dom rapidly. For a single ion, however, it will be necessary to make all three principal axes of the ellipsoidal potential well different and direct the laser beam more or less along $\hat{i} + \hat{j} + \hat{k}$.

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Quantum-Mechanical Inversion of the Differential Cross Section: Determination of the He-Ne Potential

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The He-Ne potential is obtained from the measured differential cross section by a systematic inversion procedure based on the generalized opitcal theorem. The potential, obtained in the range from 2.1 to 6 Å, is in good agreement with recently proposed model potentials. The results constitute the first example of a fully direct and systematic inversion of experimental scattering data of real systems.

Molecular-beam scattering experiments are the source of some of the most accurate and detailed information on intermolecular potentials.[1] In most cases the extraction of the interaction from the data is done by assuming an explicit functional form for the potential that includes free parameters. These quantities are then varied in a trial-and-error procedure until the cross section calculated from the potential yields a good fit to the experimental data.[2] It is, of course, very desirable to replace this method by a direct, systematic inversion procedure. It was found by Buck[3] and Buck and Pauly[4] that part of this task could be achieved by applying the Firsov[5] semiclassical inversion, which generates the potential from the deflection function (or phase shifts). The deflection function itself is, however, obtained from the cross section by a fitting procedure using a presupposed functional form. The purpose of the present article is to demonstrate that a *complete* inversion of scattering data is possible for real systems. A key step in this procedure is the determination of the scattering amplitude, hence the phase shifts, from the experimental cross section by the unitarity method.[6-8] Though the method was tested for simulated and idealized input data, the *practical* application was hampered by the incomplete and inaccurate data available. The advent of a new generation of molecular-beam machines, however, made it possible to obtain very precise data with high angular and velocity resolution.[9] The measured differential cross section for the system He + Ne taken at the energy of $E = 64.4$ meV ($v = 1927$ m/s) and transfomed to the center-of-mass system is shown in Fig. 1(a). This system was chosen be-

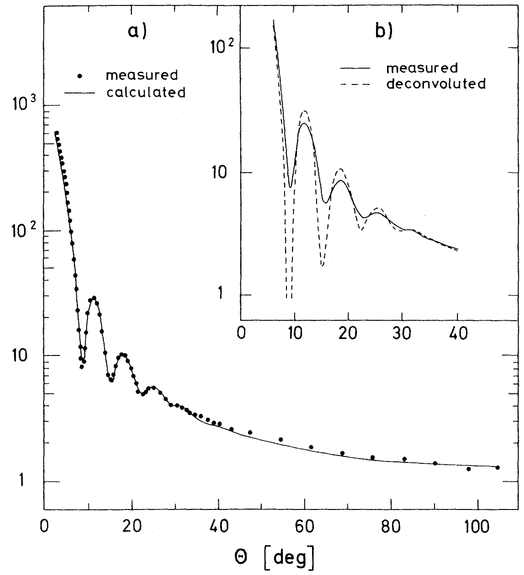

FIG. 1. Differential cross sections for HeNe at $E = 64.4$ meV in the center-of-mass system. (a) Comparison of measured and calculated values based on the potential obtained by inversion. (b) Experimental and deconvoluted cross sections.

cause the differential cross section exhibits only a few diffraction oscillations typical for light quantum systems. The data cover an angular range from 3.7° to 112.1°. Since the inversion procedure requires a complete range of angles, the experimental cross section σ_{av} is easily extrapolated to small angles using the calculated long-range part of the potential.[10] For large angles, beyond the oscillatory regime, σ_{av} is a smooth function which is extrapolated numerically to 180° using the known behavior of large-angle scattering.

The next step is the deconvolution of σ_{av}, which represents an average of the true cross section $\sigma(\theta)$ due to the finite resolution of the experimental setup. The experimental averaging is modeled by two distribution functions over velocity and angle variables with the half-widths of $\Delta v/v = 10.7\%$ and $\delta = 1.230°$, for a Gaussian in v and a rectangular distribution function in θ, respectively.[11] The algorithm used is a van Cittert iteration procedure which is described in detail in Ref. 11. To eliminate an amplification of artificial errors the cross section is fitted to a sum of Gaussian peaks centered around the measured positions of the oscillations. Since the input data is not available for all energies over the limited range of v values, it becomes necessary to assume a scaling property for the cross section: $\sigma(v,\theta) = v^{\beta}\hat{\sigma}(v^{\alpha}\theta)$. Evidence for the validity of this form was also given in Ref. 11. The constants, estimated from measurements at two neighboring collision energies, are $\alpha = 0.961$ and $\beta = 0.776$. In the present example, convergence to less 2% was found after eight iterations. Figure 1(b) shows the deconvoluted cross section $\sigma(v,\theta)$ and the experimental one $\sigma_{\mathrm{av}}(v,\theta)$. The extent of peak quenching by the experimental averaging is quite substantial. Deconvolution was successful in the present case because the peaks of $\sigma_{\mathrm{av}}(v,\theta)$ are well separated—a favorable condition for use of this procedure. Finally we note that the technical step of deconvolution is the *only* part of the inversion process where parametrized forms are used (the scaling relation; Gaussian fitting).

