identical results were obtained in cells filled with both Ne and He buffer gases and with a variation in buffer-gas density of more than an order of magnitude. In addition, the same results were obtained with both an rf discharge and H^3 as the source of electrons.

---

*Work supported by the National Science Foundation.

[1] S. J. Davis and L. C. Balling, Phys. Rev. A **6**, 1479 (1972).

[2] N. Ioli, F. Strumia, and A. Moretti, J. Opt. Soc. Am. **61**, 1251 (1971).

[3] E. L. Lewis and A. Gallagher, J. Opt. Soc. Am. (to be published).

[4] D. L. Moores and D. W. Norcross, J. Phys. B **5**, 1482 (1972); D. W. Norcross (private communication).

[5] L. C. Balling, R. J. Hanson, and F. M. Pipkin, Phys. Rev. **133**, A607 (1964).

PHYSICAL REVIEW A VOLUME 8, NUMBER 2 AUGUST 1973

Critical Screening Parameters for the Generalized Screened Coulomb Potential

Gerald J. Iafrate
US Army Electronics Technology and Devices Laboratory (ECOM), Fort Monmouth, New Jersey 07703

(Received 15 January 1973)

An approximate expression for the critical screening parameters associated with the attractive generalized screened Coulomb potential (GSCP) is obtained by utilizing the variational principle and the virial theorem. Subject to certain conditions, this expression is shown to represent a lower bound to the true critical screening parameters associated with the GSCP. Specific results are reported for the bound states n, $l = n-1$ of the Debye-Hückel potential and for the ground state and first excited state of the exponential-cosine screened Coulomb potential.

I. INTRODUCTION

The generalized screened Coulomb potential (GSCP), mathematically expressed as

$$V(s) = -(Z/s)B(\lambda s), \quad B(0) = 1, \tag{1}$$

where Z is the nuclear charge and λ is the screening parameter, represents a wide class of potentials often encountered in plasma physics[1,2] and solid-state physics.[3,4] Typical examples of the above potential are the exponential screened Coulomb potential (ESCP), commonly known as the Debye-Hückel potential, with

$$B(\lambda s) = e^{-\lambda s}, \tag{1a}$$

and the exponential-cosine screened Coulomb potential (ESCSP), with

$$B(\lambda s) = e^{-\lambda s} \cos \lambda s. \tag{1b}$$

Recently, the bound-state properties of ESCP[3-7] and ECSCP[8,9] have received considerable attention. Particular emphasis has been devoted to the calculation of the critical screening parameter λ_c, the value of λ for which a given energy level is equal to its ionization limit. In this work, we present a simple method whereby a lower bound to λ_c can be obtained for the quantum states n, $l = n - 1$ of GSCP. The method involves the minimization of the total energy with respect to hydrogenic trial wave functions that are forced to obey a subsidiary condition, namely, the virial theorem.

II. CALCULATION OF λ_c^v

We now consider the calculation of λ_c^v[10] for the general state n, l of the GSCP. The method consists of minimizing the total energy with respect to the appropriate hydrogenic wave functions subject to the virial theorem and then determining λ_c^v by choosing λ such that the total energy is equal to its ionization limit. In general, the virial theorem for this problem is established via the variational principle, whereby the trial wave functions $\psi_{n,l}(Zs)$ and λ are subjected to scale transformations[11]

$$r = \eta s \tag{2a}$$

and

$$\rho = \lambda/\eta . \tag{2b}$$

The total variational energy then becomes

$$E_v(n, l, \eta, \lambda) = \eta^2 \bar{T} + \eta \bar{V}, \tag{3}$$

where

$$\bar{T} = (\psi_{n,l}(rZ), -\tfrac{1}{2}\nabla_r^2 \psi_{n,l}(rZ))/(\psi_{n,l}(rZ), \psi_{n,l}(rZ)) \tag{4}$$

and

$$\bar{V}=(\psi_{n,l}(rZ),\{-Ze^{-\rho r}/r\}\psi_{n,l}(rZ))/(\psi_{n,l}(rZ),\psi_{n,l}(rZ)). \tag{5}$$

