been shown in Fig. 1 for energies up to 60 eV. We have also compared our results with the close-coupling calculations of Burke and Taylor,[3] the first-Born-approximation calculation of Vainshtein *et al.*,[2] the classical binary-encounter calculation of the authors,[4] and the measurements of Hughes and Hendriskson.[11] It is seen that the present calculations which are based on the polarized Born approximation including exchange yield a value of the cross section that is lower than the first-Born-approximation calculation in the low- and intermediate-energy region. Near the threshold the reduction in the cross section is about 20%. In the intermediate-energy region the present calculations give a good agreement with the experimental data and close-coupling calculations. At higher energies (≈ 55 eV) the present calculations merge with the first-Born-approximation calculations. The close-coupling calculations also tend to agree closely with the present calculations at higher energies. This is because the effect of polarization is less important at high energies. The inclusion of exchange in the polarized Born approximation produces a rather small exchange effect for the $2s$-$2p$ excitation of lithium. Thus we conclude that the inclusion of polarization improves the first-Born-approximation cross section in the low- and intermediate-energy range.

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# Energies of *s* Eigenstates in a Static Screened Coulomb Potential[*]

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Energies of the $1s$, $2s$, $3s$, and $4s$ states are obtained by a perturbation calculation and by a one-parameter variational calculation for a two-particle system interacting through a static screened Coulomb potential. The variational results are practically identical with those recently obtained by Rogers, Graboske, and Harwood by the numerical integration of the wave equation, except in the region very close to the critical screening.

## I. INTRODUCTION

The static screened Coulomb potential (SSCP)

$$V(r) = -e^2 e^{-\alpha r}/r , \tag{1.1}$$

where $\alpha$ is a screening parameter, occurs in several fields of physics. In nuclear physics it goes under the name of the Yukawa potential (with $e^2$ replaced by another coupling constant), and in plasma physics it is commonly known as the Debye-Hückel potential. Equation (1.1) also describes the potential of an impurity in a metal and in a semiconductor. The significance of $\alpha$ in these different contexts is, of course, all different.

During the last few years a number of studies[1-14] have been carried out to calculate the energy levels of an electron in such a potential and also to determine the number of bound states. Since the Schrödinger equation for Eq. (1.1) is not solvable analytically, the aforesaid investigations have employed perturbation theory,[6,13] the variational method,[2-4,12] and the actual numerical integration[5,9,14] of the differential equation. Of these, the recent results of Rogers *et al.*,[14] obtained by numerical techniques, are of high accuracy over a wide range of the screening parameter and cover 45 eigenstates. In the present paper we show that at least for "$s$" states, using analytical methods, one can obtain results quite comparable to those of Rogers *et al.*[14] except in the region very close to the critical screening. We give results for the 1*s*, 2*s*, 3*s*, and 4*s* states only, but the method can be extended to higher "*s*" states without any difficulty. The features in which the present study differs from the previous work are indicated in the following plan of the paper. We have made use of the fact that the Hulthên potential[15] is a close approximation to Eq. (1.1) for not too large values of $\alpha$. In Sec. II we outline the solution of the Schrödinger equation for the Hulthên potential. In Sec. III we carry out a first-order perturbation calculation, using the Hulthên potential as the unperturbed potential, and show that when $\alpha$ is not too large, the resulting energy values show improvement over the previous first-order perturbation calculations.[6] Section IV deals with an application of the variation method to the problem. In such calculations, of practical importance is the economy of parameters necessary to achieve a given accuracy of the eigenvalue. With a single variational parameter, we have been able to obtain energy eigenvalues which are practically identical with the best available values[14] obtained by numerical techniques, except at the very highest values of $\alpha$, and are very close to the three-parameter variational results of Harris[4] for the 1s and 2s states.

## II. EIGENFUNCTIONS AND EIGENVALUES FOR HULTHÊN POTENTIAL

For our problem, we write the Hulthên[15] potential in the form

$$V(r) = -e^2 \frac{\alpha e^{-\alpha r}}{1-e^{-\alpha r}} \ . \tag{2.1}$$

When $\alpha$ is small, it tends to the potential of Eq. (1.1). It is possible to solve the Schrödinger equation for the potential (2.1) for $l=0$ states. In the following, we adapt Hulthên's treatment to our problem.

