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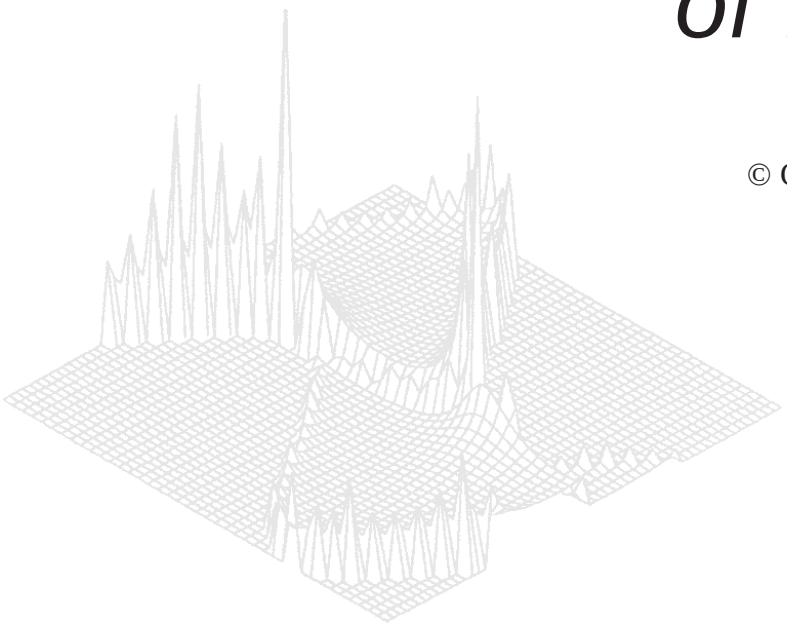
Australian Journal of Physics

Volume 50, 1997



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Aust. J. Phys., 1997, **50**, 473–82

Quantitative Theory and Accurate Experiments: Low-energy Electron Scattering by He and H_2 as Case Studies*

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Abstract

Accurate low-energy electron scattering data are needed in many fields of physics. However, accurate experiments are difficult to design and to carry out. By 1967 low-energy electron–He cross sections had been measured by two different techniques, designed to provide accurate data. Unfortunately, the data differed by amounts well outside the estimated error bars. Despite the relative simplicity of the He atom, decisive theoretical calculations on the e–He system could not be done with methods available in 1967. After a decade of development of theoretical methodology it became possible in 1979 to carry out calculations with absolute estimates of residual error limits. The results were found to agree closely with the momentum transfer cross section deduced from electron swarm data and with recent beam data by improved techniques, but were inconsistent with the original beam data of 1965. More recently, a similar conflict exists between data measured for electron-impact vibrational excitation of the hydrogen molecule by electron swarm and beam techniques. This conflict has persisted despite great progress in beam scattering techniques and in theoretical methods. A brief review of the relevant electron scattering theory will be given.

1. Introduction

Absolute values of electron scattering cross sections are needed in many subfields of physics, either to serve as a calibration standard for measurement apparatus or as input data to dynamical models of complex excited media ranging from stellar atmospheres to laser systems. Atomic He and molecular H_2 are candidates for basic standards because they are easily used in the laboratory and lend themselves to accurate theory.

Progress up to 1971 in absolute measurements and theory of total and momentum-transfer cross sections for low energy electron–He scattering was reviewed by Bederson and Kieffer (1971). For He, the low energy range extends to the first excitation threshold at $19{\cdot}818$ eV. As of 1971, two absolute measurements using different techniques had obtained results that lay outside each other's error estimates, and theory had not developed far enough to be able to resolve this difference. Developments in experimental and theoretical methodology up to this date will be summarised in Section 2 here. In the following decade, theoretical methods were developed capable of giving results within the experimental error bars. At the end of this period, new experimental techniques also evolved that

* Dedicated to Professor Robert W. Crompton on the occasion of his seventieth birthday.

