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THE EXTREMA-EFFECT IN TOTAL ELASTIC MOLECULAR BEAM SCATTERING CROSS SECTIONS FOR CHARACTERIZATION OF THE POTENTIAL WELL[*]

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ABSTRACT

The theory of the extrema-effect in elastic impact spectra is reviewed and extended. It has been shown previously that for any realistic inter-particle potential (whose well has a capacity for one or more bound states), extrema in the total elastic molecular beam scattering cross sections are expected at certain characteristic velocities. The limiting high-velocity spacing of successive extrema on a $1/v$ plot is found to be inversely proportional to the product of the well depth ϵ times the inter-particle separation r_m at the potential minimum. It is shown that the constant of proportionality is closely related to the curvature of the well, and thus to the force constant of the di-atom (or "complex" molecule). Methods are discussed for the extraction of the maximum amount of information on the shape of the potential well from measurements of the extrema-effect.

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Introduction and Review

It has been recognized[1] for some time that the most sensitive means of evaluating the intermolecular potential is the molecular beam scattering technique. Measurements of the differential and total elastic scattering cross sections, $d\sigma(\theta)/d\Omega$ and σ (sometimes designated Q) over a wide range of relative velocity v are, in principle, sufficient to allow a determination of the orientation-averaged potential function $V(r)$ over a wide range of interparticle separation r. Although formal "inversion" procedures (cross sections $\longrightarrow$ potential) are known,[2] they have not yet seen practical utilization. Rather, it has been customary[3] to assume a reasonable parametrized functional form[*] for $V(r)$ and to compute the (partial-wave) scattering phase shifts $\eta_l(k)$ and cross sections as a function of the relative velocity or the wavenumber k $(\equiv \mu v/\hbar$, where μ is the reduced mass). The calculated cross sections are then compared with observations[4] and, by suitable variation of the potential parameters, one converges on a "best set" (subject to the constraint imposed by the assumed functionality of the potential).

In general, scattering measurements at high collision energies[5] yield information primarily on the short-range, repulsive forces while thermal-energy[6] measurements are especially sensitive to the

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[*] Typically the expression for $V(r)$ involves "strength" parameters such as ϵ, the depth of the attractive well, or C, the long-range "London" attractive constant, and "size" parameters such as σ, the "collision diameter" (the zero of the potential) or r_m, the position of the minimum.

longer-range, attractive part of the potential. At a given energy, differential cross sections at the larger scattering angles (associated with collisions of small impact parameter b, e.g., $b \lesssim \sigma$) are responsive to the repulsive branch of the potential while the lower angle scattering cross sections (governed principally by collisions of large b) are affected primarily by the long-range interactions.

At thermal energies, due to the dominant influence of the long-range attractive "tail" of the potential, the angular distributions are very strongly forward peaked, so the main contribution to the total (elastic) cross section is that from very small angles. Massey and Mohr[7] derived a simple expression for the velocity dependence of the total cross section (by introducing a "random-phase" approximation for the many large phase shifts of low ℓ and a Jeffreys-Born (JB) approximation for the many small phase shifts at high ℓ), valid for a potential asymptotically of the form $V(r) \sim -C^{(6)}/r^6$:

$$Q(v) = p \cdot \left(C^{(6)}/\hbar v\right)^{2/5} \tag{1}$$

where p is a dimensionless constant[*].

However, due to the concomitant short-range forces, undulatory

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[*] Based on more recent treatments[8] a "best" value[8c] of p = 8.08 is obtained.

deviations from the monotonic $v^{-2/5}$ dependence of the total cross section are expected, i.e., extrema in the velocity dependence of Q [3b,9ab]. This so-called "extrema-effect" is due to the existence[*] of a broad maximum in the dependence of the phase shift upon the angular momentum quantum number l, which provides a significant number of non-random phases at intermediate l. The maximum phase η_m increases with decreasing k and, if the attractive well is deep enough (i.e., has a capacity for one or more bound states), $\eta_m(k)$ can pass successively through several multiples of $\pi/2$, giving rise alternately to positive and negative incremental contributions ΔQ to the random-phase-approximated Q, designated $\bar{Q}$. The increment ΔQ is found to be[10a]

$$\Delta Q = \frac{4\pi^{3/2} L_0}{k^2 \cdot (-\eta_m'')^{1/2}} \cdot \sin(2\eta_m - 3\pi/4) \tag{2}$$

where L_0 is the value of l for which η attains its maximum value, $\eta_m(k)$; $\eta_m'' = (\partial^2\eta/\partial l^2)_{L_0}$. L_0 and η_m'' are also dependent upon k. Thus the general condition for an extremum in Q is:[9b]

$$\eta_m(k_N) = \pi \cdot (N - 3/8) \tag{3}$$

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[*] This is due to the "competition" between a positive (attractive) term and a negative (repulsive) contribution to the phase shifts, characteristic of scattering by any potential with a well.

where the integer indices $N = 1, 2, \ldots$ denote maxima in Q and the half-integers $N = 1.5, 2.5 \ldots$ minima; k_N is the wavenumber of the Nth extremum.

For any realistic potential with a well, the high-energy behavior of the maximum phase in the J.-B. limit has the asymptotic form*:

$$\eta_m \sim c_1 \epsilon r_m / v \tag{4}$$

where the constant of proportionality c_1 depends somewhat upon the particular functionality of the potential. For the simplest practical two-parameter potential, the L.-J.(12,6), one finds[9a] $c_1 = 0.8432/\hbar$. Thus in the high-velocity limit, one has the following velocity dependence of the extrema:

$$N - 3/8 \sim \frac{c_1}{\pi} \epsilon r_m / v_N = A_1 / v_N \tag{5}$$

where v_N is the Nth extremum-velocity. The v_N may be determined by inspection of experimental graphs of the (oscillatory) function $\Delta Q/\bar{Q}$ vs. v^{-1} (termed[9b] elastic impact spectra). Then, from Eq. 5, a plot of $N-3/8$ vs. v_N^{-1} should pass through the origin (thus fixing the index assignments), with initial slope A_1 yielding the ϵr_m product, assuming a particular potential function with given c_1.

