

# Inversion of the Total Cross Sections for Electron-Molecule and Electron-Atom Scattering



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## Abstract

Inverse scattering theory has been applied to construct the interaction potentials from total cross sections as a function of energy for electrons scattered off of atoms and molecules. The underlying potentials are assumed to be real and energy independent and are evaluated using the Eikonal approximation and with real phase shifts determined from the total cross sections. The inversion potentials have been determined using either a high energy limit approximation or by using a fixed energy inversion method at select energies. These procedures have been used to analyse  $e^- - \text{CH}_4$ ,  $e^- - \text{SiH}_4$ ,  $e^- - \text{Kr}$  and  $e^- - \text{Xe}$  scattering data in particular.

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## I. INTRODUCTION

There are two basic approaches to extract quantitative information on the interaction of two colliding quantal particles. The most common one is the direct approach in which an interaction between two quantal systems is assumed and used in making direct solutions of the Schrödinger equations; the asymptotic properties of the wave functions from which allow comparisons with measured data. The alternative approach is to use inverse scattering theory [1] and, with one of many methods of application, construct the (Schrödinger) interaction specifically from the measured data. In so doing there is essentially no *a priori* assumption made about the shape of that potential. Inversion methods usually belong to one of two classes; those with energy as the spectral parameter and angular momentum fixed and those vice versa. Of the latter, the fixed energy schemes, we have found that the fully quantal and semiclassical WKB inversion schemes of Lipperheide-Fiedeldej type [2,3] have been most useful in practice. Those schemes have been used extensively in recent years to analyse the elastic scattering cross sections from the scattering of two nuclei [3,4] as well as of two atoms and of electrons from water molecules [5].

While most of the applications of inverse scattering theory take differential cross section data as the starting point, Miller [6] has shown that it is also possible to obtain potentials by inversion of the total cross section. His method is based on an eikonal approximation and on the assumption that the potential is local and independent of energy (i.e. there is no underlying nonlocality). It has been used [7] to specify an interaction for the He-He atomic system. Our interest lies in the fact that many total cross section measurements have been made from the scattering of electrons from atoms and molecules. In some cases those measurements span a wide energy range. For example, recent measurements at energies up to 4 keV have been reported [8-10]. We are not aware of any previous inversion analyses of the total cross sections for electron scattering and so herein we investigate the feasibility of such and compare a select set of inversion results with those obtained by direct analyses of the same data.

The inversion procedures that we have used are presented in brief in section II as they are predicated upon the detailed presentations given elsewhere [3,6]. The results of our applications to the analyses of electron scattering from the molecules CH<sub>4</sub> and SiH<sub>4</sub> and from the inert gas atoms of Kr and Xe are then presented and discussed in section III. Conclusions we can draw are given finally in section IV.

## II. INVERSION THEORY AND METHODS

All current direct and inverse methods of analysis of scattering data are two stage processes, in which the link between the measured data and the interaction potential is the scattering matrix,  $S_l(k)$ , or equivalently, the scattering phase shifts,  $\delta_l(k) [= (1/2i) \ln(S_l(k))]$ . For the scattering of spinless particles, only real half-integer values of the angular momentum variable  $\lambda$  (i.e.  $\lambda = l + \frac{1}{2}$ ), are required and the total scattering cross sections for an energy  $E (= \frac{\hbar^2}{2\mu} k^2)$ , are given by

$$\sigma(k) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l(k)) . \quad (1)$$

The inversion method described in detail by Miller [6] is based upon a representation of the phase shift function,

$$\delta_l(k) \rightarrow \eta(t, k) = -\frac{\omega(t)}{2k} , \quad (2)$$

wherein  $t$  is the impact parameter function, ( $t = \lambda/k$ ). Then upon converting the partial wave sum to an integral, the total cross section can be found from

$$\sigma(k) = 4\pi \int_0^{\infty} 2t \sin^2 \left( \frac{\omega(t)}{2k} \right) dt , \quad (3)$$

or, if  $\omega(t)$  is a monotonic function of  $t$ , from

$$\sigma(k) = \frac{2\pi}{k} \int_0^{\infty} t^2(\omega) \sin^2 \left( \frac{\omega}{k} \right) d\omega . \quad (4)$$