10.1071/PH96068 0004-9506/97/030473$05.00

significantly reduced the experimental uncertainty. The low energy data reviewed by Nesbet (1980) have remained a generally accepted standard since that time. The theoretical and experimental methods developed in the decade between these two reviews will be outlined in Section 3.

The step from He, the simplest closed-shell atom, to molecular hydrogen, the simplest molecule, is far from trivial either for theory or experiment. Although data from theory and experiment are consistent for purely rotational excitation, in analogy to the situation for He, it became clear by 1987 that there was a significant discrepancy between theory and experiment for cross sections starting at the first vibrational excitation threshold (Morrison *et al.* 1987). New and very carefully designed experimental measurements were carried out and successfully compared with refined theoretical calculations, strongly indicating that the discrepancy in data would be eliminated (Buckman *et al.* 1990) if the electron swarm data could be rejected. The latter question remains unresolved, and a recent experiment has confirmed and extended the validity of the swarm data. This situation is discussed in Section 4, together with a discussion of the theoretical resources available for quantifying vibrational excitation. At present, theory by itself cannot yet claim to produce definitive results for molecular vibrational excitations, with well-defined error estimates.

2. e–He: 1967

Bederson and Kieffer (1971) reviewed the status of absolute measurements of low energy electron–helium scattering cross sections. Two experiments by different techniques were considered by their design and error analyses to provide the most reliable data. The first experiment (Golden and Bandel 1965) used an updated version of the original apparatus of Ramsauer (1921). An electron beam in a perpendicular static magnetic field passes through an energy selector into a scattering sector. Transmitted electronic current and scattered current are measured separately, and their ratio, together with the path length through the scattering sector and the scattering gas density, determine the absolute total cross section at the selected energy. Data were obtained by Golden and Bandel for energies from $0{\cdot}4$ to 28 eV, with an estimated probable error of $\pm 3\%$. The largest single probable error, $\pm 2\%$, is due to uncertainty of the gas pressure.

The second experiment (Crompton *et al.* 1967) used an electron swarm technique to determine the absolute momentum-transfer cross section over a range of electron energies. Steady-state values of the drift velocity, the ratio of diffusion coefficient to mobility, and the magnetic drift velocity were determined in a drift tube for accelerating potentials corresponding to ratios E/N of electric field strength to gas number density in a range that allowed determination of the momentum-transfer cross section for electrons with kinetic energies from $0{\cdot}02$ to $3{\cdot}0$ eV. Statistical theory is required to relate the measured transport data to electron scattering cross sections. This requires solution of the Boltzmann equation for a nonequilibrium steady state to determine the electronic distribution function, giving number density as a function of electron kinetic energy. Below the threshold for excitation processes, only the elastic momentum-transfer cross section enters the derived formulas for the measured transport properties as a function of E/N. Crompton *et al.* estimated the error in their derived cross sections to be less than $\pm 2\%$.

In terms of the differential cross section $d\sigma/d\Omega$ as a function of scattering angle, the total cross section is defined as

$$\sigma_T = \int (d\sigma/d\Omega) d\Omega \,, \tag{1}$$

while the momentum-transfer cross section is

$$\sigma_M = \int (d\sigma/d\Omega)(1 - \cos\theta) d\Omega \,. \tag{2}$$

The additional factor arises from scattering into the electron beam in a material with many scattering centres. In order to compare accurate experimental data for σ_T and σ_M, the differential cross section must be known to comparable accuracy. This requirement is somewhat reduced by noting that the ratio σ_M/σ_T is unity for isotropic scattering (hence in the limit of zero energy), so that only the significantly smaller ratio $\int (d\sigma/d\Omega)\cos\theta / \int (d\sigma/d\Omega)$ is required, with correspondingly reduced relative accuracy. At the time of these measurements, theoretical calculations of electron–helium cross sections had been reported by LaBahn and Callaway (1966), who used a version of the polarised orbital method (described below) to model target polarisation response. Using these calculations, the most accurate available at that time, to deduce σ_M from the values of σ_T measured by Golden and Bandel, Crompton *et al.* found that their values of σ_M exceeded those deduced from the Golden–Bandel data by approximately 10% over the energy range common to both experiments.