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*In "reduced" notation, Eq. 4 may be written

$$\eta_m^* \sim a_1 / K \tag{4'}$$

where the "reduced phase" $\eta^* \equiv \eta / k r_m$ and the reduced collision energy $K \equiv E/\epsilon = \frac{1}{2} \mu v^2 / \epsilon$.

The extrema-effect has been used (somewhat as follows) to characterize the potential well for a number of alkali and noble gas systems.[11] First, $C^{(6)}$ is deduced from $\bar{Q}(v_r)$ (via Eq. 1). Then from the elastic impact spectrum and the resulting N (v_N^{-1}) plot, the ϵr_m product is evaluated, assuming a L.-J.(12,6) functionality (i.e., a specified c_1). Since for this potential $C^{(6)} = 2\epsilon r_m^6$, ϵ and r_m may be separately obtained. These may serve as initial values in an iterative computational procedure, in which the potential constants as well as functionality can be altered, and the successively computed $\Delta Q/\bar{Q}\,(v)$ curves compared with experiment.

The amplitude of the oscillations in $\Delta Q/\bar{Q}$ is well approximated[10] by the semiclassical relation

$$U \equiv \frac{|\Delta Q|_{max}}{\bar{Q}} = \frac{4\pi^{3/2} L_o}{k^2 \bar{Q}\cdot(-\eta_m'')^{1/2}} = \frac{4\beta_o}{\bar{Q}}\cdot\left[\frac{2\pi}{-\theta_o' A}\right]^{1/2} \tag{6}$$

where $\beta = (l+\frac{1}{2})/A \cong l/A$ is the reduced impact parameter (β_o the value corresponding to L_o) and $\theta_o' = (\partial\theta/\partial\beta)_{\beta_o}$ is the slope of the classical deflection function $\theta(\beta)$ at its zero, β_o.

Thus, given accurate experimental amplitudes one may extract the ratio $\beta_o/(-\theta_m')^{1/2}$, which is sensitive to the assumed functional form of the potential. Unfortunately, due to the blurring effect of even residual beam velocity distributions the observed amplitude $U(\bar{v})$ is smaller than the true $U(v)$, so that it is difficult to improve substantially on the initial value of ϵr_m

It should be noted that once the indices N are correctly assigned from a $N(v_N^{-1})$ plot it becomes possible to deduce directly from the experimental extrema-velocities, via Eq. 3, absolute values*/ of the maximum phase shift η_m as a function of k or v. The experimental results may be fitted to a power series in reciprocal velocity and ratios of successive coefficients compared with calculations based on various assumed functional forms of V(r).

The important constant of proportionality c_1 (between the experimental initial slope, A_1, and the desired ϵr_m product) is not fully independent of the shape of the potential. It will be shown that (for a given ϵ and r_m) the constant is governed primarily by the curvature of the potential at its minimum.**/

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*/ The extrema-effect appears to be the only example of a direct experimental method for the determination of an absolute scattering phase shift; ordinarily it has been assumed that experiment can only reveal phase shifts modulo π.

**/ In Ref. 10b, useful tables are presented listing the three extrema-quantities η_m^*, β_o and θ_o' as a function of K for the Kihara (α,12,6) potential with the "core" parameter in the range $-0.3 \leq \alpha \leq 0.5$; similar calculations for the L.-J. (n,6) potential were summarized by an "equivalence" table, i.e., $n \leftrightarrow \alpha$ for which the extrema-quantities were essentially identical. The experiments of Rol and Rothe[12] on the Li-Kr system which had been analyzed in Ref. 11a in terms of a L.-J.(12,6) function, were re-analyzed and a "best fit" of $\Delta Q/\bar{Q}(v)$ obtained with $\alpha = 0.2$, corresponding to n = 23. The inference might be drawn that the repulsive index, n, of the interaction is deducible from extrema measurements. It is suggested that a more correct interpretation of the re-analysis is that the curvature of the well is greater than that of a L.-J.(12-6) well of the same ϵ and r_m.

Considerations on the Maximum Phase Shift and the Curvature of the Well

Within the framework of the semiclassical treatment of scattering, the JWKBL phase shift is independent of V(r) for $r < r_o$, the classical turning point of the radial motion. It is recalled[7, 9c] that

$$\eta_\ell^{JWKBL}(k) = k\left[\int_{r_o}^{\infty}[F(r)]^{1/2}dr - \int_{b}^{\infty}[F^{(o)}(r)]^{1/2}dr\right] \tag{7}$$

where $F(r) \equiv 1 - \frac{V_{eff}(r)}{E}$, $V_{eff}(r) = V(r) + Eb^2/r^2$ (the effective potential), $F^{(o)}(r) = 1 - b^2/r^2$ and $\ell \cong kb$; the outermost* zero of F(r), i.e., $F(r_o) = 0$, defines the turning point. For all impact parameters $b > \sigma$ (the zero of the potential), the centrifugal potential is sufficiently great that $r_o > \sigma$. This follows since for $V(r_o) \geqslant 0$,

$$r_o = b\left[1 - V(r_o)/E\right]^{-1/2} \geqslant b > \sigma\ , \tag{8}$$

while for $V(r_o) < 0$, $r_o > \sigma$ (trivially).
As an illustration, Fig. 1 shows the "reduced" classical turning points $z_o \equiv r_o/r_m$ plotted vs. $\beta = b/r_m$ at various reduced energies $K = E/\epsilon$, for an Exp (14,6) potential. Thus, provided**

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* Quantum mechanically some penetration of the wavefunction (and, for collision energies below the classical critical value for orbiting, tunneling through the centrifugal barrier) occurs, but this is of secondary importance in the present connection.

