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Variational solution of Schrödinger's equation for the static screened Coulomb potential[*]

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A variational method is used to obtain solutions to Schrödinger's equation for a particle in a static screened Coulomb potential. Energy eigenvalues are obtained for the lowest 45 states. The analytic wave functions generated by this method are used to obtain the probabilities for spontaneous emission in the dipole approximation as a function of screening length, for transitions between the six lowest states.

I. INTRODUCTION

Numerous authors[1-7] in the past have attempted to find solutions of Schrödinger's equation for a particle in a screened Coulomb potential. Probably the most extensive investigation on the subject is that by Rogers *et al.*[7] The wide interest in the problem stems from its application to problems in atomic, solid-state, and astrophysics. In particular, the well-known stellar-opacity code of Cox[8] makes use of the solution to first order in the screening length (the so-called "depression of the continuum"). We were primarily motivated by a desire to provide improved energy levels for opacity calculations but more important still to point out an omission in all such calculations, viz., the fact that transition probabilities may be significantly changed by screening effects due to free charged particles. This stimulated us to seek a method of solution which would (i) provide better energy levels than all other existing methods, (ii) enable transition probabilities to be readily calculated, and (iii) be easily reproducible by other workers in this general area. In Sec. II, we present a variational calculation of the energy eigenvalues as a function of screening length. Next, we discuss several reasons why we consider the variational method to be more advantageous than the numerical-integration technique used by Rogers *et al.*[7] In Sec. III we calculate spontaneous-emission probabilities in the dipole approximation for transitions between the lowest six states as a function of the Debye-Hückel screening length. To our knowledge this is the first calculation of such transition probabilities for a particle in a Debye-Hückel potential.

II. ENERGY LEVELS

The general form of our variational solution of Schrödinger's radial equation for a particle in a screened Coulomb potential is

TABLE I. Binding energies of states $1s$-$3d$ for static screened potential with $Z=1$ (in units of rydbergs).

D/a_0 \ State	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
1500	0.9987	0.2487	0.2487	0.1098	0.1098	0.1098
1000	0.9980	0.2480	0.2480	0.1091	0.1091	0.1091
700	0.9971	0.2472	0.2472	0.1083	0.1083	0.1083
500	0.9960	0.2460	0.2460	0.1072	0.1072	0.1072
200	0.9900	0.2401	0.2401	0.1014	0.1014	0.1014
100	0.9801	0.2306	0.2305	0.092 40	0.092 31	0.092 12
70	0.9717	0.2226	0.2224	0.085 12	0.084 94	0.084 58
40	0.9509	0.2036	0.2030	0.068 66	0.068 16	0.067 15
30	0.9350	0.1895	0.1886	0.057 44	0.056 62	0.054 94
20	0.9036	0.1635	0.1615	0.038 71	0.037 12	0.033 83
15	0.8731	0.1400	0.1366	0.024 32	0.021 95	0.016 95
9	0.7951	0.088 31	0.080 31	0.003 19	0.000 25	
8	0.7718	0.075 08	0.065 54	0.000 79		
7	0.7424	0.059 94	0.048 45			
5	0.6536	0.024 22	0.008 20			

$$R_{nl}(r) = \sum_{i} \sum_{k=l}^{n-1} a_{ik} r^{k} e^{-\alpha_i r} , \qquad (1)$$

where a_{ik} and α_i are parameters. The termination value of $n-1$ in the summation was chosen initially because it was observed that it corresponded to the termination value for the Coulomb potential. The justification for this termination value of k depended on whether or not the desired stability in the eigenenergies was achieved with the use of only those terms. As it turned out in the calculations, it was not even necessary to use all the terms in the k summation below this prechosen termination value of $n-1$. Use of the first several terms proved sufficient for our desired stability.

The various nonlinear parameters α_i are chosen input data, whereas the linear parameters a_{ik} are evaluated numerically in the course of diagonalization of the Hamiltonian. With regard to the choice of α_i values, we were guided by the fact that, for the hydrogen Coulomb wave functions, $\alpha = (2|\epsilon|)^{1/2} = n^{-1}$. Note that we conform to the eigenfunction and eigenenergy labeling of the Coulomb potential, that is, the lowest s state is denoted by $1s$, the second-lowest s state by $2s$, etc., although the numerical value is no longer associated with a "principal quantum number." This particular choice of the trial solution satisfies the

TABLE II. Binding energies of states $4s$–$9l$ for the static screened potential with $Z=1$ (in units of rydbergs × 10).