The radial Schrödinger equation for $l=0$, for the potential (2.1), is

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + e^2\frac{\alpha e^{-\alpha r}}{1-e^{-\alpha r}} + E\right)\psi_n(r) = 0 \ , \tag{2.2}$$

where $\psi_n(r) = rR_n(r)$. Using atomic units (unit of length $a_0 = \hbar^2/me^2$ and unit of energy $= -me^4/\hbar^2$), Eq. (2.2) can be written as

$$\left(\frac{1d^2}{2dr^2} + \frac{\delta e^{-\delta r}}{1-e^{-\delta r}} - \frac{a_n^2\delta^2}{2}\right)\psi_n(r) = 0 \ , \tag{2.3}$$

where $\delta = \alpha a_0$, a dimensionless quantity, and for $E$ we have substituted

$$E = \tfrac{1}{2}a_n^2\delta^2 \ . \tag{2.4}$$

For solving (2.3) we make the transformation

$$\psi_n(r) = e^{-a_n\delta r}\phi_n(r), \quad y = 1-e^{-\delta r} \tag{2.5}$$

and substitute

$$\beta_n = 1 + 2a_n \ . \tag{2.6}$$

Then (2.3) becomes

$$y(1-y)\frac{d^2\phi_n}{dy^2} - \beta y\frac{d\phi_n}{dy} + \frac{2}{\delta}\phi_n = 0 \ . \tag{2.7}$$

The solution of the differential equation (2.7) has the form

$$\phi_n = y^\rho \sum_{\nu=0}^{\infty} c_\nu y^\nu = \sum_{\nu=0}^{\infty} c_\nu y^{\nu+\rho} \ .$$

Substituting it in (2.7), we get the following recursion relation for $c_\nu$'s:

$$c_{\nu+1} = \frac{\nu(\nu-1)+\beta_n\nu - 2/\delta}{\nu(\nu+1)} c_\nu, \quad \nu \geq 1 \ . \tag{2.8}$$

To have physical meaning, the wave function $\phi(r)$ must be finite, so that the infinite series should terminate somewhere—say, at $\nu = n$—to become a polynomial; thus $c_\nu = 0$ for $\nu > n$. This gives

$$n(n-1) + \beta_n n - 2/\delta = 0$$

or

$$\beta_n = 2/n\delta - n + 1 \ . \tag{2.9}$$

Using (2.6), this gives

$$a_n = \tfrac{1}{2}(2/n\delta - n) \ . \tag{2.10}$$

In conjunction with (2.4), this gives the eigenvalue. The normalized eigenfunction is found to be

$$\psi_n(r) = \left[\frac{\delta(\beta_n-1)(\beta_n+2n-1)}{2(\beta_n+n-1)}\right]^{1/2} e^{-a_n\delta r}$$

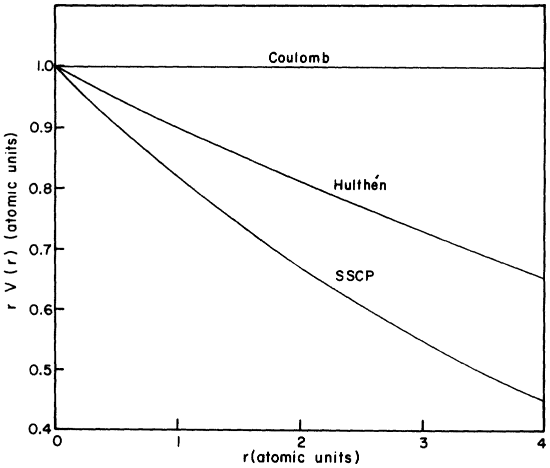

FIG. 1. Product $rV(r)$ as a function of $r$, for the Coulomb potential, the Hulthên potential, and the SSCP, for $\delta = 0.2$.

