

# The Quantum Mechanical Inverse Scattering Problem at Fixed Energy and Some Recent Applications\*

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## Abstract

Much of the information on electronic, atomic, nuclear and particle physics is obtained in scattering experiments. The inverse scattering problem is to deduce the interaction between the colliding particles, or what their constitution is, from the observed data. Inverse scattering techniques at fixed energy which have lent themselves to practical application are reviewed. Some recent applications, in particular to electron–atom scattering, are discussed. New results for e–He scattering at 30 eV are presented.

## 1. Introduction

Much of what we know about electronic, atomic, nuclear and particle physics is information gathered from scattering experiments. Inferring the structure of particles involved in the experiment or, as is often the case, the nature of the interaction between the particles, is an inverse problem. The quantum mechanical inverse scattering problem is one of long standing. The recent text by Chadan and Sabatier (1989) summarises the general status of the field admirably. Here we confine ourselves to the inverse problem at fixed energy as opposed to the idea of constructing the underlying potential from a single phase shift, given for all energies. The latter approach is intrinsically unnatural and unsatisfactory since this information is not available at all energies and the assumed nonrelativistic kinematics are no longer valid at high energies. We initially mention those fixed energy inversion methods which have lent themselves to practical applications and then consider two of these in more detail.

The Newton–Sabatier method, reviewed by Chadan and Sabatier (1989), was applied to practical problems by Coudray (1977), with later modifications by Münchow and Scheid (1980) and applications to heavy ion scattering by May *et al.* (1984).

The inverse problem at fixed energy can also be solved by discretisation of the Schrödinger equation using finite difference methods. Early work here was due to Case and Kac (1973) and Case (1973). Subsequent developments are due to Zacharév and co-workers (1977) and Hooshyar *et al.* (1982, 1984). Hooshyar *et al.* have applied their method to  $n^{-16}\text{O}$  and  $n^{-40}\text{Ca}$  scattering at low

\* Dedicated to Professor Ian McCarthy on the occasion of his sixtieth birthday.

energies and to nucleon–nucleon scattering. Numerical and other difficulties are encountered at high energies. Inversion techniques, based initially on the fixed energy analogue of the Bargmann (1949) potentials, have been developed and applied with considerable success by Lipperheide, Fiedeldey and co-workers (Lipperheide and Fiedeldey 1978, 1981; Bürger *et al.* 1983; Naidoo *et al.* 1984; Leeb *et al.* 1985; Lipperheide *et al.* 1985).

The semiclassical WKB approach to fixed energy inversion was discussed in detail by Vollmer (1969) with application to atom–atom scattering data. Kujawski (1973) applied semiclassical inversion to real data obtained from scattering of 104 MeV  $\alpha$  particles by  $^{12}\text{C}$  and  $^{90}\text{Zr}$ . Inversion of molecular scattering data using semiclassical methods was reviewed by Buck (1974). This approach requires a smooth interpolation of the phase shifts and that used in the Lipperheide–Fiedeldey quantal inversion method has been used with considerable success for WKB inversion—for example Fiedeldey *et al.* (1984) and Allen and Bürger (1984). Ambiguities associated with semiclassical analysis have been discussed by Cuer (1979).

Other inversion methods at fixed energy which have led to numerical methods are those due to Malyarov *et al.* (1975), the 'peeling' inversion method due to Shapiro and Gerber (1976) and the variational approach of Kermode *et al.* (1986).

As emphasised by Chadan and Sabatier (1989) the solution of an inverse scattering problem involves the consideration of all possible solutions. Aspects of the ill-posedness of the problem, and methods which allow us to select physically meaningful solutions (regularisation) are crucial, as has been reviewed by Sabatier (1985) and Turchin (1985).

In the next section we outline two of the fixed energy inversion methods which have been particularly successful in terms of applications, namely the Lipperheide–Fiedeldey and WKB inversion techniques.