State D/a_0	1500	1000	700	500	200	100	70	40	30	20	15
$4s$	0.6118	0.6052	0.5969	0.5859	0.5307	0.4471	0.3831	0.2501	0.1701	0.0618	0.0099
$4p$	0.6118	0.6052	0.5969	0.5859	0.5305	0.4463	0.3814	0.2459	0.1638	0.0520	0.0013
$4d$	0.6118	0.6052	0.5969	0.5858	0.5301	0.4446	0.3782	0.2374	0.1507	0.0316	
$4f$	0.6117	0.6052	0.5968	0.5857	0.5294	0.4420	0.3732	0.2244	0.1302		
$5s$	0.3868	0.3804	0.3722	0.3615	0.3088	0.2332	0.1792	0.0805	0.0337		
$5p$	0.3868	0.3804	0.3722	0.3614	0.3086	0.2324	0.1778	0.0773	0.0296		
$5d$	0.3868	0.3803	0.3721	0.3613	0.3081	0.2309	0.1749	0.0708	0.0212		
$5f$	0.3868	0.3803	0.3721	0.3612	0.3075	0.2285	0.1705	0.0607	0.0082		
$5g$	0.3868	0.3803	0.3720	0.3611	0.3066	0.2253	0.1646	0.0465			
$6s$	0.2647	0.2583	0.2503	0.2399	0.1901	0.1235	0.0802	0.0163	0.0005		
$6p$	0.2647	0.2583	0.2503	0.2398	0.1899	0.1228	0.0790	0.0143			
$6d$	0.2647	0.2583	0.2502	0.2397	0.1895	0.1214	0.0766	0.0102			
$6f$	0.2647	0.2582	0.2502	0.2396	0.1889	0.1193	0.0730	0.0040			
$6g$	0.2646	0.2582	0.2501	0.2395	0.1880	0.1165	0.0679				
$6h$	0.2646	0.2582	0.2500	0.2393	0.1870	0.1128	0.0614				
$7s$	0.1911	0.1848	0.1770	0.1669	0.1204	0.0634	0.0311	0.0002			
$7p$	0.1911	0.1848	0.1769	0.1668	0.1202	0.0628	0.0302				
$7d$	0.1911	0.1848	0.1769	0.1668	0.1198	0.0616	0.0283				
$7f$	0.1910	0.1847	0.1768	0.1667	0.1192	0.0598	0.0254				
$7g$	0.1910	0.1847	0.1768	0.1665	0.1184	0.0573	0.0215				
$7h$	0.1910	0.1847	0.1767	0.1663	0.1174	0.0541	0.0163				
$7i$	0.1910	0.1846	0.1766	0.1661	0.1162	0.0502	0.0097				
$8s$	0.1433	0.1372	0.1295	0.1198	0.0769	0.0299	0.0084				
$8p$	0.1433	0.1372	0.1295	0.1198	0.0767	0.0294	0.0078				
$8d$	0.1433	0.1371	0.1295	0.1197	0.0764	0.0283	0.0065				
$8f$	0.1433	0.1371	0.1294	0.1196	0.0758	0.0268	0.0046				
$8g$	0.1433	0.1371	0.1294	0.1195	0.0751	0.0248	0.0019				
$8h$	0.1433	0.1370	0.1293	0.1193	0.0742	0.0221					
$8i$	0.1432	0.1370	0.1292	0.1191	0.0730	0.0188					
$8k$	0.1432	0.1369	0.1290	0.1189	0.0717	0.0148					
$9s$	0.1107	0.1047	0.0973	0.0880	0.0488	0.0117	0.0006				
$9p$	0.1107	0.1046	0.0972	0.0879	0.0486	0.0113					
$9d$	0.1106	0.1046	0.0972	0.0878	0.0483	0.0106					
$9f$	0.1106	0.1046	0.0971	0.0877	0.0478	0.0094					
$9g$	0.1106	0.1045	0.0970	0.0876	0.0471	0.0078					
$9h$	0.1106	0.1045	0.0969	0.0874	0.0462	0.0058					
$9i$	0.1106	0.1044	0.0968	0.0872	0.0452	0.0033					
$9k$	0.1105	0.1044	0.0967	0.0870	0.0440	0.0002					
$9l$	0.1105	0.1043	0.0966	0.0867	0.0426						

condition that the radial function associated with a particular Y_{lm} must have the asymptotic behavior r^l as $r \to 0$.