** For all practical potentials this inequality is found to be satisfied. E.g., for the L.J. (n,6) potential it is readily shown that $\beta_o > \sigma/r_m$ for all $n > 7$.

$\beta_o > \sigma/r_m$, the maximum phase η_m is independent of V(r) for all positive (repulsive) values of the potential. Strictly, then, it is not possible to acquire information dealing with the repulsion (V(r) > 0) from measurements of the extrema-effect. The entire information content of such experiments is confined to the attractive well.* This suggests that a suitable description of the potential from the viewpoint of the extrema analysis is one which specifies (in addition to ϵ and r_m) the curvature of the well. Thus, if V(r) is expanded around the minimum it is plausible that the leading (quadratic) term may be deducible from extrema measurements.

All the semi-empirical potential functions** are readily expanded:

$$V^*(\zeta) = -1 + \tfrac{1}{2}\varkappa\zeta^2 + \sum_{n=3}^{N} \frac{\zeta^n}{n!} f^{(n)}(0) \tag{9}$$

where $V^* \equiv V/\epsilon$ is the reduced potential, $\zeta \equiv z - 1$ is the "reduced displacement", $\varkappa \equiv \left(\partial^2 V^*/\partial\zeta^2\right)_0$ is the "reduced curvature" and $f^{(n)}(0) = \left(\partial^n V^*/\partial\zeta^n\right)_0$.

In conventional terminology the force constant is $k = 4\pi c^2\mu\omega_e = \varkappa\epsilon/r_m^2 = \varkappa D_e/r_e^2$ where the spectroscopic symbols have their usual

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* Of course, from a knowledge of the shape of the well (i.e., curvature at the minimum) one may estimate the ratio σ/r_m and the slope of V(r) near $r = \sigma$.

** Expansion coefficients for the L.-J.(n,6), Exp. (α,6) and Morse (a) potentials have been published.[13] Convergence of (9) is achieved only if $0 < z < 2$.

meanings. One expects, of course, that in addition to the curvature, further higher-order terms in Eq. 9 are required for accurate determination of η_m^*.[*] However, the principal dependence of $\eta_m^*(K)$ should be upon $\varkappa$; i.e., the coefficient of the leading term (a_1 in Eq. 4') should be well correlated with $\varkappa$.

The maximum reduced phase may be expanded in powers of $K^{-\frac{1}{2}}$ (extending Eq. 4'):

$$\eta_m^* = \sum_{n=1}^{N} a_n K^{-(n+1)/2} \tag{10}$$

where the dimensionless a_n coefficients are (within the framework of the semiclassical approximation) independent of μ , ϵ and r_m , depending only on the "shape" of the potential.

As will be shown, a_1 is a slowly-varying function of $\varkappa$ over a rather wide range of $\varkappa$; thus ϵr_m may be estimated to within about ±10 per cent directly from an experimental value of A_1 . Of course, if the ϵ and r_m were known sufficiently well from independent considerations (e.g. to $\pm$ 1 per cent in the ϵr_m product), then from the experimental A_1 and the known dependence of a_1 upon $\varkappa$ one could deduce the curvature of the well (and the di-atom force constant).

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[*] Auxiliary calculations have shown that the potential must be known out to z = 2 in order to achieve the requisite accuracy in η_m^* .

Computational Procedures

Semiclassical reduced phases $\eta^{*JWKBL}(\beta, K)$ were computed via Eq. 7 for three commonly used potentials, following procedures similar to those used earlier[14], but with improved accuracy of quadrature. The resulting η^* values were numerically accurate to within about ± 0.00001, independent of any systematic errors associated with the approximation (Eq. 7) itself.

The potentials were expressed in the reduced forms

Potential 1: $$V_{LJ}^* = \left(\frac{6}{n-6}\right)\left(\frac{r_m}{r}\right)^n - \left(\frac{n}{n-6}\right)\left(\frac{r_m}{r}\right)^6 \qquad (11.1)$$

Potential 2: $$V_K^* = \left(\frac{1-\alpha}{r/r_m - \alpha}\right)^{12} - 2\left(\frac{1-\alpha}{r/r_m - \alpha}\right)^6 \qquad (11.2)$$

Potential 3: $$V_E^* = \left(\frac{6}{\alpha-6}\right)\exp\left[-\alpha\left(r/r_m - 1\right)\right] - \left(\frac{\alpha}{\alpha-6}\right)\left(\frac{r_m}{r}\right)^6 \qquad (11.3)$$

The range of K investigated was from 1.2 to 100 (lower K's would introduce the complication of three turning points[15] (classical orbiting), while for higher K's the η_m^* values are so small that the percentage error is larger than desired. In general the range of β was restricted to the region in the neighborhood of β_o (e.g. $.8 < \beta < 1.3$); the maximum in the

$\eta^*(\beta)$ curve was obtained by a 3-point Aitken interpolation which also yielded β_o and $\left(\partial^2\eta^*/\partial\beta^2\right)_o$

For the eventual purpose of correlation of these results with curvature $\mathcal{K}$, the following equivalence relationships between potential parameters and $\mathcal{K}$ have been used:

Potential 1: $$\mathcal{K} = 6n \qquad (12.1)$$

Potential 2: $$\mathcal{K} = \frac{72}{(1-\alpha_K)^2} \qquad (12.2)$$

Potential 3: $$\mathcal{K} = 6\alpha_E\left(\frac{\alpha_E - 7}{\alpha_E - 6}\right) \qquad (12.3)$$

Fig. 2 is a nomograph relating the various indices n, α_K, α_E, with $\mathcal{K}$. (Included also is the Morse function with index a_M).