## 2. Fixed Energy Inversion

### (a) Lipperheide–Fiedeldey Quantal Inversion

The simplest of the methods developed and applied by Lipperheide, Fiedeldey and co-workers (Lipperheide and Fiedeldey 1978; Bürger *et al.* 1983) is based on the following representation for the scattering function:

$$S_{\text{rat}}(\lambda) = \prod_{n=1}^N \frac{\lambda^2 - \beta_n^2}{\lambda^2 - \alpha_n^2}, \quad (1)$$

where  $\lambda = l + \frac{1}{2}$  and the  $\alpha_n$  and  $\beta_n$  are complex parameters (for the case of a real potential  $\beta_n = \alpha_n^*$ ). Using this representation we can interpolate between  $2N$  phase shifts at the physical  $l$  values by means of  $N$  pairs of parameters  $\{\alpha_n, \beta_n\}$ . However, the conditions  $\text{Im} \alpha_n^2 > 0$ ,  $\text{Im} \beta_n^2 < 0$  must be satisfied if one is to obtain a regular potential.

The potential  $V(r)$  is determined iteratively:

$$V(r) = V_N(r), \quad (2)$$

where

$$V_n(r) = V_{n-1}(r) + V^{(n)}(r), \quad n = 1, 2, \dots, N, \quad (3)$$

$$V^{(n)}(r) = \frac{2}{r}(\beta_n^2 - \alpha_n^2) \frac{d}{dr} \left\{ \frac{1}{r} \left( \frac{1}{\{L_{\beta_n}^{n-1}(r)\}^- - \{L_{\alpha_n}^{n-1}(r)\}^+} \right) \right\}. \quad (4)$$

The  $\{L_\lambda^n(r)\}^\pm$  are the logarithmic derivatives of the Jost solutions  $\{f_\lambda^n(r)\}^\pm$  to the potential  $V_n(r)$ . In the case where  $\text{Im} \alpha_n^2 < 0$  or  $\text{Im} \beta_n^2 > 0$  we must use a nonrational scattering function of the form

$$S_{\text{nonrat}}(\lambda) = \left\| \frac{\sigma_{\beta_n}^{(0)} - \sigma_{\alpha_m}^{(0)}}{\beta_n^2 - \alpha_m^2} - \frac{\sigma_\lambda^{(0)} - \sigma_{\alpha_m}^{(0)}}{\lambda^2 - \alpha_m^2} \frac{\sigma_{\beta_n}^{(0)}}{\sigma_\lambda^{(0)}} \right\| \left/ \left\| \frac{\sigma_{\beta_n}^{(0)} - \sigma_{\alpha_m}^{(0)}}{\beta_n^2 - \alpha_m^2} - \frac{\sigma_\lambda^{(0)} - \sigma_{\alpha_m}^{(0)}}{\lambda^2 - \alpha_m^2} \right\| \right., \quad (5)$$

with  $\sigma_\lambda^{(0)} = \exp\{-i\pi(\lambda - \frac{1}{2})\}$ . In this case the  $\{L_\lambda^n(r)\}^\pm$  are the logarithmic derivatives of the regular solutions  $\phi_\lambda^n(r)$ . Fitting phase shifts to the nonrational scattering function directly is not always straightforward. However, if  $|\text{Im} \alpha_n|, |\text{Im} \beta_n|$  are sufficiently large (approximately  $\geq 2$ ) then  $S_{\text{nonrat}}(\lambda) = S_{\text{rat}}(\lambda)$  for real  $\lambda$ , so that the fitting can be done via equation (1), which is straightforward. The two schemes can be combined by writing  $S(\lambda)$  as a product of rational and nonrational scattering functions (Naidoo *et al.* 1984).

The error in the (complex) potential is given by (Leeb *et al.* 1985)

$$(\Delta V(r))_e^2 = \langle [\Delta V(r)]^2 \rangle = \sum_{n,m=1}^{4N} \frac{\partial V(r)}{\partial a_n} \frac{\partial V(r)}{\partial a_m} \Big|_{\hat{a}} \epsilon_{nm}, \quad (6)$$

where  $\mathbf{a} = \{a_n\}$  is the set of all the real and imaginary parts of the  $2N$  complex parameters  $\alpha_n$  and  $\beta_n$ , and  $\epsilon_{nm}$  is an error matrix. For a real potential the sum runs to  $2N$ .