A Fourier sine transform of that equation yields

$$t^2(\omega) = \frac{1}{\pi^2} \int_0^\infty \frac{1}{k} \sigma(k) \sin\left(\frac{\omega}{k}\right) dk, \quad (5)$$

from which Miller [6] determined an inversion potential to be

$$V_M(r) = \frac{\hbar^2}{\pi\mu} \int_0^{\omega_0} \frac{1}{\sqrt{t^2(\omega) - r^2}} d\omega. \quad (6)$$

The upper integration limit is that value at which the radicand vanishes. Thereby this approach is appropriate for small radii in contradistinction to other fixed energy inversion methods [2,3] which are more reliable in defining the long ranged character of potentials.

Thus the remaining problem is to specify the impact parameter function,  $t(\omega)$ , from the data. We shall restrict consideration to monotonic forms, but note that the approach can be made with nonmonotonic functions too [6]. Clearly the impact parameter function can be found numerically (from Eq.5) by making the Fourier sine transform of the cross section data for all relevant values of  $\omega$ . But we have found it more convenient to adopt a two parameter functional form, namely

$$t^2(\omega) = \frac{a}{\omega(b^2 + \omega^2)^2}, \quad (7)$$

as then the cross section, Eq.4, takes the analytic form,

$$\begin{aligned} \sigma(k) &= \frac{\pi^2 a}{b^4 k} \left[ 1 - \left(1 + \frac{b}{2k}\right) e^{-b/k} \right], \\ &\rightarrow \frac{\pi^2 a}{2b^3 k^2} + \mathcal{O}(k^{-4}) \dots \text{ as } k \rightarrow \infty. \end{aligned} \quad (8)$$

The parameter values,  $(a, b)$ , can then be determined by a chisquare minimisation search to find a 'best fit' to the measured data. Therewith we also have the phase shift function,  $\eta(t, k)$ , at each energy and so we can apply the fixed energy WKB scheme [3-5] at select single values of energy to define an inversion potential as well.

The fixed energy WKB scheme is based upon the Sabatier transform [1] whereby the inversion potential is defined in terms of a quasipotential, viz

$$V_{WKB}(r) = E \left[ 1 - e\left(\frac{-q(\sigma)}{E}\right) \right] \quad (9)$$

so long as there is a 1:1 correspondence between  $r$  and dimensionless variable  $\sigma$  from the transcendental equation

$$r = \frac{1}{k} \sigma e^{\left(\frac{Q(\sigma)}{2E}\right)}. \quad (10)$$

The quasipotential is defined from the deflection function,

$$\Theta(\lambda, k) = 2 \frac{d}{d\lambda} \eta(t(\lambda), k), \quad (11)$$

by the Abel integral transform [1],

$$\begin{aligned} Q(\sigma) &= \frac{2E}{\pi} \int_{\sigma}^{\infty} \frac{\Theta(\lambda, k)}{\sqrt{\lambda^2 - \sigma^2}} d\lambda \\ &= \frac{4E}{\pi} \frac{1}{\sigma} \frac{d}{d\sigma} \left( \int_0^{\infty} \frac{\eta(t(\lambda), k)}{\sqrt{\lambda^2 - \sigma^2}} \lambda d\lambda \right); \end{aligned} \quad (12)$$

an integral that is analytic if the S-function, which relates simply to the phase shift function, can be specified by one of a set of functions [11]. We have found that the rational form,

$$S(\lambda, k) = \prod_{n=1}^N \left( \frac{\lambda^2 - \beta_n^2}{\lambda^2 - \alpha_n^2} \right), \quad (13)$$

is particularly convenient as then

$$Q(\sigma) = 2iE \sum_{n=1}^N \left[ \frac{1}{\sqrt{\sigma^2 - \alpha_n^2}} - \frac{1}{\sqrt{\sigma^2 - \beta_n^2}} \right]. \quad (14)$$