Following up the original swarm experiment of 1967, Crompton *et al.* (1970*a*) measured drift velocities at 77 K, obtaining results in agreement with the 1967 experiment within 1%, and extending the scattering energy range down to $0 \cdot 008$ eV. This made it possible to compare the indicated momentum-transfer cross section with an analytic formula derived using effective range theory (O'Malley 1963). In the lowest energy range ($0 \cdot 008$–$0 \cdot 1$ eV), the data of Crompton *et al.* implied a value $1 \cdot 18 a_0$ (Bohr units) for the scattering length, defined as minus the threshold limit of the ratio of s-wave phase shift to the electron wave number. In retrospect, this agrees very closely with the value $1 \cdot 1835 a_0$ obtained with an estimated accuracy of $0 \cdot 5$% by accurate variational calculations whose results were adjusted to be consistent with the current recommended experimental value of the static electric dipole polarisability of He (Nesbet 1980). This comparison suggests that the actual residual error in these swarm experiments was much smaller than the published estimate of 2%. It is interesting to note that O'Malley (1963) deduced a value of $1 \cdot 19 a_0$ for the scattering length, combining measurements of σ_T by Ramsauer and Kollath (1929, 1932) with the known value of the dipole polarisability, and averaging out low-energy fluctuations in these data, now known to be an artifact. Neither the Golden and Bandel data nor that of Crompton *et al.* showed these low-energy structures. An extrapolation to lower energies of the Golden–Bandel data (Golden 1966) gave $1 \cdot 15 a_0$ for the scattering length.

A refined version of the polarised orbital method (EPOM, for extended polarised orbital method) was used by Callaway *et al.* (1968) to compute electron–He cross sections, which were compared to both the beam and swarm data. Bederson and Kieffer used phase shifts from these calculations to convert σ_M from the

swarm data to σ_T. This transformed total cross section was found to be in good agreement with the direct EPOM calculation (within 6%), while the Golden–Bandel cross section was about 9% less than the transformed swarm data. An independent theoretical calculation, using a variational method that takes polarisation response into account (Michels *et al.* 1969), was in close agreement with the EPOM calculations, and much closer to the swarm data than to the Golden–Bandel cross section.

Reviewing this situation in 1971, Bederson and Kieffer found that neither set of experimental data could be rejected. However, the theory required for interconversion of σ_T and σ_M was sufficiently accurate to imply a true inconsistency between the error estimates of the beam and swarm experiments. These authors concluded that the helium total cross section, as measured in transmission by beams techniques, had not yet been determined to better than 10–15%, while the precision of the swarm data could not be improved within the then current limitations of theory and experiment.

3. e–He: 1979

Much of the subsequent progress in resolving this inconsistency was due to recasting the question of accurate cross sections into the much more tractable question of accurate phase shifts. The differential cross section for elastic scattering by He is defined by $d\sigma/d\Omega = |f(\theta)|^2$, where the scattering amplitude, expressed in terms of partial-wave phase shifts η_ℓ, is

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\exp(i\eta_\ell)\sin\eta_\ell P_\ell(\cos\theta)\,. \tag{3}$$

Here k is the electron momentum in atomic units, and P_ℓ is a Legendre polynomial (see, for example, Nesbet 1980). The partial-wave Born approximation is valid for an effective one-electron scattering problem when the classical centrifugal potential dominates the scattering potential. This must always be true for sufficiently large angular quantum numbers ℓ. Because the dominant potential for an electron scattered by a neutral atom at low scattering energies is the polarisation potential, $-\alpha_d/2r^4$ in Hartree atomic units, where α_d is the static dipole polarisability, high-ℓ phase shifts are determined by α_d. Thompson (1966) derived a simple formula for the sum of partial-wave contributions to the scattering amplitude, given known accurate values of low-order ($\ell \leq \ell_0$) phase shifts and using the Born approximation to close the sum for $\ell > \ell_0$. This implies closed summation formulas for the total and momentum-transfer cross sections (Thompson 1966; Nesbet 1980).