(b) WKB Inversion

The phase shifts in the WKB approximation are given in terms of the quasipotential  $Q(\sigma)$  by (Vollmer 1969):

$$\delta(\lambda) = \frac{1}{2i} \ln S(\lambda) = \frac{1}{2E} \int_\lambda^\infty \frac{Q(\sigma) d\sigma}{(\sigma^2 - \lambda^2)^{\frac{1}{2}}}, \quad (7)$$

where  $E$  is the centre-of-mass energy. Conversely, the quasipotential is given in terms of the phase shift  $\delta(\lambda)$  by

$$Q(\sigma) = \frac{4E}{\pi} \frac{1}{\sigma} \frac{d}{d\sigma} \int_\sigma^\infty \frac{\delta(\lambda) d\lambda}{(\lambda^2 - \sigma^2)^{\frac{1}{2}}} d\lambda. \quad (8)$$

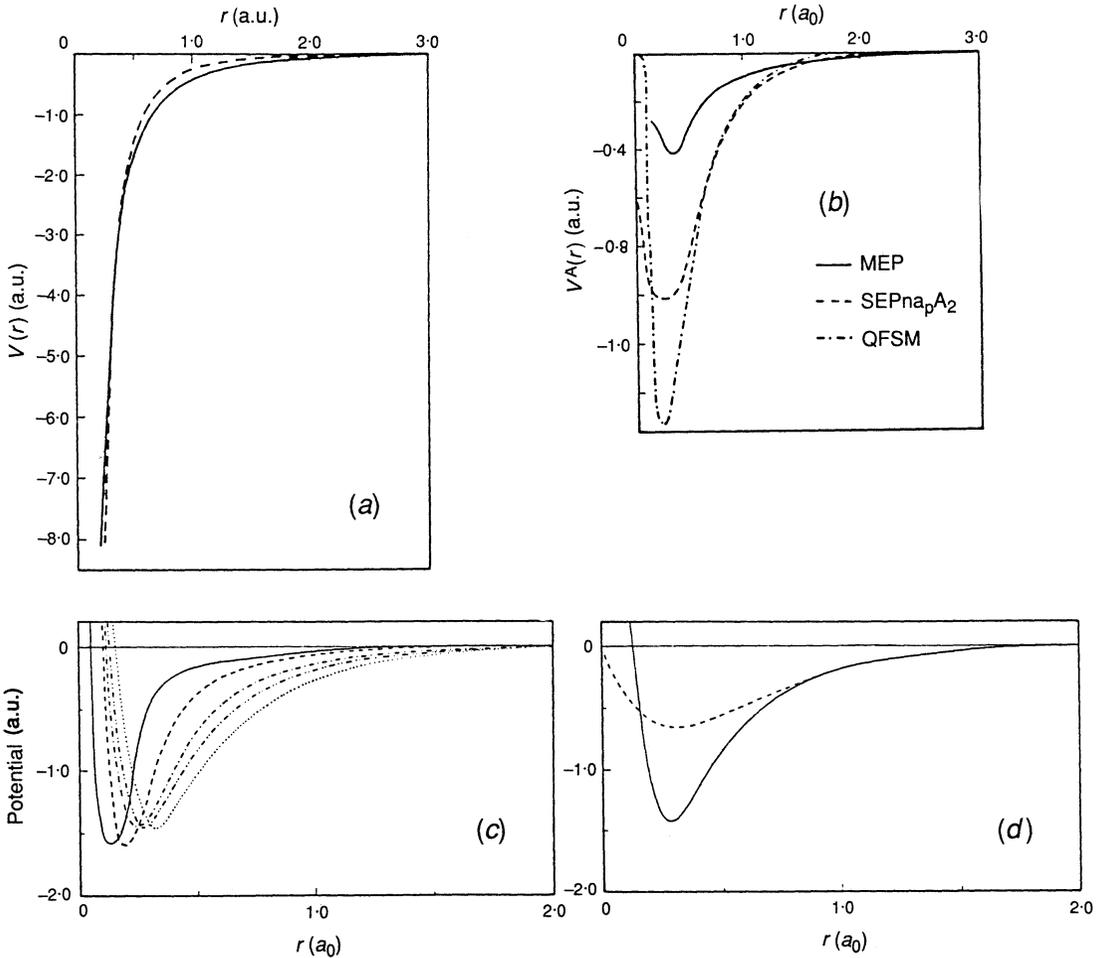
The potential  $V(\rho)$  is related to  $Q(\sigma)$  by

$$V(\rho) = E[1 - \exp\{Q(\sigma)/E\}], \quad (9)$$

where

$$\rho = \sigma \exp[Q(\sigma)/2E], \quad (10)$$

with  $\rho = kr$ . Using the representation equation (1),  $Q(\sigma)$  can be found analytically (Fiedelney *et al.* 1984) as well as the partial derivatives in equation (7) (Allen 1986).