TABLE I. Energy eigenvalues as a function of screening parameter for the 1*s* state.

| Screening parameter $\delta$ | Our results Perturbation | Our results Variational | Smith (Ref. 6) (perturbation) | Harris (Ref. 4) (three-parameter variational) | Rogers *et al.* (Ref. 14) (numerical) |
|---|---|---|---|---|---|
| 0.001 | 0.499 00 | 0.499 00 | 0.499 00 | | |
| 0.002 | 0.498 00 | 0.498 00 | 0.498 00 | | 0.498 0 |
| 0.005 | 0.495 02 | 0.495 02 | 0.495 02 | | 0.495 0 |
| 0.01 | 0.490 07 | 0.490 07 | 0.490 07 | | 0.490 1 |
| 0.02 | 0.480 30 | 0.480 30 | 0.480 30 | | 0.480 3 |
| 0.025 | 0.475 46 | 0.475 46 | 0.475 46 | | 0.475 5 |
| 0.03 | 0.470 66 | 0.470 66 | 0.470 66 | | |
| 0.04 | 0.461 17 | 0.461 17 | 0.461 17 | | |
| 0.05 | 0.451 82 | 0.451 82 | 0.451 81 | 0.451 82 | 0.451 8 |
| 0.06 | 0.442 60 | 0.442 60 | 0.442 60 | | |
| 0.07 | 0.433 51 | 0.433 52 | 0.433 51 | | |
| 0.08 | 0.424 56 | 0.424 57 | 0.424 56 | | |
| 0.09 | 0.415 74 | 0.415 75 | 0.415 73 | | |
| 0.10 | 0.407 04 | 0.407 06 | 0.407 03 | | 0.407 1 |
| 0.20 | 0.326 58 | 0.326 81 | 0.326 45 | | 0.326 8 |
| 0.25 | 0.290 43 | 0.290 92 | 0.290 12 | 0.290 92 | 0.290 9 |
| 0.30 | 0.256 74 | 0.257 63 | 0.256 14 | 0.257 64 | |
| 0.40 | 0.196 10 | 0.198 36 | 0.194 44 | 0.198 38 | |
| 0.50 | 0.143 58 | 0.148 08 | 0.140 00 | 0.148 12 | 0.148 1 |
| 0.60 | 0.098 33 | 0.106 08 | 0.091 72 | 0.106 33 | |
| 0.70 | 0.059 68 | 0.071 74 | 0.048 70 | 0.071 83 | |
| 0.80 | 0.027 08 | 0.044 59 | 0.010 20 | 0.044 70 | |
| 0.90 | 0.000 09 | 0.024 18 | −0.024 38 | 0.024 30 | |
| 1.0 | −0.021 65 | 0.010 16 | | 0.010 23 | 0.010 29 |
| 1.05 | | 0.005 44 | | 0.005 46 | |
| 1.10 | | 0.002 20 | | 0.002 12 | |
| 1.15 | | 0.000 41 | | 0 | |
| 1.20 | | 0.000 04 | | | |

$$\times \sum_{\nu=1}^{n} (-1)^{\nu-1} \binom{n-1}{\nu-1} \binom{n+\beta+\nu-2}{\nu} (1-e^{-\delta r})^{\nu} \,. \tag{2.11}$$

## III. PERTURBATION CALCULATION

The SSCP, Eq. (1.1), can be written as a Hulthén potential plus a perturbation $U(r)$:

$$V(r) = \frac{\delta e^{-\delta r}}{1-e^{-\delta r}} + \left( \frac{e^{-\delta r}}{r} - \frac{\delta e^{-\delta r}}{1-e^{-\delta r}} \right) \tag{3.1}$$

$$= \frac{\delta e^{-\delta r}}{1-e^{-\delta r}} + U(r) \,. \tag{3.2}$$

Now $U(r)$ is treated as a perturbing potential. The eigenvalues for the unperturbed Hulthén potential are known from Eq. (2.4). In Fig. 1, we show the SSCP, the Hulthén potential, and the Coulomb potential. Note that the choice of the Hulthén potential as the unperturbed potential is a better one than that of a Coulomb potential[6] for the same.

