(1976).
[10]R. J. Spindler, J. Quant. Spectrosc. Radiat. Transfer 9, 1041 (1969).
[11]E. M. Purcell, Astrophys. J. 116, 457 (1952).
[12]W. K. Bischel, P. J. Kelley, and C. K. Rhodes, Phys. Rev. A 13, 1829 (1976).

Evidence for a Resonance in e^+-H S-Wave Scattering

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Using the coordinate rotation method with Pekeris trial functions, we find evidence that a resonance occurs in e^+-H S-wave scattering at a complex energy ($-0.257\,374 - i\,0.000\,067$) Ry. No lower resonance is found in the calculation.

Since the prediction by Mittleman[1] of an infinite sequence of resonances in positron-hydrogen scattering below the excitation thresholds, there have been some attempts (described by Wakid[2]) to locate the lowest such resonance, and some associated controversy.[3] Apparently these previous calculations either had a basis set which was too restricted to locate the resonance accurately or else used procedures which could generate nonphysical resonances. We present here a general method which couples sparse-matrix techniques for large basis sets with a stable, numerically convergent procedure to obtain an estimate for the lowest resonance location which appears to be accurate to six significant figures.

We shall describe the e^+-H system by means of the Hamiltonian

$$H(\vec{\mathbf{r}}) = -\nabla_1^2 - \nabla_2^2 - \frac{2}{r_1} + \frac{2}{r^2} - \frac{2}{|\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|},$$

where $\vec{\mathbf{r}}_1$ and $\vec{\mathbf{r}}_2$ are the coordinates of electron and positron, and the proton is fixed at the origin. Define $H_\alpha(\vec{\mathbf{r}})$ by

$$H_\alpha(\vec{\mathbf{r}}) = H(\vec{\mathbf{r}}e^{i\alpha}),$$

where each component of the coordinate vector is multiplied by a factor $e^{i\alpha}$, $\alpha > 0$. It has been shown rigorously[4] that the spectrum of H_α consists of a series of rays, making an angle -2α with the positive real axis, that start from each of the thresholds in the problem. These thresholds are those associated with the hydrogen atom at $-n^{-2}$, $n = 1, 2, \ldots$, and those connected with positronium at $-0.5m^{-2}$, $m = 1, 2, \ldots$. In addition, there may be discrete points in that part of the complex plane swept out by the rays as α is increased to its chosen value from zero, and also points on the real axis below $E = -1$ corresponding to three-body bound states.

It is very likely that the complex discrete points are associated with resonances, as would be the case for short-range potentials,[5] and this correspondence certainly occurs in the case of e^--H scattering.[6] We assume it to be true in the present case.

If E_r, $\mathrm{Im}E_r < 0$, is a discrete point in the spectrum of H_α, then there is a normalizable function ψ such that

$$H_\alpha\psi = E_r\psi.$$

A variational estimate of E_r may be found by approximating ψ by a linear combination of normalizable basis functions $\varphi_i(r)$, so that

$$\psi \approx \psi_t = \sum_{i=1}^{N} c_i \varphi_i,$$

and finding a stationary value of $[E_r]$, where

$$[E_r] = \frac{\int d^3r_1 d^3r_2 \psi_t H_\alpha \psi_t}{\int d^3r_1 d^3r_2 \psi_t \psi_t}.$$

If the coefficients c_i are varied, the problem reduces to the calculation of the eigenvalues $\lambda(k)$, $k = 1, \ldots, N$, given by

$$\sum_{j=1}^{N} H_{ij} x_j^{(k)} = \lambda^{(k)} \sum_{j=1}^{N} N_{ij} x_j^{(k)}, \quad i = 1, \ldots, N, \qquad (1)$$

where

$$H_{ij} = \int d^3r_1 d^3r_2 \, \varphi_i H_\alpha \varphi_j, \quad N_{ij} = \int d^3r_1 d^3r_2 \, \varphi_i \varphi_j.$$

With the use of Hylleraas trial functions, this approach has located several resonances in e^--H scattering.[6,7] After the main results of this Let-

ter were obtained, we learned that the method had been applied[3] to the S-wave e^+-H system, with the conclusion that no resonance could be found below the H($n=2$) threshold $E=-0.25$. In that work, it appears that no more than 56 basis functions had been used. We report here a calculation with considerably more basis functions which provides very strong evidence for the existence of a resonance just below the H($n=2$) threshold.