**Fig. 1.** (a) Inverted potentials obtained by quantum mechanical inversion for e-He scattering at 19 eV (solid curve) and 2 eV (dashed curve).

(b) Comparison of the absorptive parts  $V^A(r)$  of the potential obtained by inversion from the MEP model, the  $SEPn_pA_2$  potential, and the QFSM potential for e-He scattering at 200 eV.

(c) Local exchange potentials for e-He scattering obtained by inversion which are exact within the static exchange approximation at 19 eV (dotted curve), 30 eV (dash-double dot), 50 eV (dash-dot), 100 eV (dashed), and 200 eV (solid).

(d) Local exchange potential for e-He scattering at 30 eV (solid curve) obtained by inversion compared with the exchange potential of Furness and McCarthy (1973) at the same energy (dashed curve).

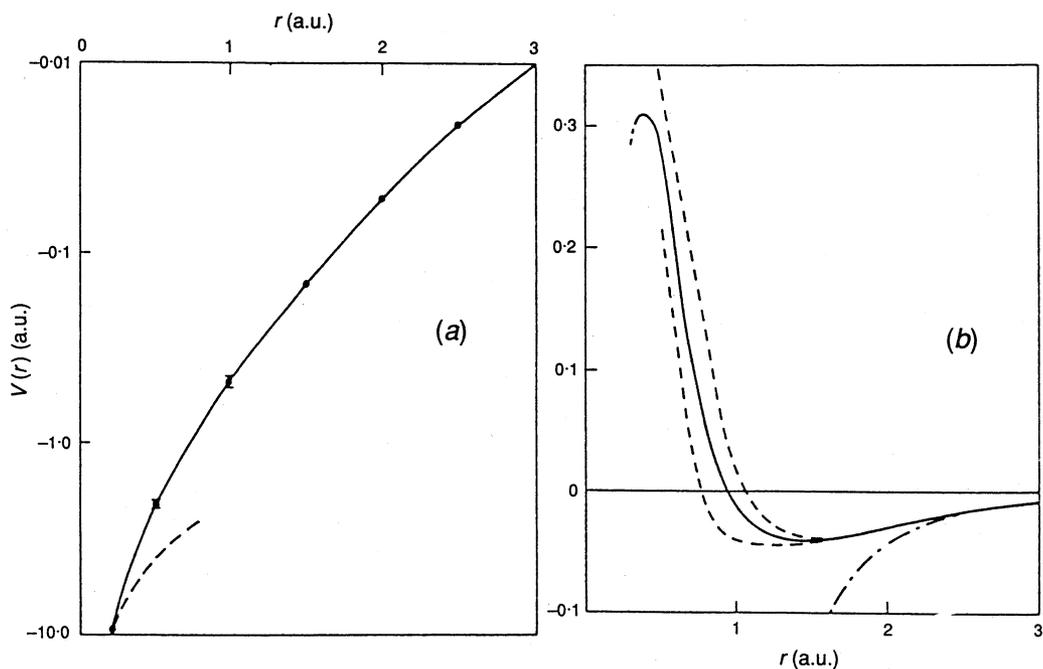
### 3. Applications to Electron–Atom Scattering

Inverse scattering techniques were first applied to electron–atom scattering by Bürger *et al.* (1983) who used both fully quantal Lipperheide–Fiedeldej and semiclassical WKB inversion methods to obtain local potentials for e–He scattering for incident energies of 2 and 19 eV. The quantum mechanical results are shown in Fig. 1*a*. These potentials, obtained without any *a priori* assumptions about their analytic form, are in agreement with our physical expectations both in the tail and at short range. The incoming electron sees a polarisation potential at large distances and the Coulomb potential due to the nuclear protons at small distances (see Bürger *et al.* 1983 for these comparisons). There is a weak energy dependence of the local potential at intermediate distances which is a manifestation of the nonlocal exchange interaction.

