

Phase shifts of the static screened Coulomb potential

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Phase shifts and their weighted sum over angular momentum are reconsidered for the static screened Coulomb potential (SSCP). Results are given for both an attractive and a repulsive SSCP. The numerical results are derived in the present work from two independent and simple techniques based upon the Numerov method and the variable-phase approach, respectively, applied to the Sturm-Liouville form of the Schrödinger equation. Special emphasis is given to the high-density low-temperature domain ($\lambda_D < 10$ a.u.). Excellent agreement is found with results obtained previously by Rogers using the WKB approximation.

I. INTRODUCTION

In order to evaluate the statistical properties of dense two-component plasmas through the two-body interaction part of the partition function of interacting Boltzmann particles,

$$z_{\text{int}} = \sum_l (2l+1) \left[\sum_n e^{-E_{nl}/k_B T} + \pi^{-1} \int_0^\infty dk \frac{d\delta_l(k)}{dk} \exp\left(-\frac{\hbar^2 k^2}{2\mu k_B T}\right) \right], \quad (1)$$

(μ = reduced mass of the considered pair) we need to know the bound-state energies E_{nl} (attractive case only) and also the phase shifts $\delta_l(k)$ of the Schrödinger equation for the static screened Coulomb potential (Debye)

$$V(r) = \pm e^2 e^{-r/\lambda_D}/r. \quad (2)$$

Although considerable attention² has been given to the computation of the eigenvalues E_{nl} , equally important phase shifts have been relatively neglected. In an important recent paper, Rogers³ obtained very accurate $\delta_l(k)$ data through a clever mixing of the WKB approximation with difference techniques for the wave functions of the Schrödinger equation taken in the form

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + \left(k^2 - \frac{l(l+1)}{r^2} - V(r) \right) R(r) = 0. \quad (3)$$

We intend to come back to this problem with two main motivations: first, to confirm and to clarify the reasons for Rogers's success; second, to obtain phase shifts with an accuracy comparable to Rogers's results through different but sufficiently simple numerical techniques to be used by a non-specialist in the art of solving Schrödinger equations. In view of our special interest in plasmas with a few particles in the Debye sphere, we focus our attention on small values of λ_D ($10 < a_0$).

II. THE SSCP SCHRÖDINGER EQUATION

In order to easily check results of Rogers with simple but still accurate methods, it is convenient to start from the Sturm-Liouville form of the radial Schrödinger equation,

$$\frac{d^2 \psi_l}{dr^2} + \left(\epsilon - U(r) - \frac{l(l+1)}{r^2} \right) \psi_l = 0, \quad (4)$$

r being measured in units of the Bohr radius, with

$$\epsilon = (2\mu/\hbar^2)E = k^2, \quad U(r) = (2\mu/\hbar^2)V(r),$$

μ being the reduced mass of the interacting pair.

The free solutions [$U(r)=0$] of Eq. (4) are⁴

$$\psi_l^0(r) = kr j_l(kr) = \left(\frac{1}{2}\pi kr\right)^{1/2} J_{l+1/2}(kr) \quad (5a)$$

and

$$\phi_l^0(r) = kr n_l(kr) = \left(\frac{1}{2}\pi kr\right)^{1/2} J_{-l-1/2}(kr), \quad (5b)$$

in terms of the spherical Bessel $n_l(x)$ and Neumann functions $n_l(x)$. Therefore, the asymptotic ($r \rightarrow \infty$) solutions of Eq. (4) may be written as

$$\begin{aligned} \psi_l(kr) &= A_l kr j_l(kr) + B_l kr n_l(kr) \\ &= C_l kr [\cos\delta_l(k) j_l(kr) - \sin\delta_l(k) n_l(kr)], \end{aligned} \quad (6)$$

where

$$\tan\delta_l(k) = B_l/A_l, \quad (7)$$

and

$$\lim_{r \rightarrow \infty} \psi_l(r) = C_l \sin\left[kr - \frac{1}{2}l\pi + \delta_l(k)\right]. \quad (8)$$

In what follows we shall solve numerically the Sturm-Liouville differential equation (4) with a wave function iterated until the r value fulfilling

$$|u(r)| \ll \left| k^2 - \frac{l(l+1)}{r^2} \right|, \quad |r| \gg k[l(l+1)]^{1/2}, \quad (9)$$

is reached, and then equals it at two distinct asymptotic points r_1 and r_2 with a free solution.

