has shown that this can be expected to hold in general.

Figure 3 shows a plot of the Clinton potential for HCl. Included in the figure are a plot of the corresponding Morse potential and the RKR turning points for the first eleven vibrational levels. The latter are derived from Jarman's³ formulation of the RKR method. For levels $v=6$ through 10 the eigenvalues are obtained from spectroscopic constants¹³ based upon experimental values for levels $v=0$ through 5. Since such an extrapolation can lead to serious errors the higher turning points must be accepted with some reserve.

The Morse potential lies below the RKR throughout the whole range plotted here, but the Clinton lies below the RKR for $r > r_e$, and above

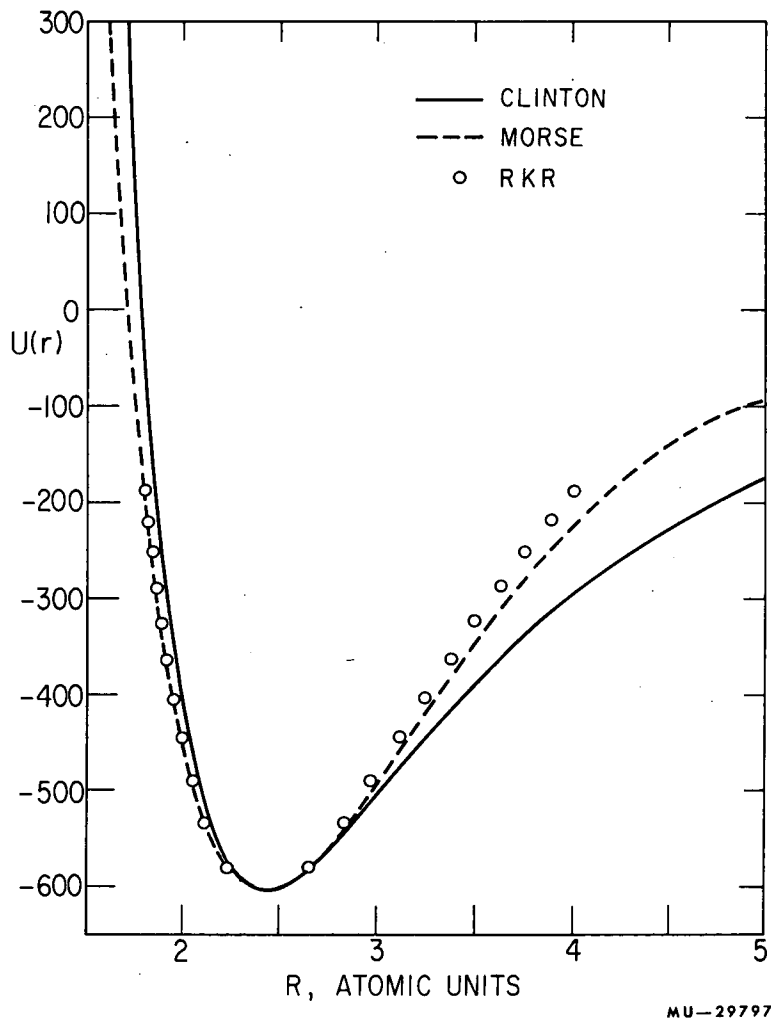


Fig. 3. The Clinton potential for HCl. The Morse potential and the classical turning points obtained from the Rydberg-Klein-Rees procedure are included for comparison.

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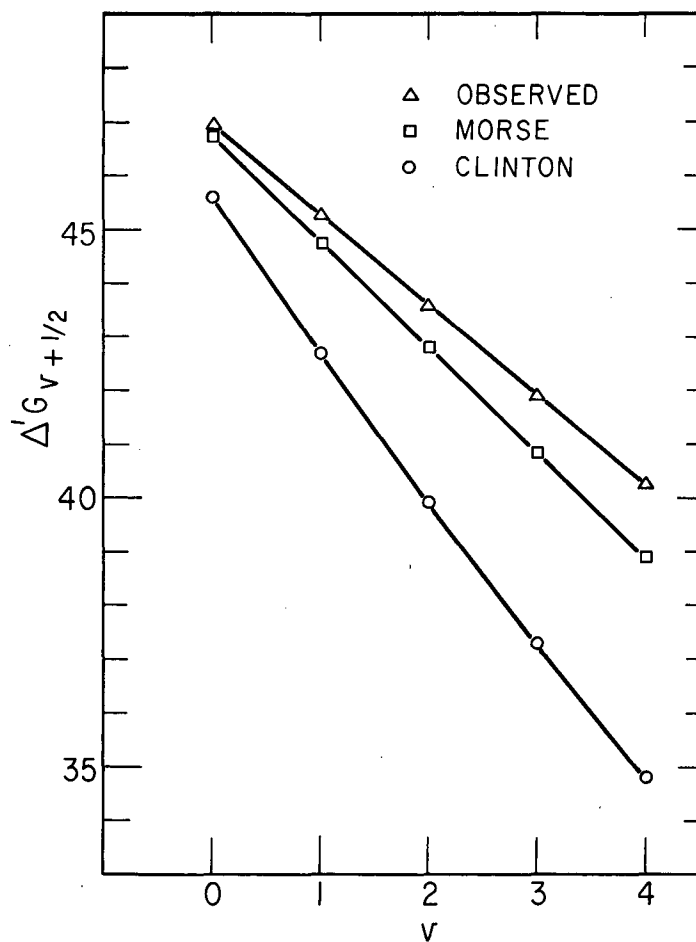
for $r < r_e$. On both sides of r_e the Clinton curve deviates from the RKR points much more than does the Morse. While it is quite possible that a reliable extension of the RKR points to the dissociation limit would come closer to the Clinton value for r_c than to the Morse value, it is by no means apparent that it will do so from the points plotted here.