The maximum phases η^*_m(K) were computed for various values of these indices over a range of $\mathcal{K}$ from 48-108 for potentials (1)-(3). The results were expressed in terms of power series in $K^{-\frac{1}{2}}$ according to Eq. 10; the coefficients were evaluated by a modified Aitken polynomial method. A four-term expansion fitted the values to within about $\pm$.1 per cent. It was found that, aside from the a_1 (obtained theoretically by the JB procedure), the expansion coefficients depended only very slightly on $\mathcal{K}$. Moreover these higher coefficients (a_2-a_4) are essentially invariant to the functional form of the potential. Since a simple set of constant expansion coefficients (see Results), along with the theoretical values of a_1, can be used to reproduce the tables of $\eta_m^*(K)$ to within a maximum deviation of 0.3 per cent, these tables will not be presented.*

Results

Fig. 3 shows a sample of the behavior of η_m^* as a function of $1/K$ for the three potentials, each at three specified (common) values of curvature κ. The curves are seen to group together according to curvature.

The deviation from the high energy, limiting behavior (eq. 4') is best shown in graphs of the product $\eta_m^* K$ vs. $1/K$, as illustrated in Fig. 4 for the same set of calculations. Here again the "family" structure is apparent, curvature being the dominant factor. Note that the ordinate intercept of the curve (via extrapolation) gives a "computationally evaluated" a_1. These agree (± 0.1 %) with the JB-calculated a_1 values (see Appendix).

The constants of the semi-empirical equations for η_m^* (following the form of Eq. 11) are presented in Table I.

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* By introducing a slight κ dependence in the expansion coefficients a_3 and a_4 the maximum deviation can be decreased by about a factor of two.

Table I

Expansion Coefficients (a_1-a_4) for $\eta_m^*(\kappa)$ According to Eq. 10

a_1

κ	Potential 1	Potential 2	Potential 3
48	.47000	.47421	.45208
60	.44113	.44432	.43063
72	.42156	.42156	.41462
84	.40727	.40338	.40232
96	.39630	.38838	.39257
108	.38757	.37568	.38465
120	.38043	.36474	.37808
132	.37446	.35515	.37253
144	.36938	.34666	.36776

$$a_2 = 2.0 \times 10^{-3}$$

$$a_3 = -1.90 \times 10^{-1}$$

$$a_4 = 8.8 \times 10^{-2}$$

The a_1 coefficients listed are the theoretical (J.-B.) values, while the higher coefficients were evaluated by the Aitken fitting procedure mentioned earlier. The a_1's could be expressed in closed form only for potential 1. The analysis for the other two potentials involved the solution of transcendental equations and power series expansions (see appendix). The $\mathcal{K}$-dependence of the important parameter a_1 is shown in Fig. 5. Here $a_1(\mathcal{K})$ shows a broad region ($70 \leq \mathcal{K} \leq 130$) in which (a) the slope is essentially constant ($da_1/d\mathcal{K} \cong -9 \times 10^{-4}$) and (b) the results for the three potentials are very similar.

Conclusions

The excellence of the correlation of a_1 with $\mathcal{K}$, nearly independent of the particular functionality of the potential, confirms the suggestion that the third "characterization parameter" of the potential should be the curvature of the well. Since the higher order coefficients (a_2-a_4) are found to be completely invariant to the functionality of the potential and essentially independent of $\mathcal{K}$, an experimental determination of the ratios a_2/a_1 and a_3/a_1 (from plots of Nv_N vs. v_N^{-1}) should allow (via Table I) an estimate of $\mathcal{K}$ and thus the di-atom force constant.

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Appendix

High-energy limiting forms for the extrema-quantities η_m^* and β_0 may be obtained from the J.-B. approximation for the phase shift[9,10a,16]. These were obtained in closed form only for potential 1. In this case

$$\eta_m^{JB} = \frac{3\pi}{32}\left(\frac{m}{m-1}\right)\frac{1}{K}\left[\frac{32}{5\pi}\left(\frac{m-1}{m}\right)f(m)\right]^{\frac{5}{6-m}} \qquad \text{(A-1)}$$

$$\beta_0 = \left[\frac{32}{5\pi}\left(\frac{m-1}{m}\right)f(m)\right]^{\frac{1}{m-6}} \qquad \text{(A-2)}$$

where[16]

$$f(m) = \tfrac{1}{2}\pi\,\Gamma\tfrac{1}{2}(m-1)/\Gamma\tfrac{1}{2}m \quad . \qquad \text{(A-3)}$$

For potential 2

$$\eta^{*JB} = \frac{(1-\alpha)^6}{K}\int_\beta^\infty\left\{\frac{1}{x^5\sqrt{x^2-\beta^2(1-\alpha/x)^6}} - \frac{(1-\alpha)^6}{2x^{11}\sqrt{x^2-\beta^2(1-\alpha/x)^{12}}}\right\}dx \qquad \text{(A-4)}$$

The integrals were evaluated by expanding the factor of $(1-\alpha/x)^{-m}$ in a convergent power series. Then η^* can then be written in the form

$$\eta^{*JB} = \frac{(1-\alpha)^6}{K}\Bigg\{\frac{3}{16}\frac{\pi}{\beta^5} - (1-\alpha)^6 \frac{63}{1024}\frac{\pi}{\beta^{11}}$$

$$+ \sum_{k=1,3,5,\cdots}\Bigg[\frac{(k+5)!}{120\,k!}\,\alpha^k \frac{\left(\frac{k+3}{2}\right)!\; 2^{\left(\frac{k+3}{2}\right)}}{1\cdot 3 \cdots (k+4)\,\beta^{k+5}}$$

$$+ \frac{(k+6)!}{120(k+1)!}\,\alpha^{k+1}\,\frac{(k+5)!}{\left[\left(\frac{k+5}{2}\right)!\right]^2}\,\frac{\pi}{(2\beta)^{k+6}}$$

$$- \frac{(1-\alpha)^6}{2}\,\frac{(k+11)!}{11!\,k!}\,\alpha^k\,\frac{\left(\frac{k+9}{2}\right)!\; 2^{\left(\frac{k+9}{2}\right)}}{1\cdot 3\cdots(k+10)\,\beta^{k+11}} \tag{A-5}$$

$$- \frac{(1-\alpha)^6}{2}\,\frac{(k+12)!}{11!\,(k+1)!}\,\alpha^{k+1}\,\frac{(k+11)!}{\left[\left(\frac{k+11}{2}\right)!\right]^2}\,\frac{\pi}{(2\beta)^{k+12}}\Bigg]\Bigg\}$$