Therefore the standard procedure yields⁴

$$\tan \delta_l(k) = \frac{r_1 \psi_l(kr_2) j_l(kr_1) - r_2 \psi_l(kr_1) j_l(kr_2)}{r_1 \psi_l(kr_2) n_l(kr_1) - r_2 \psi_l(kr_1) n_l(kr_2)}. \quad (10)$$

The Sturm-Liouville expression displayed in Eq. (4) suggests strongly the use of standard difference techniques.⁵ For our own purposes, we found it very convenient to apply the well-known Numerov procedure to Eq. (4) given as

$$\frac{d^2 \psi}{dr^2} = [A(r) - \epsilon] \psi(r) = f(r) \psi(r), \quad (11)$$

with a discrete mesh of unit step Δr and $\psi_j = \psi(j\Delta r)$, j being an integer.

III. VARIABLE-PHASE APPROACH

A. Preliminary remarks

A completely different approach to the phase-shift problem is afforded by the variable-phase approach,⁶ which disregards the scattered wave function. It is a complete and coherent alternative to the Schrödinger problem based upon the simple observation that any linear second-order differential equation may be transformed into an equivalent first-order nonlinear differential equation. This procedure will enable us to replace the Sturm-Liouville equation for the wave function with a differential equation for the phase shift alone. This approach is meaningful only for potentials sufficiently regular at $r=0$ with

$$\lim_{r \rightarrow 0} V(r) = V_0 r^{-m}, \quad m < 2, \quad (12)$$

(in this paper we have $V_0 = \pm e^2$, $m=1$) such that Eq. (4) has two independent solutions respectively proportional to r^{-l} and r^{l+1} when $r \rightarrow 0$. The condition (12) allows us to select a regular solution satisfying

$$\lim_{r \rightarrow 0} \psi_l(r) = \text{const} \times r^{l+1},$$

the asymptotic expression of which defines a phase shift δ_l , when it is compared to the asymptotic behavior of the free solution

$$\lim_{r \rightarrow \infty} \psi_l(r) = \text{const} \times \sin(kr - \frac{1}{2}l\pi + \delta_l). \quad (13)$$

The angular ambiguity in the definition of δ_l is finally removed by the condition

$$\lim_{k \rightarrow \infty} \delta_l(k) = 0.$$

B. Phase-shift expression

In order to derive the phase-shift differential equation, we consider Eq. (4) in the alternative integral expression

$$\psi_l(r) = \hat{j}_l(kr) - \frac{1}{k} \int_0^r ds [\hat{j}_l(kr) \hat{n}_l(ks) - \hat{j}_l(ks) \hat{n}_l(kr)] \times U(s) \psi_l(s). \quad (14)$$

$\hat{j}_l(x)$ and $\hat{n}_l(x)$ denote the Ricatti-Bessel functions:

$$\hat{j}_l(x) = (\frac{1}{2}\pi x)^{1/2} J_{l+1/2}(x), \quad (15)$$

$$\hat{n}_l(x) = (-)^{l+1} (\frac{1}{2}\pi x)^{1/2} J_{-(l+1/2)}(x),$$

with

$$\lim_{x \rightarrow 0} \hat{j}_l(x) = \left(\frac{x^{l+1}}{(2l+1)!!} \right) [1 + O(x^2)], \quad (16)$$