Turning now to the more direct and quantitative comparisons, Fig. 4 shows the eigenvalue separation, or ΔG curve, for the Clinton, the Morse and experiment. The Morse points lie on a straight line since all terms in powers of $(v + 1/2)$ beyond the second are zero. This is not the case for the Clinton potential or for experiment. The vibrational term values for the Clinton potential are well-represented by the equation

$$G(v) = 48.68621 (v + 1/2) - 1.56656 (v + 1/2)^2 + 2.4649 \times 10^{-2} (v + 1/2)^3 - 1.76 \times 10^{-4} (v + 1/2)^4. \quad (11)$$

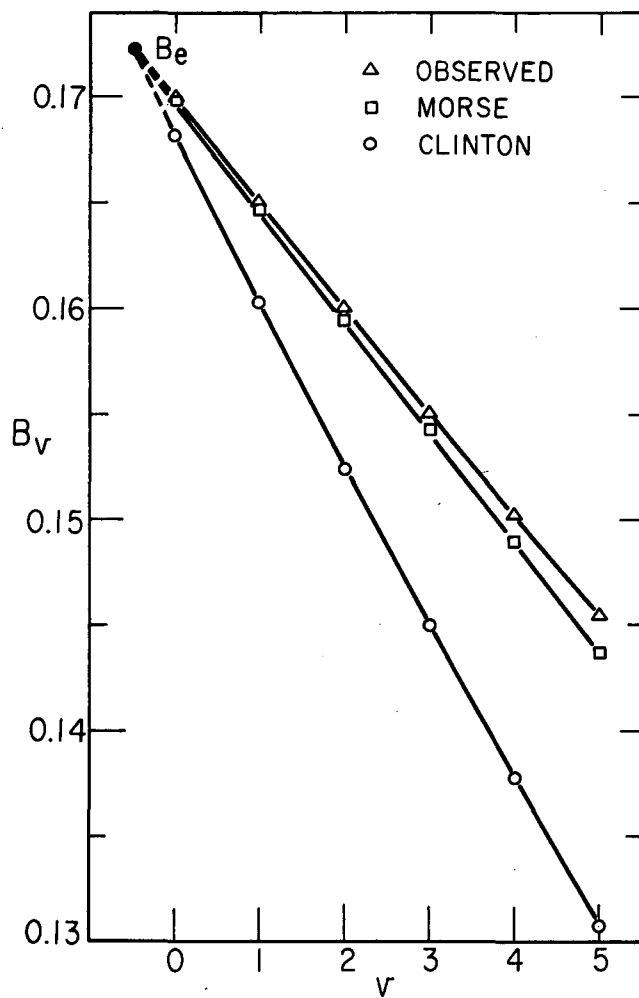
It was noted earlier that in certain cases the value of $\omega_e x_e$ might not provide an adequate approximation to the eigenvalues of the potential. The Clinton potential affords an example of this. The value of $\omega_e y_e$, which is almost an order of magnitude above experiment, contributes significantly to the energy for higher v (e.g., about 10% of the contribution of the second term for $v=5$).

Since the rotational constant D_v is very small in comparison to B_v for all the values of v investigated here, the comparison between calculated and experimental rotational eigenvalues can be made most simply through the corresponding B_v values. These are shown in Fig. 5.



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Fig. 4. Vibrational eigenvalue separations for HCl computed from the Morse and Clinton potentials compared with experiment.



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Fig. 5. Rotational constants B_v predicted by the Morse and Clinton potentials compared with experiment. The two calculated sets extrapolate to the experimental value of $B_e (= 1/r_e^2)$ at $v = 1/2$ since the experimental value of r_e was used in defining both.

As for the rotationless states, the Morse is much superior to the Clinton in the prediction of eigenvalues.

In order to be sure that this test of the Clinton potential was not being made on an atypical molecule, the same comparisons were made for the LiH, CO, and HF molecules. In every case the results were entirely analogous to those obtained with HCl.

Conclusion

The numerical integration of Schroedinger's radial equation by Cooley's⁷ procedure provides a method of testing potential functions which is direct, rapid and applicable to any function. Besides furnishing accurate eigenvalues it gives the eigenfunctions, from which all other properties implicit in the potential model may be calculated, e.g., the expectation values of powers of r . The usefulness of the numerical procedure is not restricted to the testing of potential functions. It also provides a convenient method of generating eigenfunctions for use in calculating properties of a molecule which depend only in part upon the potential curve. The vibration-rotation interaction is such a property, and a subsequent publication will deal with its evaluation by numerical methods.

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