The significance of phase-shift analysis in determining consistent and accurate cross sections was greatly clarified by crossed-beam measurements of the angular distribution of electrons elastically scattered by helium (Andrick 1973; Andrick and Bitsch 1975). The experimental design was intended to make the scattering volume (intersection of the electron and target gas beams) very nearly independent of scattering angle. Thus the relative angular dependence at a given energy was quite accurate, but the absolute differential cross section was not measured directly. Thompson's formula for the scattering amplitude was used by Andrick and Bitsch to parametrise their measured angular distributions in terms of phase

shifts. This fit disclosed the very important fact that the d-wave phase shift is given by the Born approximation to an accuracy on the order of 1% throughout the low-energy range. It follows from the argument given above that results within the error limits of the disputed cross section data depend only on accurate values of the s- and p-wave phase shifts. Having verified the accuracy of the partial-wave Born formula for the d-wave phase shift, Andrick and Bitsch fitted their angular distribution data for energies 2–19 eV to Thompson's formula with $\ell_0 = 1$, using $\alpha_d = 1 \cdot 39$a.u. for the dipole polarisability, to determine η_0 and η_1. This fit does not require absolute normalisation of the differential cross section, and uses the data independently for each scattering energy. Using the closure formulas of Thompson, cross sections are determined within an error due only to the inaccuracy of the measured angular distributions, although Andrick and Bitsch assigned error limits of $\pm 5\%$ to their reported cross sections. Subsequent comparison with differential cross sections from accurate variational calculations (Nesbet 1979*a*, 1979*b*) indicated that the measured angular distributions of Andrick and Bitsch were in fact accurate to within roughly $0 \cdot 5\%$. Phase shifts η_0 and η_1 fitted to the experimental angular distribution data were consistent with theoretical phase shifts computed by methods that included target-atom polarisation. The implied σ_T was approximately 10% greater than the data of Golden and Bandel, and hence in good agreement with the transformed cross section obtained by Bederson and Kieffer from the swarm data of Crompton *et al.*

These results emphasise the importance of the polarisation response in theoretical calculations. In the polarised orbital method (POM) of Temkin (1957), an effective potential is computed as a model of the true optical potential that formally represents polarisation response. This model implies a penetration effect, taken into account in the EPOM formalism of Callaway *et al.* (1968). Duxler *et al.* (1971) reported calculations of e–He scattering, using the full formalism of Temkin. The computed p-wave phase shift agreed better with the Andrick–Bitsch data than did any other theoretical phase shift then available.

A quite different theoretical approach first appeared in calculations by Michels *et al.* (1969), and later with some refinements in calculations by Sinfailam and Nesbet (1972). These calculations used variational methods, replacing the Rayleigh–Schrödinger variational principle familiar for the bound state of atoms and molecules with fixed-energy methods based on the Kohn (1948) variational principle. By augmenting standard bound-state basis sets with continuum functions that have correct asymptotic behaviour for open scattering channels, these variational methods could exploit existing computer programs designed for so-called 'configuration interaction' (CI) calculations of electronic correlation. In this approach, the polarisation response is represented by specific configurations in which a dipole transition of a continuum channel function is coupled to a dipole response transition of the target atom. Partial-wave phase shifts for e–He scattering computed by Sinfailam and Nesbet (1972) agreed closely with POM and EPOM results and were consistent with the experimental phase shifts of Andrick and Bitsch. These calculations were carried out in a continuum Bethe–Goldstone (BG) approximation, which is an independent-pair model for the bound-continuum interaction. The computed BG phase shifts were used by Milloy and Crompton (1977) to convert new swarm data, in the energy range 4–12 eV, to an equivalent total cross section. Comparison with σ_M computed

from phase shifts by Andrick and Bitsch and with σ_T from the data of Golden and Bandel supports the the conclusion by Andrick and Bitsch that the latter data are affected by a systematic error of about -10%.