This form of S-function has been used with success in WKB inversion studies of nuclear, atomic and molecular scattering (differential) cross sections [4,5] and we now apply it by finding the optimal smallest set of complex pole/zero pairs by a (second) chisquare fit to the relevant phase shift function, Eq.2, obtained from the total cross section data. A purely real inversion potential results by restricting the parameter values of the poles and zeroes in this form of quasipotential to be complex conjugate pairs.

### III. RESULTS OF DISCUSSION

The inversion procedures based upon the total cross sections from electron atom and electron molecule scattering have been used to determine inversion potentials for the interactions of electrons with Kr and Xe inert gas atoms [8] and with the CH<sub>4</sub> and SiH<sub>4</sub>

molecules [9,10]. Total (elastic scattering) cross section data for all have been taken in the range 70-80 eV up to 4 keV. The data were all fit using the two parameter form for the impact parameter function, Eq.7, and the optimal parameter values are listed for each case in the table. The measure of quality of fit is given in the first of the columns (designated 'data') listing chisquare per data point ( $\chi^2/N$ ) values. Inverting the impact parameter functions gives the phase shift functions per Eq.2 and to check that a quality fit to the data has been retained, those phase shift functions were used in the partial wave summations of Eq.1 to compare with the data a second time. The results of those comparisons are listed in the second column of  $\chi^2/N$  values, designated as 'refit' in the table. Clearly the adopted form for the phase shift function retains the quality of fit to data quite well and the integral formula Eq. 3 is therefore a reliable approximation with these data sets. The last column of  $\chi^2/N$  values are those we obtained by using the WKB inversion potential obtained from the phase shift functions at a fixed energy of 1000 eV to recalculate the total cross sections in the range 80 to 400 eV by direct solution of the Schrödinger equations. The column of numbers, designated 'inversion' reflect a retained quality of fit to the measured data. Those 'inversion' fits to the atomic and molecular scattering data are displayed in Fig. 1. Clearly they are particularly good for the higher energy data, notably with wave numbers in excess of  $10 \text{ \AA}^{-1}$ . To obtain the inversion (WKB) potentials, four pole/zero pairs were required in the specifying the rational form of the S-function so that the phase shifts were well fit (to better than 1 part in 10000) for all partial waves up to  $l = 200$ . Also, fixed energy WKB analyses were made at lower energies for the molecular scattering cases, at 100 and 400eV specifically, to note any residual energy dependence in the inversion potentials that might reflect upon the validity of the diverse approximations that have been used.

The results of our analyses of the molecular scattering data are shown in Fig. 2. In the main feature of the diagram, the WKB inversion potential (1000 eV) results are displayed by the solid and dashed curves respectively. They are virtually identical to the results one obtains by using the Miller prescription, Eq. 6. In this figure, the inversion results are also compared with theoretical calculations. The potential displayed by the dotted curve

is a sum of static, polarization and exchange potentials for the  $e^- - \text{CH}_4$  system [12] while the sum of static and polarization potentials for the  $e^- - \text{SiH}_4$  system [13] is given by the dot-dashed curve. The inversion potentials are evidently larger than the model calculations both for  $e^- - \text{CH}_4$  and  $e^- - \text{SiH}_4$  at radii greater than 1 a.u. but note that the ordinate scale is logarithmic. That stresses the smoothness of the two inversion potentials. The two theoretical model potentials have bumps due to the static components. The good fits of our inversion studies show that there is no evidence (data signature) in the total cross sections that such bumps need exist, but given that they are physical, then other data will be needed to test their attributes.