As basis functions, we have used the same linear combinations of Hylleraas functions used by Pekeris[8] for the helium atom, namely φ_{lmn} given by

$$\varphi_{lmn}(r_1,r_2,r_{12}) = \exp[-a(r_1+r_2)]L_l^{(0)}(u)L_m^{(0)}(v)L_n^{(0)}(w),$$

with $u=a(r_2+r_{12}-r_1)$, $v=a(r_1+r_{12}-r_2)$, $w=2a(r_1+r_2-r_{12})$. Here $L_1^{(0)}$ is a Laguerre polynomial, $r_{12}=|\vec{r}_1-\vec{r}_2|$, and a is a real, positive constant. For a number of values of Ω, we used all basis functions satisfying $l+m+n\leq\Omega$, $0\leq l,m,n$.

The advantage of this form of basis function is that the matrices H_{ij},N_{ij} are found to be sparse, each with no more than 57 nonzero elements in any row. Also, the matrix N_{ij} does not appear to be ill-conditioned as is the case when Hylleraas functions are used.

We expect that most of the eigenvalues $\lambda^{(k)}$ from (1) will be close to the rays of the continuous spectrum, and these are of no interest. To search for possible resonances, we have used the method of inverse interation (also used by Reinhardt[9] in similar circumstances). For a particular choice of λ and $y_j^{(0)}$, the sequence of vectors $y_j^{(p)}$ is constructed by

$$y^{(p+1)}=(\lambda N-H)^{-1}Ny^{(p)}.$$

For $p\to\infty$ it may be shown that

$$y_j^{(p)}\approx \text{const}(\lambda-\lambda^{(k)})^{-p}x_j^{(k)},$$

where $\lambda^{(k)}$ is the eigenvalue of H_{ij} nearest to λ. In this way the eigenvalue nearest to λ may be found by solving a succession of linear equations, and, moreover, it may be asserted that in general no other eigenvalue exists inside a circle in the complex plane, center λ, passing through $\lambda^{(k)}$.

The sparseness of the matrices H_{ij},N_{ij} has been used to make the solution of the linear equations feasible for large basis sets.[10]

For all values of Ω (between 8 and 14), a, and α that have been studied, an eigenvalue is found in the vicinity of $E=-0.257$, provided a suitable value of λ was chosen. No eigenvalues that appear to be associated with resonances were found at smaller values of E.

As an indication of how the procedure converges for $\Omega=10$, eigenvalues for a number of rotation angles are presented in Fig. 1 for $a=0.25$ and 0.35. The resonance location is assumed to be near the point where the rate of change of the eigenvalue with respect to α is smallest. This empirical procedure is described by Doolen,[11] where it is applied successfully to the e^--H case.

This appears to be confirmed by the data given in Table I, which gives a sequence of eigenvalues for $\Omega=10$–14, with $a=0.25$, $\alpha=0.3$. These values of a and α were near the point where the rate of change of eigenvalue with respect to α was smallest, for all Ω considered. Our conclusion is that H_α has an eigenvalue at $E=-0.257\,374-0.000\,067i$ to within an error of no more than 10^{-6} in each part.

Our result is consistent with a prediction made by a calculation based on M-matrix theory,[12] which involves the calculation of a generalized

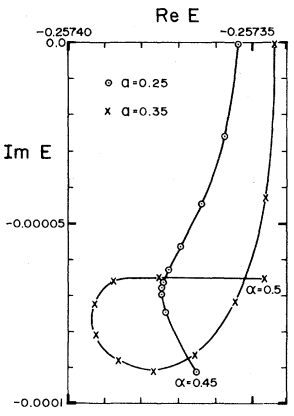

FIG. 1. Eigenvalues for $\Omega=10$, $a=0.25$, 0.35, and different α. Values of α differing by 0.05 rad are connected. For $\alpha=0$, the eigenvalues are real.

TABLE I. Location of an approximate eigenvalue of H_α calculated with $\alpha=0.3$, $a=0.25$, for $\Omega=10$–14.