$$\lim_{x \rightarrow 0} \hat{n}_l(x) = -x^{-l} (2l-1)!! [1 + O(x^2)].$$

Following Calagero, let us introduce the scattering functions

$$S_l(r) = -k^{-1} \int_0^r dr' U(r') \hat{j}_l(kr') \psi_l(r'), \quad (17a)$$

$$C_l(r) = 1 - k^{-1} \int_0^r dr' U(r') \hat{j}_l(kr') \psi_l(r'), \quad (17b)$$

such that

$$\psi_l(r) = C_l(r) \hat{j}_l(kr) - S_l(r) \hat{n}_l(kr) \quad (18)$$

displays the asymptotic behavior

$$\lim_{r \rightarrow \infty} \psi_l(r) = C_l(\infty) \sin(kr - \frac{1}{2}l\pi) + S_l(\infty) \cos(kr - \frac{1}{2}l\pi) \quad (19)$$

obtained with the aid of ($x \gg l$)

$$\lim_{x \rightarrow \infty} \hat{j}_l(x) = \sin(x - \frac{1}{2}l\pi),$$

$$\lim_{x \rightarrow \infty} \hat{n}_l(x) = -\cos(x - \frac{1}{2}l\pi).$$

Therefore Eq. (19) may be given the form $\psi_l = \text{const} \times \sin(kr - \frac{1}{2}l\pi + \delta_l)$ with

$$\tan \delta_l = S_l(\infty) / C_l(\infty), \quad (20)$$

showing that the asymptotic values of S_l and C_l give, together with the condition $\lim_{k \rightarrow \infty} \delta_l(k) = 0$, the required phase shift.

Moreover the behavior of S_l and C_l at $r=0$ gives

$$\lim_{r \rightarrow 0} \frac{S_l(r)}{C_l(r)} = \frac{V_0 r^{-m}}{k^2 (2l+3-m)} \frac{(kr)^{2l+3}}{[(2l+1)!!]^2}, \quad (21)$$

while Eq. (20) shows

$$\lim_{r \rightarrow \infty} S_l(r) / C_l(r) = \tan \delta_l. \quad (22)$$

As a consequence, we are allowed to introduce the so-called phase function $t_l(r) = S_l / C_l(r)$ vanishing at the origin and equal to $\tan \delta_l$ at $r = \infty$.

C. Differential equation for the phase-shift function

We differentiate the equations that define the auxiliary functions S_l and C_l . We also use Eq. (14)

to substitute in the right-hand side. We thus secure the following system of two coupled first-order linear equations

$$S'_i(r) = -k^{-1}U(r)\hat{j}_i(kr) \times [C_i(r)\hat{j}_i(kr) - S_i(r)\hat{n}_i(kr)], \quad (23a)$$

$$C'_i(r) = -k^{-1}U(r)\hat{n}_i(kr) \times [C_i(r)\hat{j}_i(kr) - S_i(r)\hat{n}_i(kr)]. \quad (23b)$$

Now, we multiply the first equation by $C_i(r)$ and the second by $S_i(r)$, subtract the second equation from the first and divide by $C_i^2(r)$. In this manner we obtain

$$t'_i(r) = \frac{S'_i C_i - S_i C'_i}{C_i^2} = -k^{-1}U(r)[\hat{j}_i(kr) - t_i(r)\hat{n}_i(kr)]^2, \quad (24)$$

which is the required equation. This is a generalized Riccati equation, i.e., the simpler nonlinear differential equation. As is well-known the solution of a Riccati equation need not be bounded, it may have poles. This may happen in our case too, as implied by $t_i(r) = S_i(r)C_i^{-1}(r)$ and the fact that $C_i(r)$ might vanish. Therefore, we now make a further step, introducing another function $\delta_i(r)$ such that

$$t_i(r) = \tan \delta_i(r), \quad (25)$$

with

$$\lim_{r \rightarrow 0} \delta_i(r) = -\frac{V_0 r^{-m}}{k^2} \frac{(kr)^{2l+1}}{(2l+3-m)[(2l+1)!!]^2} \quad (26)$$

and

$$\lim_{r \rightarrow \infty} \delta_i(r) \equiv \delta_i(\infty) = \delta_i.$$

Inserting Eq. (25) into Eq. (24) we find for $\delta_i(r)$ the differential equation

$$\delta'_i(r) = -k^{-1}U(r)[\cos \delta_i(r)\hat{j}_i(kr) - \sin \delta_i(r)\hat{n}_i(kr)]^2, \quad (27)$$

easily solvable with the aid of the Runge-Kutta method and a variable step technique for the r values satisfying inequalities (9).