In general, 14 of the Slater-type orbitals were used to obtain at least seven-figure stability, although only two were needed for the ground state to obtain stability to the quoted figures. Good agreement is obtained between our variational results and the results obtained by Rogers *et al.*,[7] except for some particular cases noted below. We also find that, as expected, the binding energies of the states decrease with decreasing screening length. In addition, we agree with the conclusion of Rogers *et al.*[7] that, contrary to the remark of Rouse,[6] the number of bound energy states for a particle moving in a screened Coulomb potential is finite. In fact, this has been proved analytically by several authors.[9] Tables I and II give the binding energies with $Z = 1$ for the values of the screening length D for which some differences between our method and that of Rogers *et al.*[7] have been found. The crossing of the energy eigenvalues for different levels in the case of strong screening as described by Rogers *et al.*[7] is confirmed by us. Some slight differences are noted in the energies of some of the higher levels but these are usually only discrepancies in the last figure. The only major differences are as follows. Bound states not reported in Rogers *et al.*[7] but found in our calculations are: for $D = 100$, the $9i$

TABLE III. Transition probabilities $A_{ll'}$ for static screened potential.

Transitions D	$2p \to 1s$	$2p \to 2s$	$3s \to 2p$	$3p \to 1s$	$3p \to 2s$	$3p \to 3s$	$3d \to 2p$	$3d \to 3p$
1000 Wavelength	1215.0 Å		6561.5 Å	1025.2 Å	6561.4 Å		6561.4 Å	
$A_{ll'}$ [a]	6.27(0) [b]		6.33(−2)	1.68(0)	2.25(−1)		6.48(−1)	
700 Wavelength	1215.0 Å		6561.7 Å	1025.2 Å	6561.9 Å		6561.6 Å	
$A_{ll'}$	6.27(0)		6.33(−2)	1.68(0)	2.25(−1)		6.48(−1)	
500 Wavelength	1215.0 Å		6562.7 Å	1025.2 Å	6562.3 Å		6562.2 Å	
$A_{ll'}$	6.27(0)		6.33(−2)	1.68(0)	2.25(−1)		6.48(−1)	
300 Wavelength	1215.1 Å		6565.5 Å	1025.3 Å	6564.5 Å		6564.0 Å	
$A_{ll'}$	6.27(0)		6.32(−2)	1.68(0)	2.25(−1)		6.47(−1)	
200 Wavelength	1215.2 Å		6570.8 Å	1025.5 Å	6568.6 Å		6567.4 Å	
$A_{ll'}$	6.27(0)		6.30(−2)	1.67(0)	2.24(−1)		6.46(−1)	
100 Wavelength	1215.6 Å	948.03 μ	6599.0 Å	1026.4 Å	6590.0 Å	995.86 μ	6585.8 Å	497.14 μ
$A_{ll'}$	6.26(0)	2.14(−10)	6.23(−2)	1.66(0)	2.21(−1)	1.12(−9)	6.39(−1)	6.77(−9)
80 Wavelength	1215.9 Å	612.69 μ	6619.5 Å	1027.0 Å	6605.7 Å	651.50 μ	6599.4 Å	324.96 μ
$A_{ll'}$	6.25(0)	7.97(−10)	6.19(−2)	1.65(0)	2.19(−1)	4.02(−9)	6.35(−1)	2.45(−8)
60 Wavelength	1216.5 Å	350.26 μ	6663.1 Å	1028.4 Å	6638.8 Å	380.12 μ	6628.1 Å	189.26 μ
$A_{ll'}$	6.23(0)	4.28(−9)	6.09(−2)	1.63(0)	2.15(−1)	2.05(−8)	6.26(−1)	1.26(−7)
40 Wavelength	1218.4 Å	160.75 μ	6784.0 Å	1032.3 Å	6730.5 Å	181.82 μ	6708.5 Å	90.084 μ
$A_{ll'}$	6.18(0)	4.47(−8)	5.83(−2)	1.57(0)	2.04(−1)	1.94(−7)	6.01(−1)	1.21(−6)
30 Wavelength	1220.9 Å	93.348 μ	6949.8 Å	1037.5 Å	6855.4 Å	110.21 μ	6819.3 Å	54.125 μ
$A_{ll'}$	6.12(0)	2.30(−7)	5.50(−2)	1.51(0)	1.91(−1)	9.05(−7)	5.67(−1)	5.85(−6)