Ω	No. of basis functions	ReE	ImE
10	286	−0.257 374 4	−0.000 067 6
11	364	−0.257 373 3	−0.000 067 4
12	455	−0.257 374 5	−0.000 067 1
13	560	−0.257 374 0	−0.000 067 7
14	680	−0.257 374 1	−0.000 067 7

scattering length at $E = -0.25$. This approach gives a series of resonances, one of which is at $E = -0.2569 - 0.000\,06i$.

The present calculation demonstrates the power of the coordinate rotation method in finding resonance positions when coupled with the inverse iteration technique for solving the generalized eigenvalue problem and with a judicious choice of basis functions which generate a sparse matrix.

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[1]M. H. Mittleman, Phys. Rev. 152, 76 (1966).
[2]S. E. A. Wakid, Phys. Lett. 54A, 103 (1975).
[3]A. K. Bhatia and R. J. Drachman, to be published.
[4]E. Balslev and J. M. Combes, Commun. Math. Phys. 22, 280 (1971); B. Simon, Commun. Math. Phys. 27, 1 (1972).
[5]B. Simon, Ann. Math. (N.Y.) 97, 247 (1973).
[6]G. D. Doolen, J. Nuttall, and R. W. Stagat, Phys. Rev. A 5, 1612 (1974).
[7]Y. K. Ho, to be published.
[8]C. L. Pekeris, Phys. Rev. 112, 1649 (1958).
[9]W. P. Reinhardt, private communication.
[10]L. T. Choo, Ph.D. thesis, University of Western Ontario, 1977 (unpublished).
[11]G. D. Doolen, J. Phys. B 8, 525 (1975).
[12]L. T. Choo, M. C. Crocker, and J. Nuttall, to be published.

Z Oscillations in the Excitation of $2s$ Vacancies in Ne III Measured by Radiative Decay

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Collisional excitation of neon atoms in light sources such as electric discharges, beam-foil interactions, etc., leads to a statistical population of the excited multiplets. This communication shows an anomalously high singlet-to-triplet ratio when the $2s2p^5\,{}^1P, {}^3P$ levels in Ne III are populated by impact of 100-keV projectiles (helium to potassium). Further, an oscillatory sturcture has been observed as a function of the element number of the projectile.

Measurements of the population of singlet and triplet states[1] in earlier atomic collision studies have resulted in a better understanding of the collision process at low velocities.[2] We present here experimental measurements of the singlet-to-triplet ratio of the secondary radiation emitted when neon atoms have been excited by ion impact in the hundred keV range. The experimental results have been qualitatively explained on the basis of the molecular-orbital (MO) model[3] and may further contribute to the understanding of collision processes at high velocities.

The present investigation deals with the $2s$-vacancy states ($2s2p^5\,{}^1P, {}^3P$) in Ne III produced in single collisions between projectiles with atomic numbers ranging from 2 to 19 and a thin neon-gas target. The projectiles produced by a 600-keV electromagnetic, heavy-ion accelerator were directed into a differentially pumped gas cell, where the pressure of ultrapure neon gas was kept below 1 mTorr to ensure single-collision conditions. The light emitted perpendicular to the beam was focused onto the entrance slit of a 2-m grazing-incidence spectrometer (McPherson, model 247) by an ellipsoidal gold mirror. The monochromator was equipped with a 600-lines/mm grating and a Channeltron detector. The wavelengths depopulating Ne III ($2s2p^5\,{}^1P, {}^3P$) were 370 and 488–490 Å, respectively, and, because of the low spectral intensity, several scans (365–510 Å) had to be accumulated in a multichannel analyzer operating in the multiscaling mode.

The population ratio of the $2s2p^5\,{}^1P$ to the $2s2p^5\,{}^3P$ level was measured by the radiative decay. This singlet-to-triplet ratio, S/T, with values in the range from 0.4 to 5.5 exhibit a pronounced oscillatory structure with peak values for Z equal to 4 and 15 (Fig. 1). As will be discussed in a forthcoming publication, the S/T ratio is a function of the initial ion energy. Thus for $P^+ \rightarrow$ Ne, the S/T ratio varies from 4.6 at 100 keV to 1.2 at 1.1 MeV, while for $Ne^+ \rightarrow$ Ne a value of 0.40 ± 0.04 very close to the statistical value was measured at 100 keV.

The discussion is based upon the Barat-Lichten diabatic correlation rules[4] with the relevant schematic correlation diagrams for the MO model shown in Fig. 2. The formation of Ne III ($2s2p^5\,{}^1P$,