IV. NUMERICAL RESULTS

In order to ease the computation of quantities of physical interest, we rewrite Eq. (1) after an integration by parts in the form¹

$$Z_{\text{int}} = \sum_l (2l+1) \sum_n (e^{-E_{nl}/k_B T} - 1) + \frac{\pi \hbar^2}{\mu k_B T} \int_0^\infty k G_B(k) e^{-\hbar^2 k^2 / 2\mu k_B T}, \quad (28)$$

with

$$G_B(k) = \sum_l (2l+1) \delta_l(k), \quad (29)$$

for the Boltzmann sum phase shift. The sums (29) are evaluated under the condition that the first neglected term is smaller than 10^{-8} times the sum of the foregoing ones.⁷ We specialize our calculations to two important physical systems: electron-proton ($\mu \approx m_e$) and electron-electron ($\mu = \frac{1}{2}m_e$) pairs. In both cases, the quantities of physical interest, i.e., the scattered wave function $\psi_i(r)$ in the Numerov method, and the phase shift function $\delta_i(r)$ of the variable phase are considered for $r \geq R_0$ with

$$|U(R_0)| < \frac{1}{10^n} \left| k^2 - \frac{l(l+1)}{R_0^2} \right|, \quad R_0 \gg k[l(l+1)]^{1/2}, \quad (30)$$

which makes them R_0 -independent for $n \geq 7$. Our $G_B^-(k)$ values⁹ for the electron-proton system are given in Table I with significant figures common

TABLE I. Boltzmann-sum phase shifts (π rad) for the electron-proton system with k in a.u. Each entry $A n$ means $A \times 10^n$. The data below the double straight are obtained only through the Numerov method.

$k \backslash \lambda_D$	1	2	3	4	5	6
10^{-4}	9.996 42 -1	9.999 373 -1	1.001 20	1.999 18	4.999 55	5.000 06
10^{-3}	9.964 -1	9.993 7 -1	1.0120	1.9918	4.9955	
1.5×10^{-3}	9.946 4 -1	9.996 60 -1	1.018 00	1.987 76	4.993 34	
4.7×10^{-3}	9.832 2 -1	9.970 62 -1	1.055 49	1.961 94	4.978 94	
10^{-2}	9.643 9 -1	9.937 96 -1	1.111 15	1.921 51	4.953 60	
1.5×10^{-2}	9.467 86 -1	9.908 04 -1	1.153 4	1.888 40	4.926 9	
4.7×10^{-2}	8.420 90 -1	9.765 9 -1	1.2800	2.0605	4.7035	
10^{-1}	7.139 8 -1	9.923 01 -1	1.581 9	3.334 6	4.657 8	
1.5×10^{-1}	6.399 18 -1	1.070 0	2.050 2	3.665 2	5.244 99	
0.47	6.1820 -1	2.034 0	4.338 9	7.498 93	11.509 6	
1	9.976 9 -1	3.795 98	8.397 4	14.800	23.003	

TABLE II. Boltzmann-sum phase shifts (π rad) for the electron-electron system with k in a.u. When two data are available at the same place, the Numerov result is the upper one while the lower one is the variable phase approach.