In using the variational principle to determine η we use Eq. (3) to obtain

$$\frac{\partial E_v}{\partial\eta}=2\eta\bar{T}+\bar{V}+\eta\frac{\partial\bar{V}}{\partial\rho}\frac{\partial\rho}{\partial\eta}=0. \tag{6}$$

Letting

$$\frac{\partial\bar{V}}{\partial\rho}=\bar{V}_\rho, \tag{7}$$

and using the fact that

$$\frac{\partial\rho}{\partial\eta}=-\frac{\lambda}{\eta^2}\equiv-\frac{\rho}{\eta}, \tag{8}$$

Eq. (6) can be reexpressed as

$$2\bar{T}\eta+\bar{V}-\rho\bar{V}_\rho=0. \tag{9}$$

The determination of $\eta(\rho)$ from Eq. (9) ensures that the virial theorem is satisfied (see Appendix). In addition, selecting λ so that E_v in Eq. (3) is equal to E_I (the ionization limit), we then obtain

$$\bar{T}\eta^2+\bar{V}\eta=E_I. \tag{10}$$

Thus, Eqs. (9) and (10), together with Eq. (2b), are sufficient to determine λ_c^v. The simultaneous solutions to Eqs. (9) and (10) can be easily shown to yield

$$\bar{V}(\rho_c)\left[1+\rho_c\left(\frac{\partial}{\partial\rho}\ln\bar{V}(\rho)\right)_{\rho=\rho_c}\right]=2\rho_c\frac{E_I}{\lambda_c^v}, \tag{11}$$

as the equation determining ρ_c, η_c being given by

$$\eta_c=-\frac{\bar{V}(\rho_c)}{2\bar{T}}\left[1-\rho_c\left(\frac{\partial}{\partial\rho}\ln\bar{V}(\rho)\right)_{\rho=\rho_c}\right] \tag{12}$$

(ρ_c and η_c refer to the values of ρ and η for which $\lambda=\lambda_c^v$). It then follows from Eqs. (2b) and (12) that the approximate expression for the critical screening parameter is

$$\lambda_c^v=-\rho_c(\bar{V}(\rho_c)/\bar{T})[1-(E_I/\lambda_c^v)(\rho_c/\bar{V}(\rho_c))], \tag{13}$$

where ρ_c is determined from Eq. (11).[12] If the specific form of $B(\lambda s)$ in the GSCP dictates an ionization limit of $E_I=0$, then Eqs. (11)–(13) simplify and become

$$1+\rho_c\left(\frac{\partial}{\partial\rho}\ln\bar{V}(\rho)\right)_{\rho=\rho_c}=0, \tag{14}$$

$$\eta_c=-\bar{V}(\rho_c)/\bar{T}, \tag{15}$$

and

$$\lambda_c^v=-\rho_c(\bar{V}(\rho_c)/\bar{T}). \tag{16}$$

We note that if the trial wave function for a given state is orthogonal to all the exact wave functions corresponding to states of lower energy, then E_v for that state is an upper bound[13] to the exact energy and λ_c^v represents a lower bound to the true λ_c (now to be referred to as λ_c^T). The lower-bound theorem for λ_c follows from the argument that if

$$E_v(n,l,\eta_c,\lambda_c^v)=E_I, \tag{17a}$$

and, by the variational principle,

$$E_v(n,l,\eta_c,\lambda_c^v)>E_T(n,l,\lambda_c^v) \tag{17b}$$

(E_T referring to the true energy state for a given n, l, and λ_c^v), then

$$E_T(n,l,\lambda_c^v)<E_I, \tag{18}$$

and therefore

$$\lambda_c^v(n,l)<\lambda_c^T(n,l). \tag{19}$$

If the above-mentioned orthogonality is lacking, no such lower bound on λ_c^T can be claimed.