The results of our WKB fixed energy calculations at different energies are shown in the insert. There is practically no difference between the 400 and 1000 eV calculation results so that the implicit assumption that the underlying potential is energy independent is met. Further, the agreement indicates that the Eikonal approximation is very good at energies above 400eV. The 100 eV result does differ slightly and while we expect such as a breakdown of the high energy approximations of our inversion studies, that can also be a reflection of absorptive processes, ionisation in particular, being more important as well. In a mean field theory such are accounted by having complex, optical potentials.

The inversion and static (theoretical) potentials [14] for the scattering of electrons from the Kr and Xe atoms are displayed in Fig. 4. Therein the static potentials for  $e^- - \text{Kr}$  and  $e^- - \text{Xe}$ , displayed by the dotted and dot-dashed curves, are to be compared with the relevant inversion ones shown by the solid and dashed curves respectively. The theoretical interactions are stronger than our inversion ones at small radii ( $< 1.5$  a.u. for  $e^- - \text{Xe}$  and  $< 2$  a.u. for  $e^- - \text{Kr}$ ) but decrease much more rapidly at larger separations. Asymptotically it is known that the WKB fixed energy solutions vary as  $r^{-3}$  but that occurs at radii much larger than those for which the data are sensitive [5].

#### IV. CONCLUSION

Scattering potentials have been constructed by using inverse scattering theory with total (elastic scattering) cross section data. The theory used assumed those potentials to be real and energy independent and was implemented both in the Eikonal approximation proposed by Miller [6] and by the fixed energy WKB method that we have used in other studies. Both approaches were based upon a two parameter, monotonic form for the impact parameter function, with the WKB fixed energy scheme requiring a further mapping to specify S-functions of rational form. Good fits to the data from four interacting systems,  $e^- - \text{CH}_4$ ,  $e^- - \text{SiH}_4$ ,  $e^- - \text{Kr}$  and  $e^- - \text{Xe}$ , were found and reproduced after deducing the inversion potentials. Those potentials found by using the Miller and WKB schemes were essentially identical but they are quite different to those found by direct calculations. Other data is needed to resolve these differences and/or to validate as physical, structure observed in calculated interactions.



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## FIGURES

FIG. 1. Comparison of total cross section data from electron scattering from Xe and Kr atoms (top) and from CH<sub>4</sub> and SiH<sub>4</sub> molecules (bottom) compared with the results calculated by using the inversion potentials.

FIG. 2. The inversion potentials for e<sup>-</sup>-CH<sub>4</sub> (solid line) and e<sup>-</sup>-SiH<sub>4</sub> (dashed line) compared with the results of model calculations for e<sup>-</sup>-CH<sub>4</sub> (dotted line) and e<sup>-</sup>-SiH<sub>4</sub> (dot-dashed line). The insertion shows the inversion potentials obtained from the fixed energy set of phase shifts taken at 1000eV (solid line), 400eV (dashed line) and 100eV (dotted line) respectively.

FIG. 3. The inversion potentials for e<sup>-</sup>-Kr (solid line) and e<sup>-</sup>-Xe (dashed line) scattering compared with the calculated static potentials for Kr (dotted line) and Xe (dot-dashed line) respectively.

## TABLES

TABLE I. The parameter values of  $a$  and  $b$  in Eq. 7, and the three values of  $\chi^2/N$  from the three fitting processes that are described in the text

	a	b	$\chi^2/N$		
			data	refit	inversion
CH <sub>4</sub>	8.46209343E5	19.9649483	1.6	1.8	2.6
SiH <sub>4</sub>	2.52862651E6	23.4679661	0.7	1.0	1.3
Kr	3.66412950E7	50.3657858	0.15	0.37	0.43
Xe	2.56660989E8	77.9803248	1.2	1.9	1.2