Another important development of theoretical formalism at this time was the R-matrix method, first applied to e–He scattering by Burke and Robb (1972). As originally formulated for electron scattering, this method was not variational and was based on the single-channel close-coupling equations, which do not explicitly include the polarisation response. Results were obtained at the formal level of the static exchange (SE) approximation, equivalent to a continuum Hartree–Fock calculation. Very similar results were obtained by Sinfailam and Nesbet (1972) when the two-electron configurations of the BG model were removed from their variational calculation.

Subsequently, R-matrix calculations were extended to model polarisation response through coupling to polarisation channels constructed from target atom dipole or multipole pseudostates. Pseudostates are constructed from a first-order response function, which can be computed variationally for a given perturbing multipole field. Target-atom correlation was also incorporated into the R-matrix program. Calculations with this extended method were carried out by O'Malley *et al.* (1979) for e–He scattering in the energy range 0–$16\cdot5$ eV. These calculations included the quadrupole polarisation response. Residual errors were estimated in detail and used to provide final best estimates of the s- and p-wave phase shifts and of both cross sections σ_T and σ_M. The estimated residual error is on the order of 1% for the full energy range studied.

The BG calculations of Sinfailam and Nesbet were also extended by incorporating target-atom correlation (Nesbet 1979*a*, 1979*b*). The variational formalism allowed stepwise improvement of the target wave function, using procedures developed in accurate bound-state calculations. Configurations representing quadrupole polarisability and short-range correlation were added to the variational wave function to maintain a residual error less than $0\cdot5\%$ for η_0 and less than $0\cdot66\%$ for η_1. This ensures that the net effect of residual errors in the computed phase shifts is no greater than 1% in the differential cross section at any angle. Comparison with the best estimate results of O'Malley *et al.* (1979) shows agreement within the expected error bars for η_0 but not for η_1. The variational phase shift η_1 is closer to that computed by Sinfailam and Nesbet (1972), which was closely bracketed by POM and EPOM calculations, by Duxler *et al.* (1971) and by Callaway *et al.* (1968), respectively, and to POM calculations by Yau *et al.* (1978). More detailed comparisons are given in Nesbet (1980). The variational cross sections and those computed by O'Malley *et al.* generally agree within the stated error estimates. The scattering length, which measures the slope of η_0 at zero energy, is $1\cdot177a_0$ from the best estimate of O'Malley *et al.* while the variational result is $1\cdot1835a_0$. Both numbers are consistent with the value $1\cdot18a_0$ from the swarm data of Crompton *et al.*

The variational phase shifts were fitted to cubic spline functions to give a smooth fit for energies up to 19 eV, using effective-range formulas to ensure correct analytic behaviour for small energies, and to incorporate the accurately known dipole polarisability. The Born-closure formulas of Thompson (extended to σ_M) were used to compute differential and total cross sections. When the angular distribution data of Andrick and Bitsch are scaled by the computed

variational total cross section, they show remarkable agreement with the computed absolute differential cross sections at energies 2, 5, 12 and 19 eV. The computed momentum-transfer cross section is well within the stated error bars of Crompton *et al.* (1967, 1970*a*), and compatible with an actual experimental error of 1% or better at all energies. The computed total cross section is substantially greater than the values reported by Golden and Bandel (1965).