To take advantage of the inequality in Eq. (19), we restrict our variational calculation by using hydrogenic-state wave functions for arbitrary n, but with $l=n-1$. In this way, the trial wave function with $l=n-1$ is orthogonal to all the exact wave functions corresponding to states of lower energy with $l=0,1,2,\ldots,n-2$ due to the spherical harmonics orthogonality. The explicit form of the hydrogenic trial wave function for n, $l=n-1$ is

$$\psi_n(Zs)=N_ne^{-Zs/n}(Zs)^{n-1}Y_{n-1,m}(\theta,\phi), \tag{20}$$

which satisfies the equation

$$-\tfrac{1}{2}\nabla_s^2\psi_n(Zs)-(Z/s)\psi_n(Zs)=-\tfrac{1}{2}(Z^2/n^2)\psi_n(Zs). \tag{21}$$

Putting $\psi_n(Zs)$ of Eq. (20) into Eqs. (4) and (5), we obtain expressions for $\bar{T}$ and $\bar{V}$ as

$$\bar{T}=\tfrac{1}{2}(Z^2/n^2) \tag{22}$$

and

$$\bar{V}=-Z[(2Z/n)^{2n+1}/(2n)!]\int_0^\infty r^{2n-1}B(\rho r)e^{-2Zr/n}\,dr, \tag{23}$$

where $\bar{V}$ depends on the explicit form of $B(\rho r)$.

When $B(\rho r)$ corresponds to the ESCP [see Eq. (1a)], $\bar{V}$ in Eq. (23) reduces to

$$\bar{V}_{\text{ESCP}}=-(Z^2/n^2)[Z/(Z+n\rho/2)]^{2n}. \tag{24}$$

In addition, since the ionization limit for this potential is zero, Eq. (16) is appropriate for determining λ_c^v. In this regard, substituting $\bar{V}_{\text{ESCP}}$ of Eq. (24) into Eq. (14) yields

$$\rho_c=(Z+n\rho_c/2)/n^2. \tag{25}$$

Solving for ρ_c in Eq. (25) we see that

$$\rho_c=2Z/n(2n-1). \tag{26}$$

Utilizing Eqs. (24) and (26) in Eq. (16) results in

$$\lambda_c^v=(2Z/n^2)[(2n-1)/2n]^{2n-1}. \tag{27}$$

Comparing this value of λ_c^v to recently published numerical data[6] (see Table I) shows that the lower-bound theorem is indeed satisfied for the n, $l=n-1$ energy states.

When $B(\rho r)$ refers to the ECSCP [see Eq. (1b)], $\bar{V}$ of Eq. (23) reduces

$$\bar{V}_{\text{ECSCP}}=[Z/(2n)!\,](2Z/n)^{2n+1}\,\frac{\partial^{2n-1}}{\partial\beta^{2n-1}}\left(\frac{\beta}{\rho^2+\beta^2}\right), \tag{28}$$

where

$$\beta=(2Z/n)+\rho\,. \tag{29}$$

For this potential, the ionization limit is not zero, but is given by

$$E_I=V(s_0), \tag{30}$$

where s_0 is obtained from

$$\left.\frac{dV}{ds}\right|_{s=s_0}=0. \tag{31}$$

For the GSCP of Eq. (1), Eq. (31) becomes

$$B(R_0)-R_0\left.\frac{dB(R)}{dR}\right|_{R=R_0}=0, \tag{32}$$

with

$$R_0=\lambda s_0\,. \tag{33}$$

Notice that R_0 in Eq. (32) depends *only* on the specific form of $B(\lambda s)$ and *not* on the particular choice of λ. It then follows from Eq. (30) that

$$E_I=-\lambda Z B(R_0)/R_0, \tag{34}$$

indicating that E_I is linear in λ.