Substitution of β_o (the solution of the equation $\left(\partial\eta^*/\partial\beta = 0\right)$ in Eq. A-5 yields η_m^{*JB}. Sufficient terms were carried in the expansion to insure convergence of the value of η_m^{*JB} to $\pm.000001$. This required terms as high as $k = 40$ for low $\mathcal{K}$ (i.e. negative α).

To evaluate the corresponding quantities for potential 3 to the requisite accuracy the necessary higher order expansion terms were added to Eq. 10b of Ref. 16. This equation then becomes

$$\eta^{*JB} = \frac{3\pi}{32}\,\frac{\alpha}{\alpha-6}\,\frac{1}{K\beta^5}\Bigg\{1 - \frac{32}{\sqrt{2\pi}}\,\frac{\beta^{11/2}}{\alpha^{3/2}}\,e^{\alpha(1-\beta)}$$

$$\times\left[1 + \frac{3}{8\alpha\beta} - \frac{15}{128\alpha^2\beta^2} + \frac{105}{1024\alpha^3\beta^3} - \cdots\right]\Bigg\} \tag{A-6}$$

Again η_m^{*JB} may be evaluated by substituting β_o (found, as before, by differentiation of η^{*JB}) in Eq. A-6.

It can be seen from Eq. 4' that the expressions for a_1 are obtained directly from Eqs. A-1,5,6 by suppressing the factor $1/K$.