To determine the scattering amplitude the *unitarity method*[6] can be used to calculate $f(\theta)$ if $\sigma(\theta) = |f(\theta)|^2$ is known for all θ at fixed energy. The method is based on the unitarity equation of scattering theory.[7,12] If one writes

$$f(\theta) = f(\cos\theta) = g(\cos\theta)e^{i\alpha(\cos\theta)},\qquad g(\cos\theta) = [\sigma(\cos\theta)]^{1/2}, \tag{1}$$

the unitarity equation assumes then the form[7,8]

$$g(\cos\theta)\sin[\alpha(\cos\theta)] = (k/4\pi)\int_0^{2\pi}\int_0^{\pi} g(\cos\theta'')g(\cos\theta')\{\cos[\alpha(\cos\theta'')] - \alpha(\cos\theta')\}\sin\theta'\,d\theta'\,d\varphi', \tag{2}$$

where $\cos\theta'' = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\varphi'$, and k is the scattering wave number. In Refs. 7 and 8 conditions were established on the input $g(\cos\theta)$ under which (2) can be iteratively solved for $\alpha(\theta)$ [starting with $\alpha_0(\theta) = 0$] and the solution is unique. Tests with simulated cross sections, calculated from realistic intermolecular potentials, have shown, however, that these conditions are not satisfied (at typical experimental energies).[6] Straightforward iterations with $\alpha_0(\theta) = 0$ as zeroth-order approximation are therefore excluded as a method for solving (2). The difficulty can, however, be overcome (at least practically) by using a combined iteration-extrapolation procedure and starting from a physically reasonable zeroth-order phase $\alpha_0(\theta)$.[6] Divergence was found to arise from θ regions where an nth approximant $\alpha_n(\theta)$, when substituted on the right-hand side of (2), yields a mathematically inconsistent value

$|\sin\alpha_{n+1}(\theta)|>1$ on the left-hand side. As remedy, a modified procedure uses extrapolation to determine $\alpha_{n+1}(\theta)$ from the values at previous angles in all regions where the right-hand side of (2) exceeds or approaches the magnitude $g(\theta)$. The procedure followed in the present application is essentially the same as that used in Ref. 6 for the simulated examples. However, in the present case a large number of iterations (28) were necessary. Each iteration takes about 3.5 min on the Hebrew University CDC 6400 computer. Convergence could not be improved significantly beyond 3% (estimated by the difference between successive approximants). To determine the phase shifts one can apply the partial-wave decomposition of $f(\theta)$, which yields

$$[\exp(2i\eta_l)-1]/ik=\int_0^\pi f(\theta)P_l(\cos\theta)\sin\theta\,d\theta. \quad (3)$$

(3) was evaluated by a Gauss-Laguerre quadrature for $l\leq 50$. For larger values the known functional form $\eta_l=cl^{-n}$ was used,[13] the constants c and n being determined from the numerical η_l for $46\leq l\leq 50$. The partial-wave components from (3), readily yield $\sin 2\eta_l$ and $\cos 2\eta_l$ but not the *absolute* value of the η_l, for which an ambiguity of an $n\pi$ term remains. We determine the correct $n\pi$ multiplicity by a simple process of analytic continuation, using the fact that for a realistic intermolecular potential η_l *decreases* monotonically as l *decreases* for η_l values smaller than the maximum value. In Fig. 2 the η_l so extracted are shown by circles.