$k \backslash \lambda_D$	1	2	3	4	5
10^{-4}	-2.167 92 - 5	-6.7372 - 5	-1.256 303 - 4	-1.923 02 - 4	-2.653 076 - 4
10^{-3}	-2.167 927 - 4	-6.737 296 - 4	-1.256 336 - 3	-1.923 134 - 3	-2.653 348 - 3
	-2.167 931 - 4	-6.737 301 - 4	-1.256 337 - 3	-1.923 135 - 3	-2.053 329 - 3
1.5×10^{-3}	-3.2518 - 4	-1.010 606 - 3	-1.884 569 - 3	-2.884 91 - 3	-3.980 54 - 3
4.7×10^{-3}	-1.018 95 - 3	-3.167 15 - 3	-5.908 19 - 3	-9.0498 - 3	-1.2498 - 2
10^{-2}	-2.168 23 - 3	-6.743 51 - 3	-1.259 73 - 2	-1.934 16 - 2	-2.680 441 - 2
1.5×10^{-2}	-3.2529 - 3	-1.012 70 - 2	-1.895 993 - 2	-2.921 859 - 2	-4.070 83 - 2
		-1.0127 - 2	-1.895 99 - 2	-2.9218 - 2	-4.0708 - 2
4.7×10^{-2}	-1.022 10 - 2	-3.229 82 - 2	-6.2375 - 2	-1.006 46 - 1	-1.483 80 - 1
		-3.2298 - 2			-1.4838 - 1
10^{-1}	-2.197 72 - 2	-7.287 73 - 2	-1.517 43 - 1	-2.6452 - 1	-4.161 99 - 1
					-4.162 00 - 1
1.5×10^{-1}	-3.348 26 - 2	-1.172 19 - 1	-2.577 85 - 1	-4.6563 - 1	-7.4724 - 1
	-3.3482 - 2				
4.7×10^{-1}	-1.2011 - 1	-4.9631 - 1	-1.1586	-2.1151	-3.3686
1	-2.8993 - 1	-1.2010	-2.7487	-4.9336	-7.7557

to both methods, thus showing an excellent agreement between the results of the two numerically independent approaches. The same agreement is also obtained for the repulsive case (electron-electron) shown in Tables II and III for Boltzmann and Fermi statistics.

The Fermi-sum phase shift for particles with spin s

$$G_F^+ = (s + 1) \sum_{l, \text{odd}} (2l + 1) \delta_l(k) + s \sum_{l, \text{even}} (2l + 1) \delta_l(k)$$

fulfills the relation

(31)

$$G_F^+ \approx s \sum_{l, \text{even}} (2l + 1) \delta_l(k) = \frac{1}{2} G_B^+, \quad k \leq 0.15, \quad (32)$$

in the case of strong screening ($\lambda_D < 2a_0$) emphasized in the present work, with important relative variations when $\lambda_D \geq 3a_0$. The repulsive sum phase shifts are seen to satisfy the effective range formula

$$G_B^+ = \sum_{l=0}^{\infty} (2l + 1) a_l k^{2l+1} (-1 + \frac{1}{2} a_l r_l k^2)^{-1}, \quad k < 0.2, \quad (33)$$

where⁸

TABLE III. Fermi-sum phase shifts with the caption of Table II.