The integrals involved in obtaining the perturbation energy are somewhat complicated, but can be analytically evaluated. The final expressions for the energy eigenvalues of the 1*s*, 2*s*, 3*s*, and 4*s* states, obtained from the perturbation calculation, are

$$E_{1s} = -\frac{4-\delta^2}{8} + \frac{4-\delta^2}{\delta^2} \left[ 2\ln(1+\tfrac{1}{2}\delta) - \ln(1+\delta) \right] \quad (\delta < 2), \tag{3.3}$$

$$E_{2s} = -\frac{1-4\delta^2}{8} + \frac{1-4\delta^2}{8\delta^4} \left[ -(1-\delta)^2 \ln(1-\delta) - 2(3-\delta^2)\ln(1+\delta) - 4(1+\delta)\ln(1+2\delta) - (1+\delta)^2 \ln(1+3\delta) \right] \quad (\delta < 0.5), \tag{3.4}$$

$$\begin{aligned} E_{3s} = -\frac{4-81\delta^2}{72} + \frac{4-81\delta^2}{196\,83\delta^6} \big[ & -(1-3\delta)^2(2-3\delta)^2 \ln(1-3\delta) + 6(1-3\delta)(2-3\delta)^2 \ln(1-\tfrac{3}{2}\delta) \\ & + 2(4-9\delta^2)(10-9\delta^2)\ln(1+\tfrac{3}{2}\delta) - 3(2+3\delta)(10+15\delta-18\delta^2)\ln(1+3\delta) \\ & + 6(2+3\delta)^2(1+3\delta)\ln(1+\tfrac{9}{2}\delta) - (2+3\delta)^2(1+3\delta)^2 \ln(1+6\delta) \big] \quad (\delta < 0.22), \end{aligned} \tag{3.5}$$

TABLE II. Energy eigenvalues as a function of screening parameter for the 2s state.

| Screening parameter $\delta$ | Our results Perturbation | Our results Variational | Smith (Ref. 6) (perturbation) | Harris (Ref. 4) (three-parameter variational) | Rogers *et al.* (Ref. 14) (numerical) |
|---|---|---|---|---|---|
| 0.001 | 0.12400 | 0.12400 | 0.12400 | | |
| 0.002 | 0.12301 | 0.12301 | 0.12301 | | 0.1230 |
| 0.005 | 0.12007 | 0.12007 | 0.12007 | | 0.1201 |
| 0.01 | 0.11529 | 0.11529 | 0.11529 | | 0.1153 |
| 0.02 | 0.10615 | 0.10615 | 0.10615 | | 0.1062 |
| 0.025 | 0.10177 | 0.10178 | 0.10177 | | 0.1018 |
| 0.03 | 0.09753 | 0.09753 | 0.09752 | | |
| 0.04 | 0.08940 | 0.08941 | 0.08939 | | |
| 0.05 | 0.08173 | 0.08177 | 0.08170 | 0.08177 | 0.08175 |
| 0.06 | 0.07450 | 0.07458 | 0.07445 | | |
| 0.07 | 0.06768 | 0.06782 | 0.06759 | | |
| 0.08 | 0.06125 | 0.06146 | 0.06111 | | |
| 0.09 | 0.05519 | 0.05551 | 0.05498 | | |
| 0.10 | 0.04948 | 0.04993 | 0.04917 | 0.04993 | 0.04993 |
| 0.20 | 0.00852 | 0.01208 | 0.00521 | 0.01206 | 0.01211 |
| 0.25 | −0.00306 | 0.00336 | −0.00980 | 0.00321 | 0.00339 |
| 0.30 | | 0.00008 | | 0 | |

$$E_{4s}=-\frac{1-64\delta^2}{32}+\frac{1-64\delta^2}{589824\delta^8}\left[-(1-6\delta)^2(1-4\delta)^2(1-2\delta)^2\ln(1-6\delta)+8(1-6\delta)(1-4\delta)^2(1-2\delta)^2\ln(1-4\delta)\right.$$
$$-4(1-4\delta)(1-2\delta)^2(7-28\delta-36\delta^2)\ln(1-2\delta)-2(1-2\delta)(1+2\delta)(35-380\delta+576\delta^2)\ln(1+2\delta)$$
$$+8(1-2\delta)(1+2\delta)(1+4\delta)(7+14\delta-6\delta^2)\ln(1+4\delta)-4(1+2\delta)^2(1+4\delta)(7+28\delta-36\delta^2)\ln(1+6\delta)$$
$$\left.+8(1+2\delta)^2(1+4\delta)^2(1+6\delta)\ln(1+8\delta)-(1+2\delta)^2(1+4\delta)^2(1+6\delta)^2\ln(1+10\delta)\right]\quad(\delta<0.125). \qquad (3.6)$$