The presence of a cosine factor in $B(\lambda s)$ leads to an oscillatory behavior in the ECSCP, thereby allowing multiple values of R_0 to satisfy Eq. (32). The explicit form of Eq. (32) for this potential becomes

$$1+\tan R_0+1/R_0=0. \tag{35}$$

The first five roots of this equation have been given by Lam and Varshni,[9] the first of which is $R_0(1)=2.1712$. Thus, from Eq. (34), we see that E_I becomes

$$E_I=-\lambda Z e^{-R_0(1)}[\cos R_0(1)]/R_0(1). \tag{36}$$

This would necessitate the use of Eqs. (11) and (13) in obtaining λ_c^v. However, for purposes of comparison with Lam and Varshni,[9] we adopt their criterion that $E_I=0$ and proceed to use Eqs. (14) and (16) to calculate λ_c^v for the ground state of the ECSCP. With $n=1$, the expression for $\bar{V}$ in Eq. (28) becomes

$$\bar{V}_{\text{ECSCP}}=-16Z^4(\rho+Z)/(\rho^2+2Z\rho+2Z^2)^2\,. \tag{37}$$

TABLE I. Tabulation of λ_c/Z for the first five energy states with $l=n-1$.

n	(λ_c^v/Z) [a]	(λ_c^T/Z) [b]
1	1.0000	1.1906
2	0.2109	0.2202
3	0.0893	0.0914
4	0.0490	0.0498
5	0.0310	0.0313

[a] Data obtained from Eq. (27).

[b] Data obtained from exact numerical calculations of Ref. 6.

Putting $\bar{V}_{\text{ECSCP}}$ into Eqs. (14) and (16), we obtain

$$\rho_c=0.889Z \tag{38a}$$

and

$$\lambda_c^v=0.644Z. \tag{38b}$$

In addition, for $n=2$, $\bar{V}$ in Eq. (28) becomes

$$\bar{V}_{\text{ECSCP}}=-\tfrac{1}{4}Z^6(-4\rho^4-8Z\rho^3+4Z^3\rho+Z^4)$$
$$\times(\rho^2+2Z\rho+Z^2)^{-4}\,. \tag{39}$$

In this case, Eqs. (14) and (16) yield

$$\rho_c=0.175Z \tag{40a}$$

and

$$\lambda_c^v=0.146Z\,. \tag{40b}$$

Recently, Lam and Varshni[9] obtained critical screening parameters for numerous energy states of the ECSCP (with $Z=1$) by utilizing Hulthén-type wave functions in a variational calculation. They found, for the first two states with $l=n-1$, that

$$\lambda_c^{L-V}=0.712, \quad n=1 \tag{41}$$

$$\lambda_c^{L-V}=0.143, \quad n=2\,. \tag{42}$$

The screening parameters obtained in the present calculation for the ECSCP need not be lower than the results of Eqs. (41) and (42). This follows from the approximate nature of the calculation presented in Ref. 9. In fact, comparisons of Eq. (40b) with $Z=1$ and Eq. (42) show this to be the case.

APPENDIX: SATISFACTION OF VIRAL THEOREM

The virial theorem, for a spherically symmetric potential, is mathematically stated as

$$2\langle T\rangle=\left\langle s\,\frac{dV}{ds}\right\rangle, \tag{A1}$$

where the brackets indicate an expectation value with respect to an *exact* eigenstate of the Hamiltonian, $\mathcal{H} = T + V$. When the potential is taken to be the GSCP [see Eq. (1)], the virial theorem is reexpressed as

$$2\langle T \rangle = -\langle V \rangle + \lambda \left\langle \frac{dV}{d\lambda} \right\rangle. \tag{A2}$$

