Addendum to "Analytic perturbation theory for screened Coulomb potentials: Nonrelativistic case"*

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An analytic expression is given for screened continuum radial wave functions which extends our previous results to the case of arbitrary energy shift.

In a recent paper[1] we outlined an analytic perturbation theory for the construction of screened Coulomb radial wave functions, based on an expansion of the potential of the form

$$V(r)=(-a/r)[1+V_1\lambda r+V_2(\lambda r)^2+V_3(\lambda r)^3+\cdots]. \tag{1}$$

In Eq. (1), $a=\alpha Z$, $\lambda=1.13\alpha Z^{1/3}$ is the reciprocal of the Thomas-Fermi radius of the atom, and the coefficients V_k are chosen so that this expression is a good approximation to realistic atomic potentials in the region $\lambda r<1$. Both bound and continuum states were considered, the continuum wave function being obtained by analytic continuation from the bound-state case. In order to effect this analytic continuation, we introduced a parameter T_c which is related to the physical energy T of the continuum electron by means of the formula

$$T-T_c=\delta T=\lambda T_1+\lambda^2T_2+\lambda^3T_3+\cdots, \tag{2}$$

where, in general, the coefficients T_k may be functions of T_c. For a particular choice of these coefficients, we were able to show that the screened continuum radial wave function corresponding to the energy eigenvalue T can be written in terms of a point Coulomb wave function of shifted energy T_c plus screening corrections which are expressed as a series in λ with simple analytic coefficients. Although the result for the continuum wave function given in Ref. 1 is particularly simple because of the explicit form chosen for the energy shift, it is desirable to be able to write screened continuum wave functions for arbitrary energy shifts, since many screened results can be simply related to the corresponding point Coulomb expression of shifted energy. It is the purpose of this note to give the results for screened continuum radial wave functions using the perturbation theory presented in Ref. 1 with arbitrary energy shift.

Following Ref. 1, we define a function $s(r)$ by means of the relation

$$R(r)=Nr^le^{-ik_cr}s(r), \tag{3}$$

where $R(r)$ is the radial wave function, N is a normalization constant, and $T_c=\frac{1}{2}k_c^2$. (We choose units such that $\hbar=c=m_e=1$.) If we make a change of variable, $x=2ik_cr$, then $s(x)$ satisfies the ordinary differential equation

$$\left(x\frac{d^2}{dx^2}+(2l+2-x)\frac{d}{dx}+(-i\nu-l-1)\right)s(x)=\mathfrak{D}_{-i\nu,l}s(x)=\frac{x}{4T_c}(\delta T-\delta V)s(x), \tag{4}$$

where $\delta V=V-V_c$, δT is defined by Eq. (2), and $\nu=a/k_c$. The boundary condition on $s(x)$ is that $s(0)=1$. In the following, we will assume, as in Ref. 1, that the first-order energy shift is given by $T_1=-V_1a$, since in this case the first-order correction to the wave function vanishes.[2] This considerably simplifies the subsequent development. The remaining coefficients T_k, however, are arbitrary.

We then expand $s(x)$ as a series in λ, so that

$$s(x)=s_c(x)+\lambda^2A_2(x)+\lambda^3A_3(x)+\cdots, \tag{5}$$

where $s_c(x)$ is the unperturbed Coulomb solution. Substituting (5) into (4) and equating like powers of λ, we obtain a hierarchy of equations for the coefficients $A_k(x)$. By means of the identities between contiguous confluent hypergeometric functions, these equations can be put in the general form

$$\mathfrak{D}_{-i\nu,l}A_k(x)=\sum_{s=-k}^{k}\beta_s^k(-i\nu,l)M(l+1+i\nu-s,2l+2,x), \tag{6}$$

where $M(a,b,x)$ is a regular confluent hypergeometric function and the explicit form of the coefficients $\beta_s^k(-i\nu,l)$ depends on the values chosen for the energy-shift parameters T_k. In Ref. 1, the T_k were chosen to satisfy the condition $\beta_0^k(-i\nu,l)\equiv0$. Then, using the fact that

$$\mathfrak{D}_{i\nu,l}M(l+1+i\nu-s,2l+2,x)=-sM(l+1+i\nu-s,2l+2,x), \tag{7}$$

the solution to Eq. (6) could be written down immediately.

When the T_k are arbitrary, one also needs a solution $f(x)$ of the equation

$$\mathfrak{D}_{-i\nu,\,l}f(x)=M(l+1+i\nu,2l+2,x)\,. \tag{8}$$

By differentiating Eq. (7) for $s=0$ with respect to the parameter $i\nu$ we find that

$$f(x)=\frac{\partial}{\partial(i\nu)}M(l+1+i\nu,2l+2,x)\,. \tag{9}$$

Hence, for arbitrary energy shift, the screening corrections $A_k(x)$ can be written in the form

$$A_k(x)=\sum_{s=-k}^{k}\alpha_s^k(-i\nu,l)M(l+1+i\nu-s,2l+2,x)+\beta_0^k(-i\nu,l)\frac{\partial}{\partial(i\nu)}M(l+1+i\nu,2l+2,x)\,, \tag{10}$$

where $\alpha_s^k=-\beta_s^k/s$ for all $s\neq 0$ and α_0^k is chosen to satisfy the boundary condition $A_k(0)=0$. Aside from the fact that δT is now arbitrary, so that the relation between T and T_c is changed, Eq. (10) differs from our previous solution [cf. Eq. (19) of Ref. 1] only by the addition of the last term.[3]