The calculated energy values from the above expressions are shown in Tables I–IV, and are compared with several other calculations including those of Smith,[6] who carried out a perturbation calculation with the Coulomb potential as the unperturbed potential. We may add here a remark about the calculations. When $\delta$ is small, there are large cancellations between the terms occur-

TABLE III. Energy eigenvalues as a function of screening parameter for the 3s state.

| Screening parameter $\delta$ | Our results Perturbation | Our results Variational | Smith (Ref. 6) (perturbation) | Harris (Ref. 4) (one-parameter variational) | Rogers *et al.* (Ref. 14) (numerical) |
|---|---|---|---|---|---|
| 0.001 | 0.05456 | 0.05456 | 0.05456 | | |
| 0.002 | 0.05358 | 0.05358 | 0.05358 | | 0.0536 |
| 0.005 | 0.05072 | 0.05072 | 0.05072 | | 0.0507 |
| 0.01 | 0.04620 | 0.04620 | 0.04620 | | 0.04620 |
| 0.02 | 0.03801 | 0.03802 | 0.03800 | 0.03802 | 0.03802 |
| 0.025 | 0.03430 | 0.03433 | 0.03429 | | 0.03433 |
| 0.03 | 0.03084 | 0.03089 | 0.03080 | | |
| 0.04 | 0.02456 | 0.02469 | 0.02447 | 0.02474 | |
| 0.05 | 0.01907 | 0.01935 | 0.01888 | | 0.01935 |
| 0.06 | 0.01430 | 0.01479 | 0.01393 | 0.01499 | |
| 0.07 | 0.01017 | 0.01095 | 0.00954 | | |
| 0.08 | 0.00663 | 0.00777 | 0.00564 | 0.00829 | |
| 0.09 | 0.00361 | 0.00520 | 0.00215 | | |
| 0.10 | 0.00109 | 0.00320 | −0.00096 | 0.00425 | 0.00321 |
| 0.11 | −0.00097 | 0.00172 | | | |
| 0.12 | | 0.00072 | | 0.00230 | |
| 0.14 | | 0.00000 | | 0.00144 | |
| 0.30 | | | | −0.00001 | |

TABLE IV. Energy eigenvalues as a function of screening parameter for the 4s state.

| Screening parameter $\delta$ | Our results Perturbation | Our results Variational | Smith (Ref. 6) (perturbation) | Harris (Ref. 14) (one-parameter variational) | Rogers *et al.* (Ref. 14) (numerical) |
|---|---|---|---|---|---|
| 0.001 | 0.030 26 | 0.030 26 | 0.030 26 | | 0.030 26 |
| 0.002 | 0.029 30 | 0.029 30 | 0.029 30 | | 0.029 30 |
| 0.0025 | 0.028 82 | 0.028 82 | 0.028 82 | | 0.028 83 |
| 0.005 | 0.026 54 | 0.026 54 | 0.026 54 | | 0.026 54 |
| 0.01 | 0.022 35 | 0.022 36 | 0.022 35 | | 0.022 36 |
| 0.02 | 0.015 33 | 0.015 38 | 0.015 30 | 0.015 40 | 0.015 38 |
| 0.025 | 0.012 40 | 0.012 50 | 0.012 33 | | 0.012 51 |
| 0.03 | 0.009 80 | 0.009 99 | 0.009 67 | | |
| 0.04 | 0.005 50 | 0.005 96 | 0.005 14 | 0.006 17 | |
| 0.05 | 0.002 23 | 0.003 09 | 0.001 46 | | 0.003 09 |
| 0.06 | −0.000 15 | 0.001 24 | −0.001 55 | 0.001 98 | |
| 0.07 | | 0.000 25 | | | |
| 0.08 | | 0.000 00 | | 0.000 85 | |
| 0.10 | | | | 0.000 48 | |
| 0.12 | | | | 0.000 29 | |

ring in Eqs. (3.3)–(3.6), and an accuracy greater than 16 significant figures is required. The computer available to us (IBM 360/65) has only 16-figure accuracy in "double precision." Energy eigenvalues for such values of $\delta$ (more specifically, when $\delta < 0.0045$ for the 2s state, $\delta < 0.007$ for the 3s state, and $\delta < 0.02$ for the 4s state) were obtained by expanding the logarithmic terms.