In obtaining Eq. (A2), use has been made of the fact that

$$\frac{dB(\lambda s)}{ds} = -\frac{\lambda}{Z}\frac{dV}{d\lambda}. \tag{A3}$$

When the exact wave function for the GSCP is not known, the virial theorem may still be satisfied by utilizing a variational procedure whereby an approximate trial wave function $\psi_{n,l}(Zs)$ and λ are subjected to the scale transformation of Eq. (2).[11] If we use $\psi_{n,l}(Z\eta s)$ as a trial wave function, with η as a variational parameter, and let $\rho = \lambda/\eta$, then the approximate expectation values for T and V become

$$\langle T \rangle (\eta) = \eta^2 \overline{T} \tag{A4}$$

and

$$\langle V \rangle (\eta) = \eta \overline{V}, \tag{A5}$$

where $\overline{T}$ and $\overline{V}$ are defined by Eqs. (4) and (5). The total variational energy then becomes

$$E_v(n, l, \eta, \lambda) = \eta^2 \overline{T} + \eta \overline{V}, \tag{A6}$$

as stated in Eq. (3) and the minimum energy condition of Eq. (9) follows directly. In multiplying the expression in Eq. (9) by η, we obtain

$$2\overline{T}\eta^2 + \overline{V}\eta - \rho\eta \overline{V}_\rho = 0. \tag{A7}$$

Making use of Eqs. (2b), (8), (A4), and (A5), Eq. (A7) becomes

$$2\langle T \rangle (\eta) = -\langle V \rangle (\eta) + \lambda \left\langle \frac{dV}{d\lambda} \right\rangle (\eta). \tag{A8}$$

Hence the virial theorem is established, provided that η is chosen to satisfy Eq. (A7) .

---

[1] G. M. Harris, Phys. Rev. **125**, 1131 (1962).

[2] H. Margenau and M. Lewis, Rev. Mod. Phys. **31**, 569 (1959).

[3] J. B. Krieger, Phys. Rev. **178**, 1337 (1969).

[4] V. Bonch-Bruevich and S. Tyablikov, *The Green's Function Method in Statistical Mechanics* (Interscience, New York, 1962), p. 161.

[5] G. J. Iafrate and L. B. Mendelsohn, Phys. Rev. **182**, 244 (1969).

[6] F. Rogers, H. Grabuske, and D. Harwood, Phys. Rev. A **1**, 1577 (1970).

[7] C. R. Smith, Phys. Rev. **134**, A1235 (1964).

[8] G. J. Iafrate and L. B. Mendelsohn, Phys. Rev. A **2**, 561 (1970).

[9] C. S. Lam and Y. P. Varshni, Phys. Rev. A **6**, 1391 (1972).

[10] λ_c^v refers to the value of λ_c obtained by variational methods.

[11] P. O. Löwdin, J. Mol. Spectrosc. 3, 46 (1959).

[12] The term (E_I/λ_c^v) present in Eqs. (11) and (13) is independent of λ, as will be shown in a later discussion [see Eq. (34)].

[13] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1961), pp. 373 and 394.

PHYSICAL REVIEW A VOLUME 8, NUMBER 2 AUGUST 1973

Comment on "Length and Velocity Formulas in Approximate Oscillator-Strength Calculations"

Anthony F. Starace*
Department of Physics, Imperial College, London, S.W.7, England

(Received 30 November 1972)

A previous paper by Starace showed that the length formula for the electric-dipole matrix element is the only consistent one for calculations that solve for the exact eigenfunctions of an approximate Hamiltonian containing a nonlocal potential. It is emphasized here that disagreement between such a length-formula calculation and experiment indicates inadequacy of the approximate Hamiltonian and *not* that the velocity formula may be preferable.

Starace[1] has shown that in oscillator-strength calculations employing exact eigenfunctions of an approximate Hamiltonian containing a nonlocal potential, the matrix element for electric-dipole transitions is correctly given by the length formula and not by the velocity (or acceleration) formula. Examples of such approximate Hamiltonians are those of Hartree-Fock and configuration-inter-