Semiclassical WKB inversion of phase shifts for e–He scattering at 200 and 400 eV, calculated using matrix effective potentials (MEPs) by Thirumalai *et al.* (1982), was subsequently carried out by Allen and Bürger (1984). The absorptive parts of these equivalent local potentials (ELPs) were then compared with several competing local models for absorption such as the quasi-free scattering model (QFSM) of Staszewska *et al.* (1983). This comparison at 200 eV is shown in Fig. 1*b* where it is seen that the MEP is considerably shallower than the other models but that the minima in all the potentials occur at about the same distance from the nucleus. The energy dependence of the absorptive potential manifested itself in a deeper potential at 400 eV than at 200 eV and the radius for preferential absorption was closer to the nucleus. These results are reasonable physically and agree qualitatively with the QFSM absorption potentials of Staszewska *et al.* (1983).

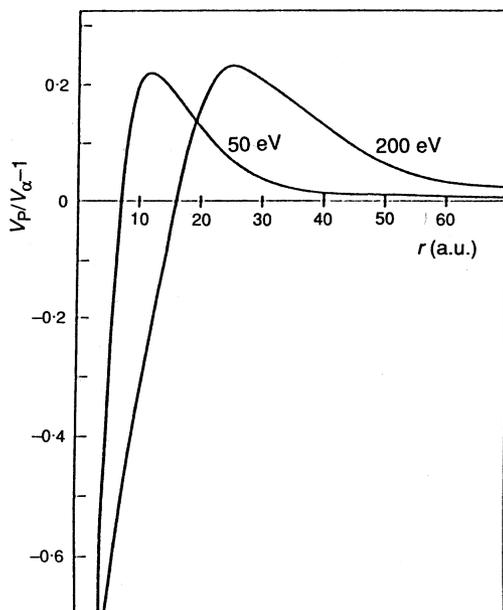
The quantum mechanical inverse scattering method was used by Holler and Allen (1986) to find local exchange potentials, exact within the context of the static exchange model, for intermediate energy electron–atom scattering. The potentials and their energy dependence are shown in Fig. 1*c* and a comparison with the semiclassical exchange potential of Furness and McCarthy (1973) is made in Fig. 1*d*.

Further developments to the quantum mechanical inversion by Leeb *et al.* (1985) allowed a rigorous analysis of the confidence intervals on the potential, taking into account the errors on the measured differential cross section. As shown by Allen (1986), within the WKB approximation, much of this error analysis can be done analytically with considerable saving in computational complexity and time. This formalism was employed to show, from the e–He data of Andrick and Bitsch (1975) at 19 eV, that the data imply that the polarisation potential behaves like  $-\alpha/r^4$  for large  $r$ , in agreement with the adiabatic polarisation potential. This WKB technique, coupled to the methods of statistical regularisation, was employed by Allen and McCarthy (1987) to extract, in a rigorous way, the local potential with error bars for e–He scattering at 19 eV, as shown in Fig. 2*a*. In obtaining this result, statistical regularisation was applied, giving equal weighting to the variational phase shifts of Nesbet (1979) (the Philipps condition). The long standing question of the behaviour of the (local) polarisation potential at short distances was addressed in this paper. The polarisation potential at short distances, shown in Fig. 2*b*, was found to be less attractive than the full adiabatic polarisation potential, as