20 Wavelength	1227.9 Å	44.206 μ	7422.2 Å	1051.6 Å	7207.9 Å	57.327 μ	7138.8 Å	27.746 μ
$A_{ll'}$	5.93(0)	2.24(−6)	4.71(−2)	1.32(0)	1.57(−1)	7.21(−6)	4.82(−1)	5.11(−5)
15 Wavelength	1237.4 Å	26.496 μ	8115.1 Å	1070.7 Å	7716.0 Å	38.464 μ	7615.8 Å	18.250 μ
$A_{ll'}$	5.69(0)	1.08(−5)	3.78(−2)	1.10(0)	1.19(−1)	2.82(−5)	3.73(−1)	2.27(−4)
12 Wavelength	1249.3 Å	18.089 μ	9101.3 Å	1094.6 Å	8425.4 Å	30.424 μ	8321.9 Å	14.279 μ
$A_{ll'}$	5.40(0)	3.57(−5)	2.80(−2)	8.34(−1)	7.97(−2)	7.22(−4)	2.41(−1)	6.96(−4)
10 Wavelength	1263.8 Å	13.425 μ	1.0516 μ	1123.7 Å	9425.7 Å	28.142 μ		
$A_{ll'}$	5.06(0)	9.30(−5)	1.84(−2)	5.26(−1)	4.29(−2)	1.32(−4)		
9 Wavelength	1274.9 Å	11.384 μ	1.1817 μ	1146.5 Å	1.0347 μ	30.942 μ		
$A_{ll'}$	4.81(0)	1.60(−4)	1.24(−2)	2.70(−1)	1.92(−2)	1.47(−4)		
8 Wavelength	1290.3 Å	9.5472 μ	1.4074 μ					
$A_{ll'}$	4.47(0)	2.91(−4)	5.74(−3)					
7 Wavelength	1313.1 Å	7.9314 μ						
$A_{ll'}$	4.00(0)	5.62(−4)						
6 Wavelength	1348.9 Å	6.5883 μ						
$A_{ll'}$	3.30(0)	1.17(−3)						
5 Wavelength	1411.9 Å	5.6910 μ						
$A_{ll'}$	2.16(0)	2.61(−3)						

[a] $A_{ll'}$ is given in units of 10^8 sec^{-1}.

[b] $1.0(-1) \equiv 1.0 \times 10^{-1}$.

and $9k$ states; for $D=70$, the $8g$ state; and for $D=15$, the $4s$ and $4p$ states. The apparent discrepancy in the results for the $3s$ state for $D=7$ which Rogers *et al.*[7] quote in their Table I and which we fail to find is obviously a cataloging error made by them since they also quote the critical screening length for the $3s$ state as being 7.171 in their Table III.

We consider that the variational method described above is more advantageous than the numerical-integration method used by Rogers *et al.*[7] in the following respects.

(i) Rogers *et al.*[7] numerically solve the radial differential equation in a transformed space (ρ space) and not in the radial coordinate space (r space). The relation between ρ and r is given by

$$\rho = (2Z/a_0)r/\lambda_{nl}\,, \tag{2}$$

where λ_{nl} is related to the eigenenergies ϵ_{nl} by

$$\epsilon_{nl} = -Z^2\hbar^2/2a_0^2\mu\lambda_{nl}^2\,. \tag{3}$$

In addition, the screening parameter d used by Rogers *et al.*[7] is related to the Debye-Huckel screening length D by

$$d = (2Z/a_0)D/\lambda_{nl}\,. \tag{4}$$

Since the relation between D and d is proportional to the unknown eigenvalue ϵ_{nl}, an initial guess must be made for d and then using the calculated value of the eigenvalue for that choice of d, the Debye-Hückel screening length D may then be determined. An iterative procedure then must be followed until the choice of d with the calculated value of ϵ_{nl} yields the desired value of D. This procedure must then be repeated for every eigenenergy. Since calculations using the above-described variational method are done in r space, the desired Debye-Hückel screening length is immediately used and a single calculation yields the number of eigenenergies determined by the number of Slater orbitals used.