$k \backslash \lambda_D$	1	2	3	4	5
10^{-4}	-1.083 96 - 5	-3.368 617 - 5	-6.281 517 - 5	-9.615 13 - 5	-1.326 541 - 4
			-6.281 515 - 5		
10^{-3}	-1.0839 - 4	-3.368 74 - 4	-6.282 145 - 4	-9.617 092 - 4	-1.327 012 - 3
				-9.617 089 - 4	
1.5×10^{-3}	-1.625 96 - 4	-5.053 34 - 4	-9.4244 - 4	-1.442 935 - 3	-1.991 41 - 3
4.7×10^{-3}	-5.0953 - 4	-1.584 55 - 3	-2.958 90 - 3	-4.5396 - 3	-6.2839 - 3
	-5.0954 - 4	-1.5845 - 3			
10^{-2}	-1.084 72 - 3	-3.381 19 - 3	-6.344 79 - 3	-9.811 78 - 3	-1.373 525 - 2
1.5×10^{-2}	-1.622 852 - 3	-5.095 27 - 3	-9.634 77 - 3	-1.508 029 - 2	-2.146 03 - 2
		-5.0953 - 3	-9.6347 - 3	-1.5080 - 2	-2.1460 - 2
4.7×10^{-2}	-5.1734 - 3	-1.709 23 - 2	-3.5578 - 2	-6.2863 - 2	-1.014 50 - 1
					-1.0145 - 1
10^{-1}	-1.157 54 - 2	-4.443 740 - 2	-1.083 62 - 1	-2.122 44 - 1	-3.596 23 - 1
1.5×10^{-1}	-1.862 52 - 2	-8.129 72 - 2	-2.095 375 - 1	-4.1201 - 1	-6.9115 - 1
		-8.129 73 - 2	-2.095 381 - 1		
4.7×10^{-1}	-9.2906 - 1	-4.5729 - 1	-1.1152	-2.0694	-3.3214
1	-2.6548 - 1	-1.1717	-2.7176	-4.9016	-7.7231

$$a_l = \frac{2^{2l}(l!)^2}{[(2l+1)!]^2} \frac{M_{2l+2}^2}{M_{2l+2} + (2/2l+2)N_{1,2l+2}} \quad (34)$$

and

$$\frac{1}{2}r_l = \frac{[(2l+1)!]^2}{2^{2l}(l!)^2(2l+3)} \left[-\frac{M_{2l+4}}{M_{2l+2}^2} + \frac{2}{(2l+1)M_{2l+2}^2} \right. \\ \left. \times \left(-2N_{1,2l+2} \frac{M_{2l+4}}{M_{2l+2}} - \frac{2}{2l-1} N_{3,2l+2} + N_{4,2l+4} \right) \right], \quad (35)$$

with

$$M_\mu = \int_0^\infty dr w(r)r^\mu,$$

$$N_{\mu,\nu} = \int_0^\infty dr w(r)r^\mu \int_0^r dr' w(r')r'^\nu, \quad (36)$$

and

$$w(r) = e^{-r/\lambda_D}/r,$$

while the attractive potential fulfills the Levinson relation $\delta_l(0) = n_l\pi$, a point already discussed at length by Rogers.³ Finally, in order to test the absolute accuracy of our calculations, we have compared our results with Rogers's previous results,³ for the attractive and repulsive cases (Tables IV and V). With the introduction of the reduced atomic units ($Z=1$) we get

$$a_\mu = \frac{\hbar^2}{\mu e^2}, \quad \epsilon = k^2 = \frac{2\mu a_\mu^2 E}{\hbar^2}, \quad U(r) = \frac{2a_\mu^2 \mu V(r)}{\hbar^2}.$$

The agreement is excellent, for we get back all of Rogers's results.³ This is an interesting result if one recalls that we solve the radial Schrödinger equation in the Sturm-Liouville form (4) instead of the expression (3) considered in Rogers's work. Moreover, we use two independent approaches with a different numerical treatment of the long-range part of the scattered wave function.

V. DISCUSSION

Although the above results look very encouraging, they do not by themselves provide any further in-

TABLE IV. Boltzmann-sum phase shifts for the electron-proton system with k in reduced atomic units. Upper data are Numerov's while the lower are the variable phase approach.

$k \backslash \lambda_D$	1	2	4	6
10^{-4}	9.997 481 - 1	9.999 55 - 1	1.999 423	5.000 048
10^{-3}	9.974 81 - 1	9.995 58 - 1	1.994 238	5.000 488
			1.994 23	5.000 48
10^{-2}	9.974 8518 - 1	9.956 10 - 1	1.943 490	5.005 15
	9.7485 - 1	9.956 - 1	1.9435	5.0050
10^{-1}	7.779 41 - 1	9.760 89 - 1	2.925 35	5.347 84
		9.7607 - 1	2.9252	5.3476
1	7.703 05 - 1		10.738 1	23.7539