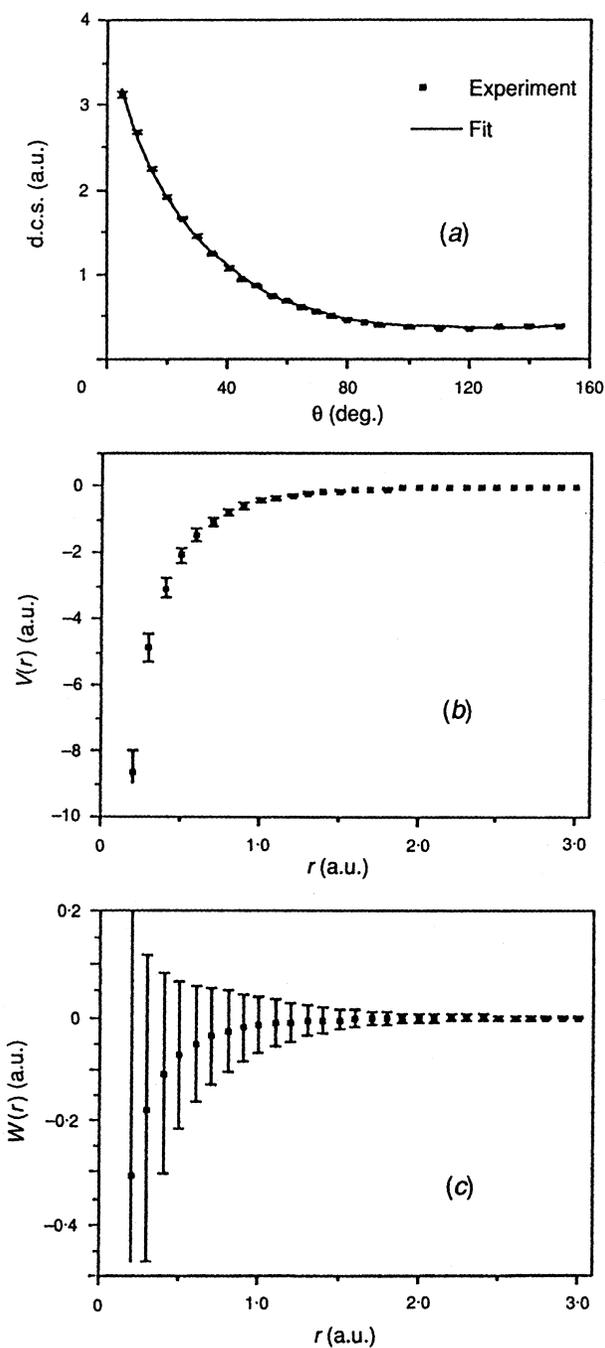


**Fig. 2.** (a) Potential for e-He scattering obtained by inversion at 19 eV when the Philipps condition is satisfied. The dashed curve shows the Coulomb potential.

(b) Polarisation potential for e-He scattering at 19 eV obtained by subtracting out the local static exchange potential from Holler and Allen (1986) (see Fig. 1c) from the potential shown in (a). The dashed curves indicate the confidence intervals. The dash-dot curve indicates the adiabatic polarisation potential  $-\alpha/2r^4$  ( $\alpha = 1.38$  a.u.).



**Fig. 3.** Phase-equivalent local potential  $V_p(r)$  for electron elastic scattering from the hydrogen 1s, 2p system plotted as  $V_p/V_\alpha - 1$  for comparison with the adiabatic potential at 50 and 200 eV.



**Fig. 4.** (a) Fit to smoothed e-He elastic differential cross section data at 30 eV using a scattering function of the form given by equation (1). (The Philipps condition is satisfied—see text.)

(b) Real part of potential obtained from the data in (a) by inversion, showing error bars.

(c) Imaginary part of potential obtained from the data in (a) by inversion, showing error bars.

discussed by McEachran and Stauffer (1983). In fact it exhibits a behaviour at short distances remarkably similar to the extended polarisation potential of Callaway *et al.* (1968).

The work just discussed prompted a theoretical investigation of the polarisation potential for dipole excitations by Allen *et al.* (1988). Here inversion techniques were employed to construct phase-equivalent local potentials to the nonlocal polarisation potential—see Fig. 3 where the phase-equivalent local polarisation potential for hydrogen is compared with the local adiabatic potential  $-\alpha/r^4$  at 50 and 200 eV.

#### 4. Application to e-He Scattering at 30 eV

In this section we present results for potentials obtained by inversion from elastic e-He scattering data at 30 eV. The starting point is the elastic differential cross section data of Brunger *et al.* (1990), normalised to and supplemented by the data of Register *et al.* (1980) in the angular range 100–150°. The parametrised phase shift analysis has been carried out as described by Leeb *et al.* (1985) and Allen and McCarthy (1987) using the parametrisation given by equation (1) and applying statistical regularisation. The data have been smoothed *a priori* using the technique described in Allen *et al.* (1987). In practice this meant that three data points were moved by 0.25 of a degree to eliminate nonstatistical errors (within the estimated errors on the angles). This 'smoothed' data set gave  $\chi^2 = 1.253$ . Statistical regularisation was applied, using the SEPna<sub>p</sub>A<sub>3</sub> model [static, exchange, polarisation, nonadiabatic, perturbative (polarisation potential), A<sub>3</sub> model for absorption] of Thirumalai *et al.* (1982) as *a priori* data. This gave a final  $\chi^2 = 1.76$  (the Philipps condition being satisfied). The experimental points and the fit for this  $\chi^2$  value are shown in Fig. 4a.