## IV. VARIATIONAL CALCULATION

Fisher and Krylovich[2] have reported results on the 1s, 2s, 2p, and 3d states from a variational calculation. The wave functions were chosen such that in the limiting cases they tended to the corresponding hydrogen functions, and had two parameters. The results of these authors are given only in a figure and it is difficult to estimate the accuracy of their results. Authors of Refs. 3, 4, and 12 have used hydrogenlike wave functions as a basis set and the exponential nuclear charge as a variational parameter. Of these, the best results are those of Harris with three variational parameters. In view of the fact that the Hulthên potential is a better approximation to the SSCP than the Coulomb potential, one anticipates that for the same number of parameters, the Hulthên wave functions would be a better choice for trial functions in our problem than the hydrogenlike wave functions.

The trial functions chosen were of the form (2.11) with $\mu$, a variational parameter, replacing $\delta$. For example, for the 1s state, the trial wave function was

$$\psi_{1s} = (4/\mu^2 - 1)^{1/2}[e^{-(1-\mu/2)r} - e^{-(1+\mu/2)r}] \; . \qquad (4.1)$$

The expressions for the energies of the 1s, 2s, 3s, and 4s states are

$$E_{1s} = (4/\mu^2 - 1)[-\tfrac{1}{8}\mu^2 - \ln(2+\delta-\mu) + 2\ln(2+\delta) - \ln(2+\delta+\mu)] \quad (2\mu - \delta < 2), \qquad (4.2)$$

$$E_{2s} = [(1-4\mu^2)/8\mu^4][-\mu^4 - (\mu-1)^2\ln(1+\delta-2\mu) + 4(1-\mu)\ln(1+\delta-\mu) - 2(3-\mu^2)\ln(1+\delta) + 4(1+\mu)\ln(1+\delta+\mu) - (1+\mu)^2\ln(1+\delta+2\mu)] \quad (3\mu - \delta < 1), \qquad (4.3)$$

$$E_{3s} = [(4-81\mu^2)/78732\mu^6][-2187\mu^6/2 - (2-6\mu)^2(2-3\mu)^2\ln(2+3\delta-9\mu) + 12(2-6\mu)(2-3\mu)^2\ln(2+3\delta-6\mu) - 12(2-3\mu)(10-15\mu-18\mu^2)\ln(2+3\delta-3\mu) + 8(4-9\mu^2)(10-9\mu^2)\ln(2+3\delta) - 12(2+3\mu)(10+15\mu-18\mu^2)\ln(2+3\delta+3\mu) + 12(2+3\mu)^2(2+6\mu)\ln(2+3\delta+6\mu) - (2+3\mu)^2(2+6\mu)^2\ln(2+3\delta+9\mu)] \quad (12\mu - 3\delta < 2), \qquad (4.4)$$

$$E_{4s} = [(1-64\mu^2)/589824\mu^8][-18432\mu^8 - (1-6\mu)^2(1-4\mu)^2(1-2\mu)^2\ln(1+2\delta-8\mu) + 8(1-6\mu)(1-4\mu)^2(1-2\mu)^2\ln(1+2\delta-6\mu) - 4(1-4\mu)(1-2\mu)^2(7-28\mu-36\mu^2)\ln(1+2\delta-4\mu) + 8(1-4\mu^2)(1-4\mu)(7-14\mu-24\mu^2)\ln(1+2\delta-2\mu) - 2(1-4\mu^2)(35-380\mu^2+576\mu^4)\ln(1+2\delta)$$

$$+8(1-4\mu^2)(1+4\mu)(7+14\mu-24\mu^2)\ln(1+2\delta+2\mu)-4(1+4\mu)(1+2\mu)^2(7+28\mu-36\mu^2)\ln(1+2\delta+4\mu)$$
$$+8(1+6\mu)(1+4\mu)^2(1+2\mu)^2\ln(1+2\delta+6\mu)-(1+6\mu)^2(1+4\mu)^2(1+2\mu)^2\ln(1+2\delta+8\mu)] \quad (10\mu-2\delta<1), \tag{4.5}$$