New experimental measurements made in this time-frame are in good agreement with the variational calculations and with the results of O'Malley *et al.* Kauppila *et al.* (1977) and Stein *et al.* (1978) used an apparatus designed for accurate transmission experiments on positron beams to measure low-energy e–He total cross sections. A curved axial magnetic field was used in the scattering chamber to guide positrons or electrons along a curved path, which eliminates high-energy particles. The measured e–He total cross sections at 0·3–31 eV are within 4% of the values deduced by Andrick and Bitsch below 19 eV, but are 12% greater than the Golden–Bandel cross sections. Kennerly and Bonham (1978) used a novel time-of-flight transmission method to measure σ_T for e–He scattering in the broad energy range 1–50 eV. Design of this experiment eliminates several of the major sources of systematic error in the Ramsauer method. Error estimates of (+3,−2)% over the energy range 2–50 eV were obtained by detailed analysis of possible error sources, with estimated error increasing below 2 eV. The results agree closely with the experiment of Kauppila *et al.* and are consistent with the accurate calculations by O'Malley *et al.* (1979) and by Nesbet (1979*a*, 1979*b*). The general conclusion from these developments (Nesbet 1980) is that the long-standing discrepancy between swarm and beam data on the low-energy e–He cross section is resolved in favour of the swarm data of Crompton *et al.* and that quantitative theory has progressed to the point that the computed differential cross section can be used as a standard with accuracy of ±1% or better in the energy range up to 19 eV.

These results of 1979 have been confirmed by more recent theory and experiment, and are still in current use for experimental calibration. Absolute elastic differential cross sections were deduced from accurate differential cross section measurements by Brunger *et al.* (1992) at 1·5, 5, 10 and 18 eV, using a refined version of phase shift analysis. The potentially very accurate convergent close-coupling (CCC) method (Bray 1994) was used for elastic cross section calculations over a large energy range (1·5 to 500 eV) by Fursa and Bray (1995).

4. e–H_2: 1987–199?

For fixed nuclei, H_2 is simply a two-centre distortion of He. Hence the theory of e–H_2 scattering should be quite similar to that for e–He scattering. The reduction from spherical to axial symmetry subdivides each spherical partial-wave component into separate terms indexed by the axial quantum number λ and by inversion parity. Matrices indexed by $\ell\lambda$ are no longer diagonal, so some of the simplicity of partial-wave analysis is lost. In a partial wave expansion, the electric dipole polarisability should dominate the high $\ell\lambda$ matrix elements. The polarisability tensor requires two independent parameters $\alpha_{\|}$ and $\alpha_{\perp}$. The molecular quadrupole moment also produces a nonspherical multipole potential, which has significant effects at low scattering energies. It must be included along with the polarisation potential in analytic approximations to high-order

scattering matrices or in Born closure formulas. Integrals required in variational methods become truly multidimensional, greatly increasing the computational effort of standard variational calculations. This argues strongly for variational R-matrix theory (Nesbet 1980), in which two-electron integrals are confined to localised functions or truncated at a molecular R-matrix boundary. The R-matrix theory must include axial dipole pseudostates for accurate treatment of the polarisation potential. Powerful analytic methods are available for the solution of non-exchange close-coupling equations outside an R-matrix boundary. Thus the loss of spherical symmetry adds complexity but does not require a fundamentally different methodology for fixed nuclei (Nesbet *et al.* 1986).

The situation is much less satisfactory when nuclear motion is taken into account, as it must be in the low-energy limit or in the vicinity of rovibrational excitation thresholds (Morrison 1988). The transfer of electronic kinetic energy into nuclear motion is a direct breakdown of the familiar Born–Oppenheimer separation, relied upon in most molecular bound-state calculations. Although many approximate methods have been tried, there is no generally accepted nonadiabatic theory of energy transfer between electrons and nuclei that is amenable to *ab initio* computations with controlled error limits. It is still necessary to estimate the absolute accuracy of theoretical models by external criteria, comparing data with alternative theory and with accurate experiments.