**Table 1. Experimental phase shifts for e-He scattering at 30 eV obtained using the parametrised and regularised phase shift analysis described in the text**

$l$	Re( $\delta_l$ )	Im( $\delta_l$ )	SEPna <sub>p</sub> A <sub>3</sub> <sup>A</sup>
0	1.600±0.038	0.038±0.042	1.521+i0.013
1	0.380±0.012	0.017±0.012	0.308+i0.029
2	0.090±0.004	0.002±0.006	0.068+i0.010

<sup>A</sup> Thirumalai *et al.* (1982).

**Table 2. Experimental integral elastic and absorptive cross sections and total cross sections compared with previously obtained experimental and theoretical values**

Cross section	Present work	Register <i>et al.</i> (1980)	Kennerly and Bonham (1978)	de Heer and Jansen (1977)
Q <sub>el</sub>	7.86±0.09	7.54	—	7.98
Q <sub>abs</sub>	0.41±4.31	—	—	0.81
Q <sub>tot</sub>	8.26±4.25	—	8.43	8.79

The phase shifts obtained, together with the associated statistical errors, are shown in Table 1, where they are compared with the SEPna<sub>p</sub>A<sub>3</sub> model. The elastic, absorptive and total cross sections are given in Table 2 where they are compared with previous results. The elastic cross section is well

determined by the scattering data, while the absorptive cross section, which is expected to be small at this energy, is not.

The interaction potential obtained by regularised inversion from the data is shown in Figs 4*b* and 4*c*. The real part of the potential is well determined by the data. However, the error bars on the relatively shallow absorptive part of the potential become large inside about one Bohr radius. Measurements of the differential cross section with smaller statistical uncertainties, over as wide a range of scattering angles as possible and at smaller intervals in the angle, would significantly improve these error bars (and also the large error bar on the absorptive cross section).

The inversion yields a local potential, whilst the underlying interaction is of course nonlocal. However, information on the nonlocality could be obtained from experiments done over a small energy range by examining the energy dependence of the local potential, which in principle allows one to extract information on the nonlocality (Fiedelley *et al.* 1985, 1986).

## 5. Conclusions

Inverse scattering methods at fixed energy leading to numerical results have been reviewed with two of the more successful approaches (the Lipperheide–Fiedelley and semiclassical WKB approaches) receiving particular attention. Phase shift analysis coupled with these inverse scattering techniques provides a rigorous way to extract physical information directly from experimental data. Statistical regularisation methods allow us to do this in a way consistent with our *a priori* knowledge of the problem.

We have discussed some previous applications of inverse scattering methods to e–He scattering and presented here for the first time a potential (with error bars) for e–He scattering at 30 eV extracted from scattering data in a rigorous way.