The energy of the 1*s*, 2*s*, 3*s*, and 4*s* states were found by minimizing each with respect to $\mu$ separately. The values of $\mu$ thus obtained are recorded in Table V and the corresponding energies are given in Tables I-IV. The wave functions for the 2*s*, 3*s*, and 4*s* states with the given values of $\mu$ are not exactly orthogonal to the eigenfunctions of the corresponding lower states, but they are close to it, except when $\delta$ is large.

## V. COMPARISON OF NUMERICAL RESULTS

Tables I–IV also show the results obtained by Smith[6] (perturbation calculation), Harris[4] (variational calculation), and Rogers *et al.*[14] (numerical integration). The values shown under "Smith" were calculated by us from his expressions. Comparison of our perturbation results with those of Smith shows that our results are better in all the four cases, as anticipated.

If we round off our variational results to four significant figures, these are practically identical with those of Rogers *et al.* except when $\delta$ is very close to $\delta_c$. Here $\delta_c$, called the critical screening parameter, is that value of $\delta$ for which the binding energy of the level in question becomes zero. The accuracy of our results slowly decreases as $\delta$ increases from 0 to $\delta_c$; consequently, our method is not very suitable for a precise determination of $\delta_c$. However, it is a small price to pay, considering that for most of the range of $\delta$ it gives results of good accuracy with a single variational parameter. For the 1*s* state, our results compare very favorably with the three-parameter variational results of Harris. For $\delta = 0.05$ and 0.25, our variational results are identical with those of Harris to five significant figures; it appears to indicate that our variational results have at least five-figure accuracy below $\delta = 0.25$. Above $\delta = 0.25$, Harris's results are slightly better than ours. However, for the 2*s* state, our results are better than Harris's three-parameter variational results. Similar is the case for the 3*s* and 4*s* states: Harris's results in these cases were obtained by a one-parameter variational treatment.

TABLE V. Best values of the parameter $\mu$.

| Screening parameter $\delta$ | Parameter $\mu$ 1*s* | 2*s* | 3*s* | 4*s* |
|---|---|---|---|---|
| 0.001 | 0.0050 | 0.0100 | 0.0151 | 0.0171 |
| 0.002 | 0.0056 | 0.0100 | 0.0151 | 0.0171 |
| 0.005 | 0.0122 | 0.0121 | 0.0151 | 0.0181 |
| 0.01 | 0.0243 | 0.0240 | 0.0234 | 0.0231 |
| 0.02 | 0.0482 | 0.0468 | 0.0448 | 0.0424 |
| 0.025 | 0.0601 | 0.0579 | 0.0549 | 0.0515 |
| 0.03 | 0.0719 | 0.0688 | 0.0647 | 0.0602 |
| 0.04 | 0.0952 | 0.0900 | 0.0834 | 0.0763 |
| 0.05 | 0.1182 | 0.1105 | 0.1011 | 0.0909 |
| 0.06 | 0.1410 | 0.1304 | 0.1178 | |
| 0.07 | 0.1636 | 0.1496 | 0.1336 | |
| 0.08 | 0.1857 | 0.1684 | 0.1486 | |
| 0.09 | 0.2077 | 0.1866 | 0.1628 | |
| 0.10 | 0.2294 | 0.2044 | 0.1763 | |
| 0.20 | 0.4357 | 0.3613 | | |
| 0.25 | 0.5326 | 0.4283 | | |
| 0.30 | 0.6262 | 0.4893 | | |
| 0.40 | 0.8051 | | | |
| 0.50 | 0.9750 | | | |
| 0.60 | 1.1376 | | | |
| 0.70 | 1.2943 | | | |
| 0.80 | 1.4460 | | | |
| 0.90 | 1.5935 | | | |
| 1.0 | 1.7373 | | | |
| 1.05 | 1.8080 | | | |
| 1.1 | 1.8780 | | | |
| 1.15 | 1.9472 | | | |
| 1.2 | 2.0158 | | | |