sight in the relative merits of the different phase-shift calculations. Moreover, as far as we know there do not exist any clear formal relationships between the corresponding approximations. This point merits further study far beyond the scope of the present paper. There are certainly difficulties in our case in view of the various second-order differential equations used as a starting point [Eq. (3) for the WKB method,³ Eqs. (4) and (27) in the present work]. However, it appears useful if not necessary to point out some possible relationships. The first one is the obvious functional similarity shown by the first-order WKB results and the phase expression (27). Second, it is of interest to comment on the relative ease and accuracy of the different techniques. Our methods (variable phase and Numerov) seem well-suited for small λ_D ($\lambda_D \approx 15a_0$) and not too large an energy ($k \leq 2$ a.u.). They are both accurate, very easy to handle, and need only a little computation. Although the WKB method⁶ works well in the whole energy range, it seems quite tedious in the small energy range. On the contrary, WKB works with an increasing accuracy when k and l increase, and it appears easier to handle. Moreover it allows the use of the pseudoanalytic sum phase shift

TABLE V. Fermi-sum phase shifts for the electron-electron system with k in reduced atomic units.

$k \backslash \lambda_D$	1	2	4	6
10^{-4}	-1.684 308 - 5	-4.807 558 - 5	-1.279 43 - 4	-2.212 29 - 4
		-4.607 556 - 5		
10^{-3}	-1.684 32 - 4	4.807 80 - 4	-1.279 80 - 3	-2.214 02 - 3
10^{-2}	-1.685 88 - 3	-4.832 28 - 3	-1.315 598 - 2	-2.382 75 - 2
		-4.832 27 - 3		
10^{-1}	-1.835 25 - 2	-6.897 14 - 2	-3.353 30 - 1	-8.720 71 - 1
		-6.897 15 - 2		
1	-4.972 22 - 1	-2.232 09	-9.014 31	

$$G = \pm \frac{2\lambda_D^2 k}{\pi} + \frac{\lambda_D}{2\pi k} \mp \frac{\ln(\lambda_D k^2 4.61^{-1})}{3\pi k^3}, \quad (37)$$

where the top sign is for an attractive potential and the bottom sign for a repulsive potential.

These features show the superiority of the WKB approximation in the large- λ_D -large- k range because our methods are not so effective in this domain. First, the Numerov method becomes increasingly inaccurate as the number of nodes in the wave function in a distance on the order of the potential's effective range increases, i.e., for increasing energy and screening length. Moreover, Calogero's Eq. (27) appears difficult to manipulate numerically when $l > 15$ [see Eq. (26)]. For small k values, only a few terms are needed in the phase-shift sum, and the above limitation does not play any role. However, it becomes harmful for large k when the l sum has to run far beyond

$l = 15$ in order to secure the required accuracy. This drawback appears to be a serious one for $\lambda_D \geq 15a_0$.

As a provisional and technical conclusion, we may state that a clever mixing of the variable phase method with the WKB approximation should certainly provide the most valuable techniques for the evaluation of phase-shift sums, as far as the accuracy and the elegance of the numerical procedure are mostly concerned.

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⁴A. Messiah, *Mécanique Quantique* (Dunod, Paris, 1959), Vol. 1, Chap. 10.

⁵D. R. Hartree, *Numerical Analysis* (Clarendon,

Oxford, 1958), p. 142.

⁶F. Calogero, *Variable Phase Approach* (Academic, New York, 1967), Chap. 3.

⁷Although this statement does not appear *a priori* as a convincing one, it is sufficient to ensure that the neglected contribution is arbitrarily small because this latter is always located far beyond the maximum of $(2l+1)\delta_l(k)$. We thank Dr. M. Lavaud for bringing this point to our attention.

⁸H. Kruger, *Z. Phys.* **204**, 114 (1967).

⁹ G^- denotes the sum phase shift for an attractive potential, while G^+ corresponds to a repulsive one.