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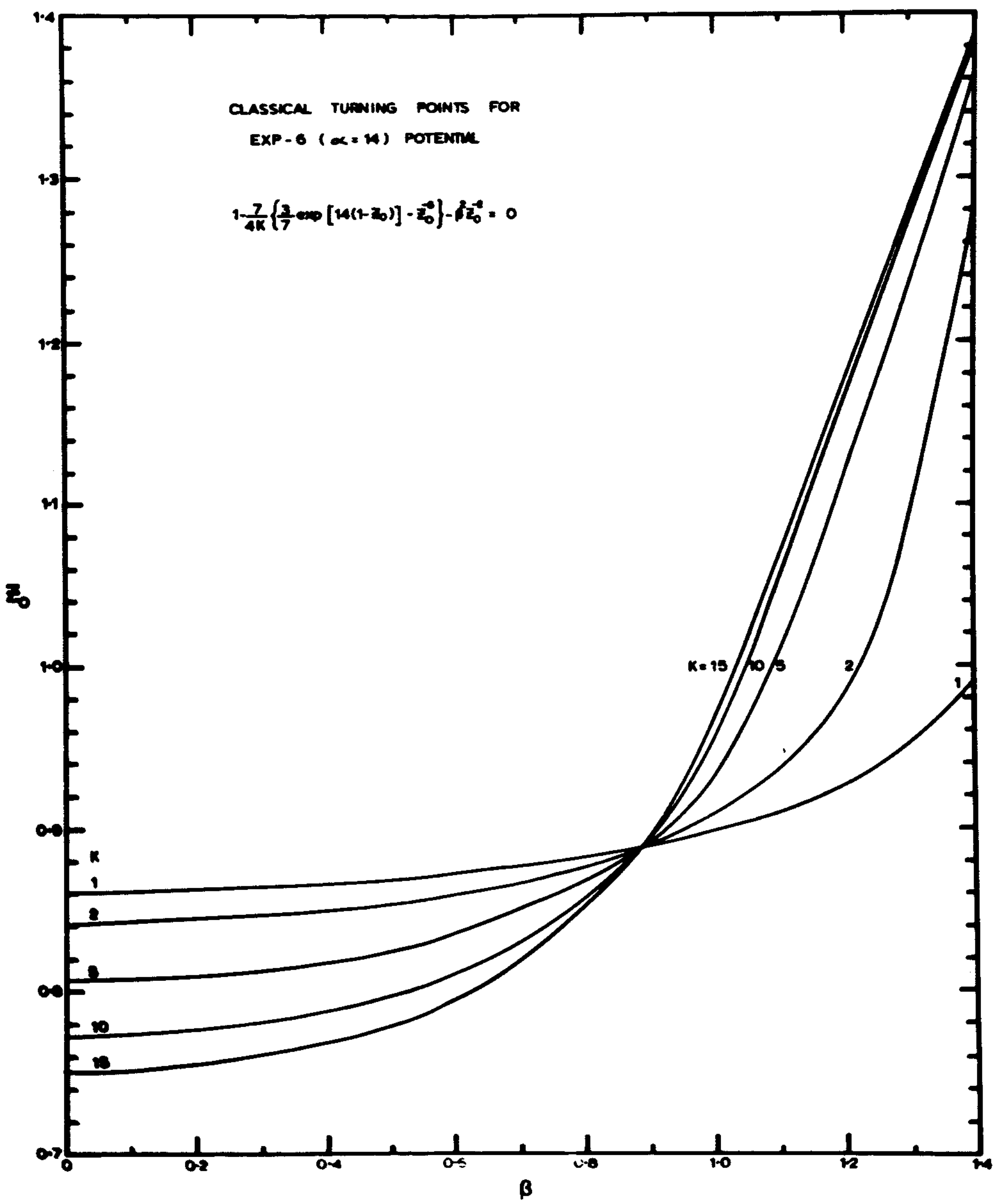
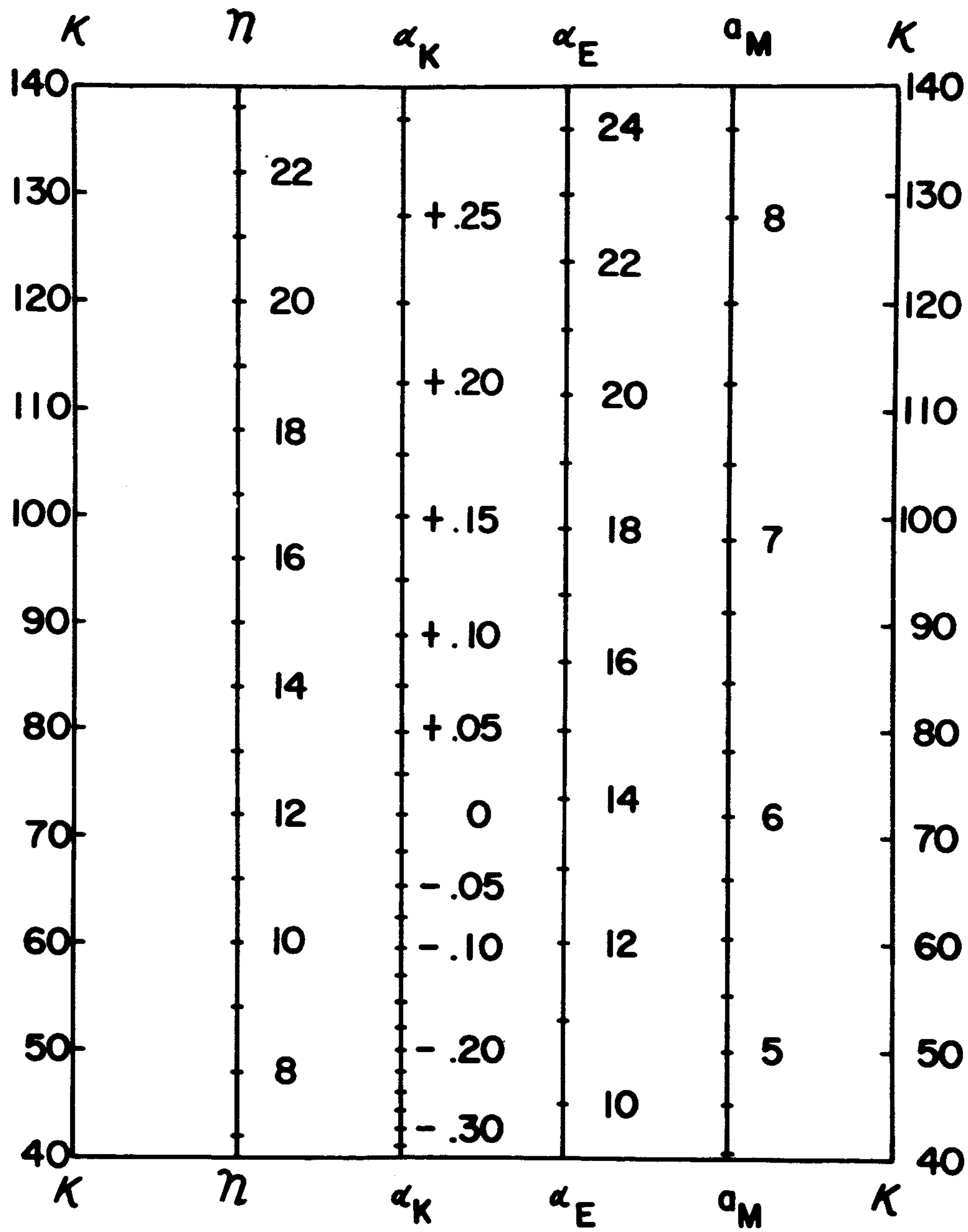
Legends for Figures

1. Reduced classical turning points for the Exp (14,6) potential as a function of reduced energy K. The curves cross at a common point when $r_o = b = \sigma$, or $z_o = \beta = \sigma/r_m$.
2. Nomograph relating the various indices of Potentials 1, 2 and 3 with the reduced curvature $\mathcal{K}$.
3. Dependence of η_m^* upon $1/K$ for Potentials 1, 2 and 3, each at the specified values of $\mathcal{K}$.
4. Dependence of $\eta_m^* K$ upon $1/K$ for Potentials 1, 2 and 3, as in Fig. 3.
5. Dependence of the a_1 parameter upon $\mathcal{K}$ for Potentials 1, 2 and 3. The expressions for $a_1(\mathcal{K})$ in the three cases are given in the Appendix.