The determination of the potential from the phase shifts is done by the Firsov method[5,14] that is known to be of good accuracy. We note, however, that quantum-mechanical inversion of the phase shift is also possible, by the recently proposed peeling method.[15] The result is shown in Fig. 2. The potential exhibits a flat well with the minimum values of $\epsilon=1.97$ meV for the depth and $R_m=2.97$ Å for the position. The zero is $R_0=2.67$ Å. The inverted potential is in good agreement with potentials proposed by semiempirical models[16] and a trial-and-error fitting of the same data based on one of these models,[9] the results of which are also shown in Fig. 2.[17] There are some small deviations in the attractive part, but less than 5% for ϵ, 1.3% for R_m, and 0.7% for R_0. These values are completely within the error limits to which these values can be determined from the present experiment [within (5–10)% for ϵ, (2–1)% for R_m, and (1.0–0.5)% for R_0]. The deviations in the repulsive part, if indeed significant, are related to the large-angle part of $\sigma_{\mathrm{av}}(\theta)$. To check the consistency of the whole procedure the experimental $\sigma_{\mathrm{av}}(\theta)$ is compared with the cross section calculated from the inversion phase shifts and averaged with the appropriate apparatus functions given above. The result is shown in Fig. 1(a). The agreement is quite good despite two small deviations around the first minimum and 55°. Whereas the first error is probably due to the deconvolution process, the deviations at large angles must be attributed to the unitarity part. However, the overall result is obviously as good as the best-fit procedures available at the moment. In addition this inversion procedure has the great advantage of making no assumptions about the special potential form.

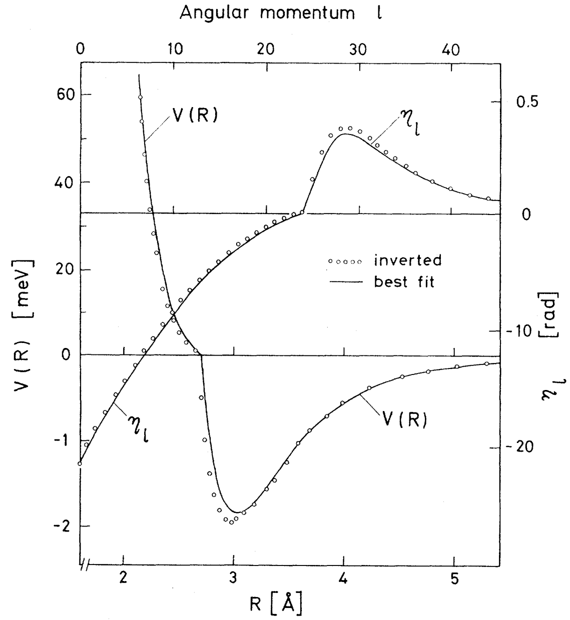

FIG. 2. Intermolecular potential $V(R)$ vs the intermolecular distance (scale: left) and scattering phase shifts η_l vs angular momentum quantum number l (scale: right) for the potential obtained by inversion and the best-fit potential. Note the change in scale between the attractive and repulsive parts of the interaction.

The above results demonstrate that direct inversion of scattering data can be a useful tool for the determination of highly accurate atom-atom potentials. It is quite conceivable that the direct inversion scheme may offer deeper insights on the sensitivity of the interaction, at various ranges, to the input data. Inversion of elastic scattering data may also stimulate further progress in the inversion of *inelastic* scattering data (e.g., leading to the determination of nonadiabatic interactions from cross sections for electronic transitions,[18] or the determination of anisotropic molecule-atom potentials from rotationally inelastic scattering data). Work in these directions is already in progress.

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Anomalous Electron Mobilities in Dense Helium Gas

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The drift velocity of electrons in helium gas at low temperatures is found to exhibit an anomalous dependence on density, similar to that which has been observed at much higher temperatures. The density and temperature dependence of the effect suggests that it arises from multiple-scattering corrections to the classical transport behavior. The effect may account for some of the phenomena which have previously been ascribed to electron localization.

In their study of electron transport through dense helium gas at 4.2°K, Levine and Sanders[1] found that the electron mobility[2] μ drops several orders of magnitude as the gas density n is varied from about 5×10^{20} to 1.5×10^{21} atoms cm^{-3}. This phenomenon has been universally interpreted as reflecting a change in the characteristic state of the electron from a free-particle–like wave function to the "bubble" state known to exist at liquid helium densities. Other workers[3,4] have extended the study of the mobility transition to higher temperatures, and several theoretical models have been proposed to account for the various observations.[1,3,5-7] In all of this work the assumption has been that at lower densities the transport properties of the electron are characterized by the simple Boltzmann equation, which yields[1]

$$\mu_0 = \frac{4}{3}\frac{e}{(2\pi m k_{\rm B}T)^{1/2}}\frac{1}{n\sigma}, \tag{1}$$

where m is the electron mass and σ is the momentum-transfer cross section in the limit of zero electron energy. The mobility transition has been viewed as arising from some new effect having little physical connection with this presumably uninteresting transport problem.

In recent measurements[8] we have observed that Eq. (1) does not in fact give a satisfactory description of the n dependence of μ at low densities. Rather, the product μn is found to decrease in an approximately linear fashion with increasing n. A typical example of our results is shown