In view of these comments, it is not surprising that quantitative theory is much more difficult to apply to e–H_2 scattering, especially above the first vibrational excitation threshold, than to e–He scattering. In a review of the H_2 situation, Morrison *et al.* (1987) compared available experimental data with theory, updating an earlier general review of electron–molecule scattering theory by Lane (1980). Theoretical calculations of rotational and vibrational excitation cross sections, using model potentials that had been checked carefully against alternative theoretical methods, were compared with beam measurements of rotational excitation cross sections by Linder and Schmidt (1971) and of total and differential vibrational excitation cross sections by Ehrhardt *et al.* (1968), Linder and Schmidt (1971) and Wong and Schulz (1974). In all cases there is close agreement between theory and the beam data. Similar general agreement is found with the pure rotational excitation cross section obtained from analysis of swarm data (Crompton *et al.* 1970*b*). In contrast, Morrison *et al.* (1987) found the integral $v = 0 \rightarrow 1$ vibrational excitation cross section derived from swarm data (Crompton *et al.* 1970*b*) to be significantly smaller than the cross section computed using the same theoretical model that had been found to agree well with available beam data on vibrational excitation.

This discrepancy was confirmed by new measurements and calculations (Buckman *et al.* 1990). England *et al.* (1988) measured the drift velocity for H_2 introduced in low concentration into Ne. Analysing these data with the well-established statistical theory implies a threshold vibrational excitation cross section for H_2 in agreement with earlier swarm experiments on pure H_2. This experiment rules out any error due to direct interaction of the hydrogen molecules. The very striking disagreement with the theoretical vibrational excitation cross section (Morrison *et al.* 1987) for electron energies from $0{\cdot}5$ to $4{\cdot}0$ eV remains unexplained. Brunger *et al.* (1990, 1991) carried out crossed-beam measurements of absolute differential cross sections for elastic scattering and rovibrational excitation of H_2. Absolute

values were determined by calibration with the now well-established e–He cross section. The elastic and $v = 0 \rightarrow 1$ excitation cross sections up to 2 eV were found to be in close agreement with improved theoretical calculations (Buckman *et al.* 1990) and to maintain the disagreement with the vibrational excitation cross section derived from swarm data. More recent calculations by the complex Kohn variational method for electrons (Rescigno *et al.* 1993), using the off-shell T-matrix approximation for vibrational excitation, confirm the large discrepancy between theory and swarm-derived data.

5. Conclusions

The preponderance of evidence supports the conclusion of Buckman *et al.* (1990) that theory and experiment are in general agreement for elastic electron scattering by H_2 and for low-energy rotational excitation. Beam experiments and theory agree well for low-energy vibrational excitation, but both disagree markedly with the vibrational excitation cross section deduced from swarm experiments. The most straightforward general conclusion is that something appears to go wrong in the statistical theory used to analyse the swarm data when vibrational excitation occurs. This conclusion would be sharpened if fully *ab initio* theoretical calculations of vibrational excitation could be carried out with internal estimates of error limits. This is much more difficult for H_2 than for He, and has not yet been done.