(ii) Since our method is based on the variational principle it has the advantage that the exact state energy exists as a lower bound to our eigenenergies. This is not true for numerical-integration techniques.

(iii) Our calculations were performed on an IBM 360-65 computer at a rate of 150 eigenenergies per minute, whereas Rogers *et al.*[7] used a CDC 6600 computer. Owing to the difference in machines, an exact comparison between the two methods of the computational time involved is not straightforward. However, a crude estimate can be obtained by comparing our calculation rate of 150 energies per minute on the IBM 360-65 with the calculation rate of Rogers *et al.*[7] which they obtained on a CDC 3600, namely, 14 eigenenergies per minute, since these two machines are roughly of comparable speed.

(iv) Our method is capable of providing analytic wave functions, and hence transition probabilities may be readily calculated.

III. SPONTANEOUS-EMISSION TRANSITION PROBABILITIES IN THE DIPOLE APPROXIMATION

In the electric dipole approximation, the probability that an atom will undergo a transition from a state l to a state l' and emit a photon of angular frequency $\omega_{ll'} = (E_l - E_{l'})/\hbar$ is given in the dipole-length representation by[10]

$$A_{l'l} = \frac{4e^2}{3\hbar c^3}\,\omega_{ll'}^3 |\langle l'|\vec{r}\,|l\rangle|^2\,. \tag{5}$$

For the screened Coulomb potential, the normal selection rules for spontaneous emission in the electric dipole approximation for a general spherically symmetric potential are valid. To our knowledge, no calculation of transition probabilities has been performed for the case of a particle in a Debye-Hückel potential. Thus, we have calculated transition probabilities for the six lowest-lying states, as a function of screening length. The results for $A_{l'l}$ are presented in Table III. Note that transitions within the same level are now possible for some values of the screening

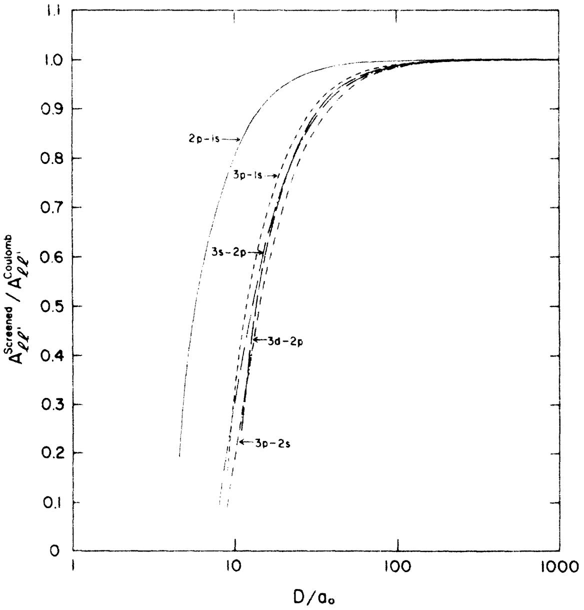

FIG. 1. Spontaneous-emission transition probabilities in the dipole approximation for the static screened Coulomb potential is shown as a function of the Debye-Hückel screening length.

length since the levels are no longer l degenerate. However, the probabilities for such transitions are very small for the large screening lengths owing to the small energy difference between the states. These transitions may be of importance for the case of very strong screening. In Fig. 1 we have plotted the transition probabilities as a function of screening length for all allowed transitions between levels for the three lowest levels.

We have also calculated the electric dipole transition probabilities in the dipole-momentum representation,[10] that is,

$$A_{l'l} = \frac{4e^2\hbar}{3\mu^2c^3}\omega_{ll'}|\langle l'|\vec{\nabla}|l\rangle|^2 . \qquad (6)$$

These results are in agreement with those obtained above in the dipole-length representation for all values of the screening length.

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