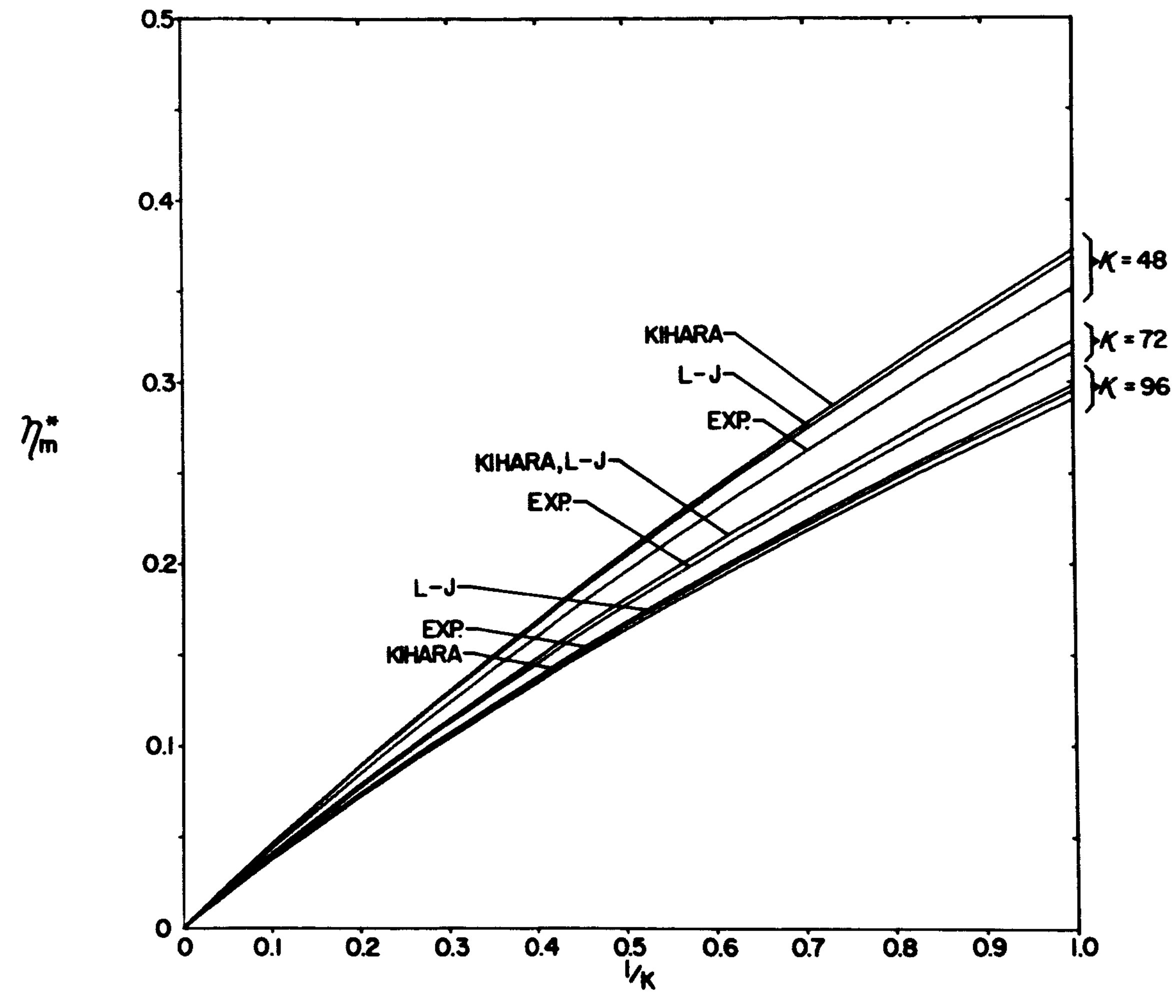
CLASSICAL TURNING POINTS FOR
EXP - 6 (α = 14) POTENTIAL
$1-\frac{7}{4K}\left\{\frac{3}{7}\exp\left[14(1-z_0)\right]-z_0^{-6}\right\}-\beta^2 z_0^{-2} = 0$
z_0
β
K
1
2
5
10
15
K = 15
10
5
2
1
0·7
0·8
0·9
1·0
1·1
1·2
1·3
1·4
0
0·2
0·4
0·6
0·8
1·0
1·2
1·4

Fig. 1



K
η
α_K
α_E
a_M
K
140
130
120
110
100
90
80
70
60
50
40
22
20
18
16
14
12
10
8
+.25
+.20
+.15
+.10
+.05
0
-.05
-.10
-.20
-.30
24
22
20
18
16
14
12
10
8
7
6
5

Fig. 2



0.5
0.4
0.3
0.2
0.1
0
η_m^*
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$1/K$
KIHARA
L-J
EXP.
KIHARA, L-J
EXP.
L-J
EXP.
KIHARA
$K = 48$
$K = 72$
$K = 96$