An obvious advantage of having the wave function of a state of a system, in a compact analytical form, is that one can conveniently calculate other physical properties of the state, besides the energy. As an illustration, we have obtained the expectation value of the radius $\langle r\rangle$ for the 1*s* state from our variational wave function, with the result

$$\langle r\rangle = (12-\mu^2)/2(4-\mu^2). \tag{5.1}$$

Figure 2 shows the variation of $\langle r\rangle$ with $\delta$. In the vicinity of $\delta_c$, the "size" of the system is seen to increase rapidly with $\delta$. Now, in plasma physics, $\delta$ is proportional to $(\rho/kT)^{1/2}$, where $\rho$ is the density of

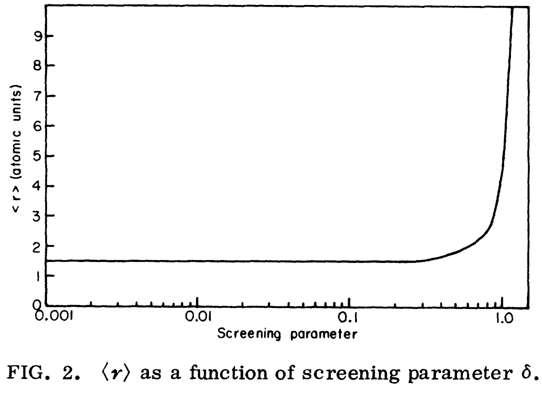

FIG. 2. $\langle r\rangle$ as a function of screening parameter $\delta$.

electrons. Clearly, beyond a certain value of $\delta$, the average radius would exceed one-half of the average internuclear separation at a given density and temperature. In this region, the approximation that the electron is bound to a single proton (or an ionized impurity) is no longer valid and one must take into account systems of the type $(\mathrm{S.C.})_2^+$, $(\mathrm{S.C.})_2$, etc. Here S. C. represents a neutral system (analogous to an H atom) in which the electron is bound in a SSCP.

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# Quasiminimum Principle for Multichannel Scattering

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A new variational principle for multichannel scattering is derived which combines certain simplifying features of both Kohn and minimum principles. The rigorous bound property of the latter is relaxed slightly to gain simplifications and efficiency, especially for collisions involving particle rearrangements. The approach is essentially equivalent to treating variationally the open-channel part of the wave function, rather than solving for it exactly as required by the minimum principle. However, variations of parameters for the open and closed channels are carried out separately using a double functional.

## I. INTRODUCTION AND SUMMARY

The variational principles for scattering problems of Kohn,[1] Hulthén,[2] and Schwinger[3] types do not provide bounds on scattering parameters. Because of this lack of bound property, scattering parameters calculated may fluctuate, often violently.[4] Nevertheless, it has been demonstrated[5] that meaningful stationary values can still be extracted by performing an extensive numerical analysis with large numbers of trial functions. The essential advantage of these methods lies in their simplicity of applications, as *all* the parameters introduced are determined variationally in a uniform fashion. There have also been several modifications of the principles to avoid the violent fluctuations due to spurious singularities. For example, the method developed by Harris[6] identifies the scattering energy to be one of these spurious points. Another approach[7] avoids the singularities altogether by analytically continuing to the complex energy values. These approaches still require a fair number of trial functions and their convergence is not always uniform. However, their applicability for simple scattering systems is reasonably well understood by now. We do not distinguish different versions of the methods and denote them in the following as the variational principles for scattering (VPS).

The minimum principles[8] and their generalizations[9] have been successfully applied to many of the low-energy scattering problems,[10–12] with the resulting bounds on scattering parameters. The procedure involved is considerably more complicated than that of the VPS, and gets rapidly worse as more reaction channels open up. Specifically, the complication arises from the requirement that the open-channel part of the scattering equations should be solved *exactly* numerically. Of course, this is necessary if the rigorous bounds are to be maintained. A recent calculation[12] of the positron-hydrogen pickup collision using the generalized varia-