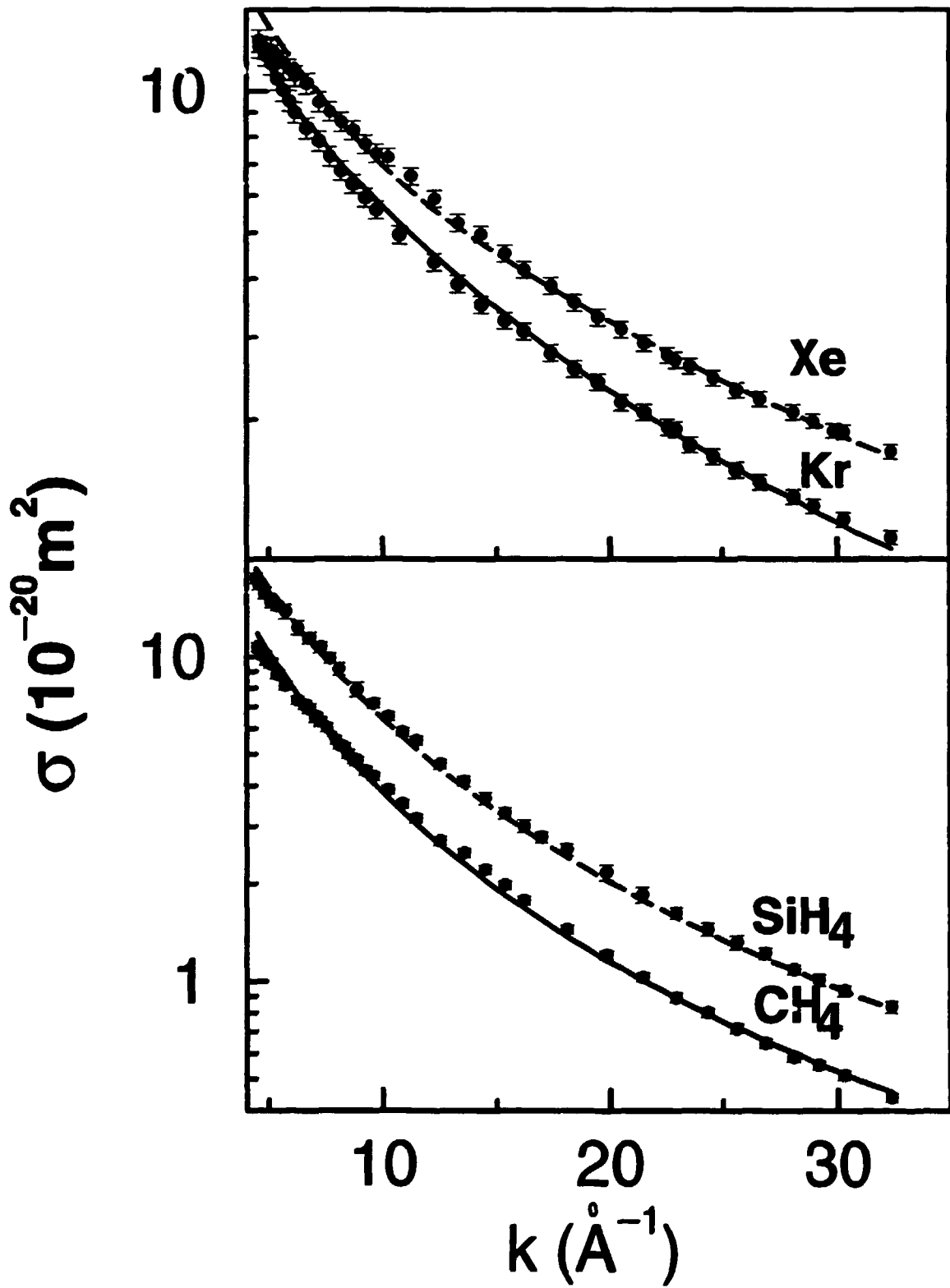


fig.1