References

Andrick, D. (1973). *Adv. At. Mol. Phys.* **9**, 207.
Andrick, D., and Bitsch, A. (1975). *J. Phys.* B **8**, 393.
Bederson, B., and Kieffer, L. J. (1971). *Rev. Mod. Phys.* **43**, 601.
Bray, I. (1994). *Phys. Rev.* A **49**, 1066.
Brunger, M. J., Buckman, S. J., and Newman, D. S. (1990). *Aust. J. Phys.* **43**, 665.
Brunger, M. J., Buckman, S. J., Newman, D. S., and Alle, D. T. (1991). *J. Phys.* B **24**, 1435.
Brunger, M. J., Buckman, S. J., Allen, L. J., McCarthy, I. E., and Ratnavelu, K. (1992). *J. Phys.* B **25**, 1823.
Buckman, S. J., Brunger, M. J., Newman, D. S., Snitchler, G., Alston, S., Norcross, D. W., Morrison, M. A., Saha, B. C., Danby, G., and Trail, W. K. (1990). *Phys. Rev. Lett.* **65**, 3253.
Burke, P. G., and Robb, W. D. (1972). *J. Phys.* B **5**, 44.
Callaway, J., La Bahn, R. W., Pu, R. T., and Duxler, W. M. (1968). *Phys. Rev.* **168**, 12.
Crompton, R. W., Elford, M. T., and Jory, R. L. (1967). *Aust. J. Phys.* **20**, 369.
Crompton, R. W., Elford, M. T., and Robertson, A. G. (1970*a*). *Aust. J. Phys.* **23**, 667.
Crompton, R. W., Gibson, D. K., and McIntosh, A. I. (1969). *Aust. J. Phys.* **22**, 715.
Crompton, R. W., Gibson, D. K., and Robertson, A. G. (1970*b*). *Phys. Rev.* A **2**, 1386.
Duxler, W. M., Poe, R. T., and La Bahn, R. W. (1971). *Phys. Rev.* A **4**, 1935.
Ehrhardt, H., Langhans, L., Linder, F., and Taylor, H. S. (1968). *Phys. Rev.* **173**, 222.
England, J. P., Elford, M. T., and Crompton, R. W. (1988). *Aust. J. Phys.* **41**, 573.
Fursa, D. V., and Bray, I. (1995). *Phys. Rev.* A **52**, 1279.
Golden, D. E. (1966). *Phys. Rev.* **151**, 48.
Golden, D. E., and Bandel, H. W. (1965). *Phys. Rev.* **138**, A14.
Kauppila, W. E., Stein, T. S., Jesion, G., Dababneh, M. S., and Pol, V. (1977). *Rev. Sci. Instrum.* **48**, 822.
Kennerly, R. E., and Bonham, R. A. (1978). *Phys. Rev.* A **17**, 1844.
Kohn, W. (1948). *Phys. Rev.* **74**, 1763.
LaBahn, R. W., and Callaway, J. (1966). *Phys. Rev.* **147**, 28.
Lane, N. F. (1980). *Rev. Mod. Phys.* **52**, 29.
Linder, F., and Schmidt, H. (1971). *Z. Naturforsch.* **26a**, 1603.

Michels, H. H., Harris, F. E., and Scolsky, R. N. (1969). *Phys. Lett.* A **28**, 467.
Milloy, H. B., and Crompton, R. W. (1977). *Phys. Rev.* A **15**, 1847.
Morrison, M. A. (1988). *Adv. At. Mol. Phys.* **24**, 51.
Morrison, M. A., Crompton, R. W., Saha, B. C., and Petrović, Z. Lj. (1987). *Aust. J. Phys.* **40**, 239.
Nesbet, R. K. (1979*a*). *J. Phys.* B **12**, L243.
Nesbet, R. K. (1979*b*). *Phys. Rev.* A **20**, 58.
Nesbet, R. K. (1980). 'Variational Methods in Electron–Atom Scattering Theory' (Plenum: New York).
Nesbet, R. K., Noble, C. J., and Morgan, L. A. (1986). *Phys. Rev.* A **34**, 2798.
O'Malley, T. F. (1963). *Phys. Rev.* **130**, 1020.
O'Malley, T. F., Burke, P. G., and Berrington, K. A. (1979). *J. Phys.* B **12**, 953.
Ramsauer, C. (1921). *Ann. Physik* **66**, 546.
Ramsauer, C., and Kollath, R. (1929). *Ann. Physik* **3**, 536.
Ramsauer, C., and Kollath, R. (1932). *Ann. Physik* **12**, 529.
Rescigno, T. N., Elza, B. K., and Lengsfield, B. H. (1993). *J. Phys.* B **26**, L567.
Sinfailam, A. L., and Nesbet, R. K. (1972). *Phys. Rev.* A **6**, 2118.
Stein, T. S., Kauppila, W. E., Pol, V., Smart, J. H., and Jesion, G. (1978). *Phys. Rev.* A **17**, 1600.
Temkin, A. (1957). *Phys. Rev.* **107**, 1004.
Thompson, D. G. (1966). *Proc. R. Soc. London* A **294**, 160.
Wong, S. F., and Schulz, G. J. (1974). *Phys. Rev. Lett.* **32**, 1089.
Yau, A. W., McEachran, R. P., and Stauffer, A. D. (1978). *J. Phys.* B **11**, 2907.

Manuscript received 14 June, accepted 15 November 1996