Fig. 3

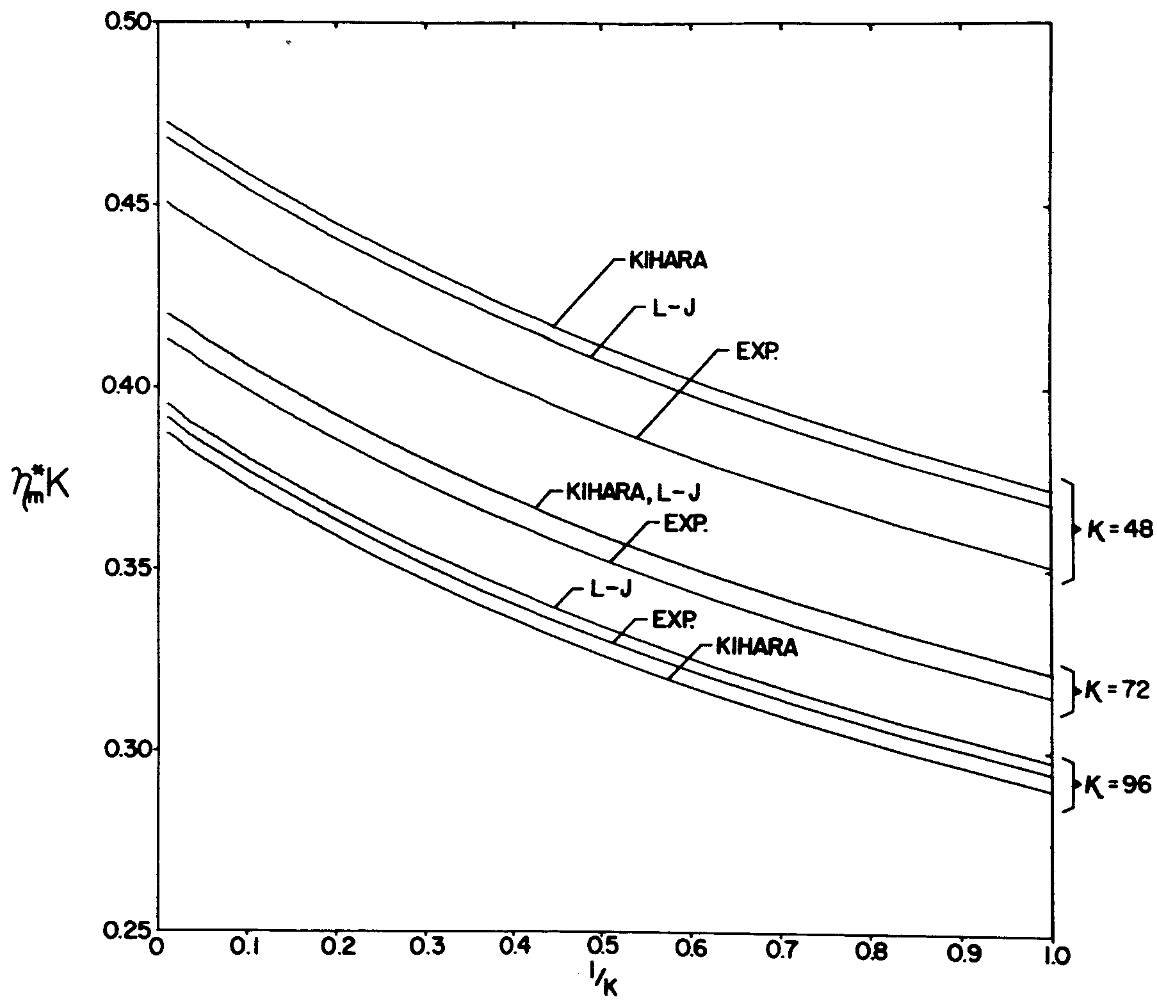
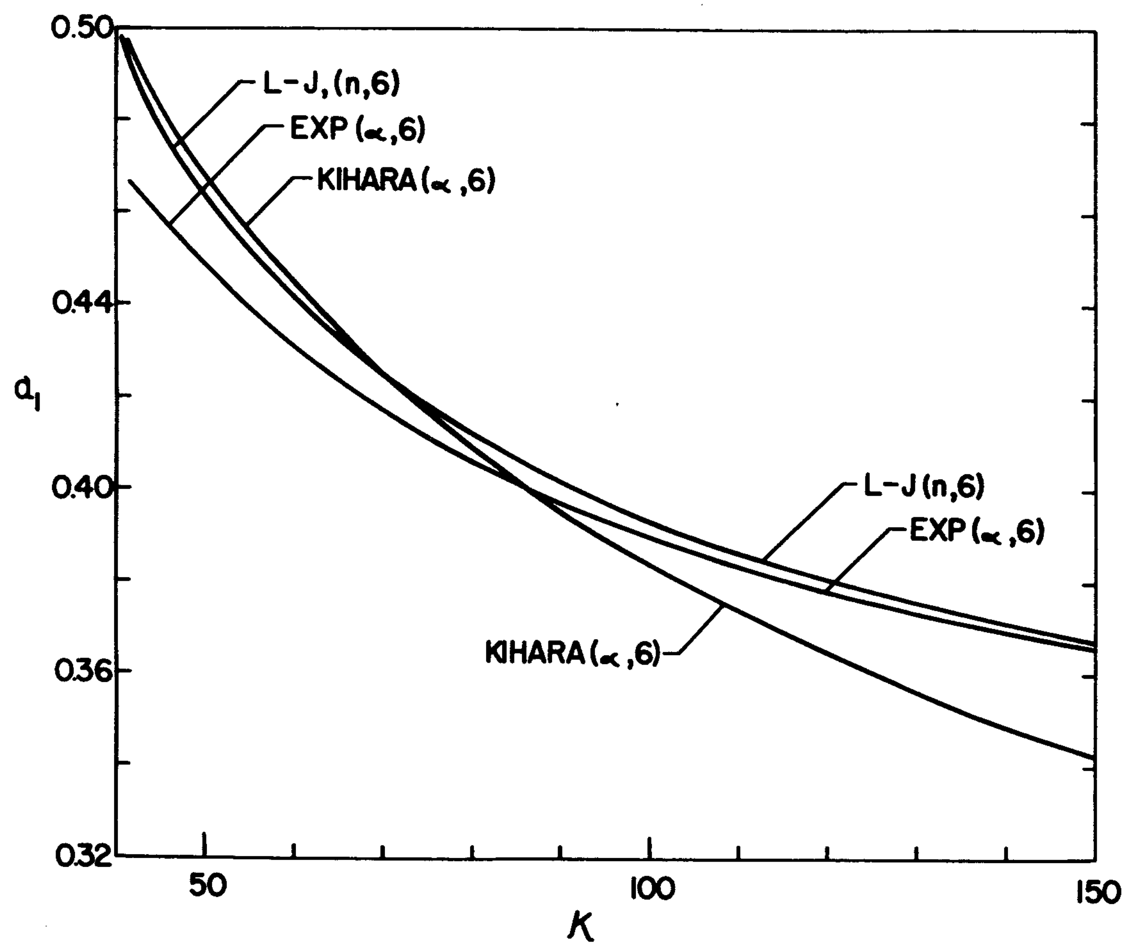

0.50
0.45
0.40
0.35
0.30
0.25
$\eta_m^* K$
KIHARA
L-J
EXP.
KIHARA, L-J
EXP.
L-J
EXP.
KIHARA
K = 48
K = 72
K = 96
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1/K

Fig. 4



0.50
0.44
0.40
0.36
0.32
d_1
50
100
150
K
L-J, (n,6)
EXP (α,6)
KIHARA (α,6)
L-J (n,6)
EXP (α,6)
KIHARA (α,6)

Fig. 5