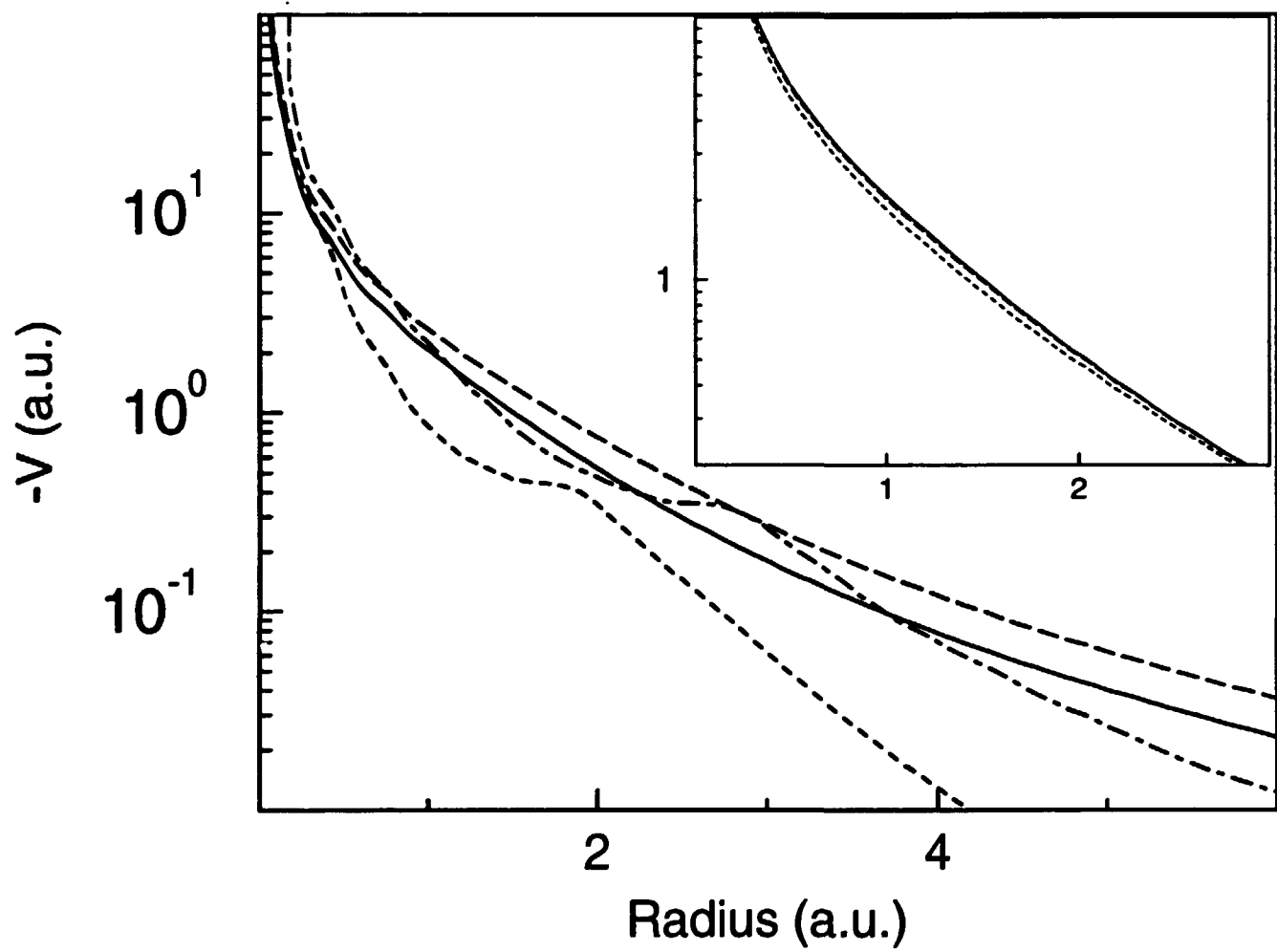


fig. 2

figs