## References

- Allen, L. J. (1986). *Phys. Rev. A* **34**, 2706.  
 Allen, L. J., Bray, I., and McCarthy, I. E. (1988). *Phys. Rev. A* **37**, 49.  
 Allen, L. J., Brunger, M. J., McCarthy, I. E., and Teubner, P. J. O. (1987). *J. Phys. B* **10**, 3741.  
 Allen, L. J., and Bürger, H. (1984). *Phys. Rev. A* **30**, 1237.  
 Allen, L. J., and McCarthy, I. E. (1987). *Phys. Rev. A* **36**, 2570.  
 Andrick, D., and Bitsch, K. (1975). *J. Phys. B* **8**, 393.  
 Bargmann, V. (1949). *Rev. Mod. Phys.* **21**, 488.  
 Brunger, M. J., McCarthy, I. E., Ratnavelu, K., Teubner, P. J. O., Weigold, A. M., Zhou, Y., and Allen, L. J. (1990). *J. Phys. B* **23**, 1325.  
 Buck, U. (1974). *Rev. Mod. Phys.* **46**, 369.  
 Bürger, H., Allen, L. J., Fiedelley, H., and Sofianos, S. A. (1983). *Phys. Lett. A* **97**, 39.  
 Callaway, J., LaBahn, R. W., Pu, R. T., and Duxler, W. M. (1968). *Phys. Rev.* **168**, 12.  
 Case, K. M. (1973). *J. Math. Phys.* **14**, 916.  
 Case, K. M., and Kac, M. (1973). *J. Math. Phys.* **14**, 594.  
 Chadan, K., and Sabatier, P. C. (1989). 'Inverse Problems in Quantum Scattering Theory' (Second Edition) (Springer: New York).  
 Coudray, C. (1977). *Lett. Nuovo Cim.* **19**, 319.  
 Cuer, M. (1979). *Ann. Phys.* **120**, 1.  
 de Heer, F. J., and Jansen, R. H. J. (1977). *J. Phys. B* **10**, 3741.  
 Fiedelley, H., Lipperheide, R., Naidoo, K., and Sofianos, S. A. (1984). *Phys. Rev. C* **30**, 434.  
 Fiedelley, H., Sofianos, S. A., Allen, L. J., and Lipperheide, R. (1985). *Phys. Rev. A* **32**, 3095.  
 Fiedelley, H., Sofianos, S. A., Allen, L. J., and Lipperheide, R. (1986). *Phys. Rev. C* **33**, 1581.

- Furness, J. D., and McCarthy, I. E. (1973). *J. Phys. B* **6**, 2280.
- Holler, E. W., and Allen, L. J. (1986). *Phys. Rev. A* **33**, 3774.
- Hooshyar, M. A., and Razavy, M. (1984). *Phys. Rev. C* **29**, 20.
- Hooshyar, M. A., Nadeau, R., and Razavy, M. (1982). *Phys. Rev. C* **25**, 1187.
- Kennerly, R. E., and Bonham, R. A. (1978). *Phys. Rev. A* **17**, 1844.
- Kermode, M. W., Cooper, S. G., and Allen, L. J. (1986). *Inverse Problems* **2**, 353.
- Kujawski, E. (1973). *Phys. Rev. C* **8**, 100.
- Leeb, H., Fiedeldey, H., and Lipperheide, R. (1985). *Phys. Rev. C* **32**, 1223.
- Lipperheide, R., and Fiedeldey, H. (1978). *Z. Phys. A* **286**, 45.
- Lipperheide, R., and Fiedeldey, H. (1981). *Z. Phys. A* **301**, 81.
- Lipperheide, R., Fiedeldey, H., and Leeb, H. (1985). *Lecture Notes in Physics* **236**, 249.
- McEachran, R. P., and Stauffer, A. D. (1983). *J. Phys. B* **16**, 255.
- Malyarov, V. V., Poplavskii, I. V., and Popushoi, M. N. (1975). *Sov. Phys. JETP* **41**, 210.
- May, K.-E., Münchow, M., and Scheid, W. (1984). *Phys. Lett.* **141**, 1.
- Münchow, M., and Scheid, W. (1980). *Phys. Rev. Lett.* **44**, 1299.
- Naidoo, K., Fiedeldey, H., Sofianos, S. A., and Lipperheide, R. (1984). *Nucl. Phys. A* **419**, 13.
- Nesbet, R. K. (1979). *Phys. Rev. A* **20**, 58.
- Register, D. F., Trajmar, S., and Srivastava, S. K. (1980). *Phys. Rev. A* **21**, 1134.
- Sabatier, P. C. (1985). *Lecture Notes in Physics* **236**, 1.
- Shapiro, M., and Gerber, R. B. (1976). *Chem. Phys.* **13**, 235.
- Staszewska, G., Schwenke, D. W., Thirumalai, D., and Truhlar, D. G. (1983). *Phys. Rev. A* **28**, 2740.
- Thirumalai, D., Truhlar, D. G., Brandt, M. A., Eades, R. A., and Dixon, D. A. (1982). *Phys. Rev. A* **25**, 2946.
- Turchin, V. F. (1985). *Lecture Notes in Physics* **236**, 33.
- Vollmer, G. (1969). *Z. Phys.* **226**, 423.
- Zakharév, B. N., Mel'nikov, V. N., Rudyak, B. V., and Suz'ko, A. A. (1977). *Sov. J. Part. Nucl.* **8**, 120.