For $k=2$ and 3, we have derived the explicit forms of the $A_k(x)$ in terms of the energy-shift parameters T_k. We find

$$\begin{aligned}A_2(x)=\frac{-\nu^2V_2}{4a^2}\Big(&\tfrac{1}{2}i\nu(l+2+i\nu)(l+1+i\nu)M(-2,x)-(l+1+i\nu)[2i\nu(1+2i\nu)+2d_2]M(-1,x)\\&-[3\nu^2(2l+3)-4(l+1)d_2]M(0,x)-4i\nu\{\tfrac{1}{2}[3\nu^2+l(l+1)]-d_2\}\frac{\partial}{\partial(i\nu)}M(0,x)\\&-(l+1-i\nu)[-2i\nu(1-2i\nu)+2d_2]M(1,x)-\tfrac{1}{2}i\nu(l+2-i\nu)(l+1-i\nu)M(2,x)\Big)\,,\end{aligned} \tag{11a}$$

$$\begin{aligned}A_3(x)=\frac{\nu^4V_3}{4a^3}\Big(&-\tfrac{1}{6}(l+3+i\nu)(l+2+i\nu)(l+1+i\nu)M(-3,x)+\tfrac{3}{2}(1+i\nu)(l+2+i\nu)(l+1+i\nu)M(-2,x)\\&+\tfrac{1}{2}(l+1+i\nu)[-15i\nu(1+i\nu)+3l(l+1)-6+4ad_3/\nu^2]M(-1,x)\\&-[10\nu^2(l+2)+\tfrac{1}{3}(l+1)(8l^2+13l-6)+4a(l+1)d_3/\nu^2]M(0,x)\\&+2i\nu\{[-5\nu^2+1-3l(l+1)]-2ad_3/\nu^2\}\frac{\partial}{\partial(i\nu)}M(0,x)\\&+\tfrac{1}{2}(l+1-i\nu)[15i\nu(1-i\nu)+3l(l+1)-6+4ad_3/\nu^2]M(1,x)\\&+\tfrac{3}{2}(1-i\nu)(l+2-i\nu)(l+1-i\nu)M(2,x)-\tfrac{1}{6}(l+3-i\nu)(l+2-i\nu)(l+1-i\nu)M(3,x)\Big)\,,\end{aligned} \tag{11b}$$

where $d_k=T_k/V_k$ and $M(s,x)=M(l+1+i\nu-s,2l+2,x)$. We note that, from Poincaré's theorem,[4] $A_k(r)$ will be analytic in k_c whenever the energy shift $\delta T(k_c)$ is analytic. Hence, although it is not evident from Eqs. (11), $A_k(x)$ will be finite at $T_c=0$ if the energy shift is finite at this point.

Having an explicit form for $A_k(x)$, we can also determine the screening corrections to the continuum normalization and the interior contribution to the phase shifts using the procedure of Ref. 1. Since the procedure is discussed there at length, we will only give here our results for the case of arbitrary energy shift.

The screened continuum normalization $N(k,l)$ can be written, as before, in terms of an expansion in λ. Through third order we find, explicitly,

$$\begin{aligned}N(k,l)=N_c(k_c,l)\left(\frac{k_c}{k}\right)^{1/2}\Big\{1&+\lambda^2\frac{V_2}{8T_c}\Big[l(l+1)(2l+1)-\Big(\frac{3a^2}{2T_c}+l(l+1)-2d_2\Big)(2l+1-\rho_l)\Big]\\&-\lambda^3\frac{aV_3}{16T_c^2}\Big[\tfrac{5}{3}l(l+1)(2l+1)+\Big(-\frac{5a^2}{2T_c}-3l(l+1)+1-\frac{2ad_3}{\nu^2}\Big)(2l+1-\rho_l)\Big]\Big\}\,,\end{aligned} \tag{12}$$

where

$$\rho_l=\nu N_c^{-2}(k_c,l)\frac{\partial}{\partial\nu}N_c^2(k_c,l)=\rho_{l-1}+\frac{2\nu^2}{l^2+\nu^2}\,,\quad \rho_0=1-\frac{2\pi\nu}{e^{2\pi\nu}-1}\,, \tag{13}$$

and $N_c(k_c,l)=(2k_c)^l\,|\Gamma(l+1+i\nu)|\,e^{\pi\nu/2}/\Gamma(2l+2)$ is the point Coulomb normalization of shifted energy. We note that the ratio $N(k,l)/N_c(k_c,l)$ is finite at $T_c=0$ if the energy shift is finite at this point. This can be seen immediately using the low-energy expansion of ρ_l,

$$\rho_l\simeq(2l+1)+\tfrac{1}{3}l(l+1)(2l+1)\nu^{-2}+\tfrac{1}{5}l(l+1)(2l+1)[l(l+1)-\tfrac{1}{3}]\nu^{-4}+O(\nu^{-6})\,, \tag{14}$$

in which contributions of the form $e^{-2\pi\nu}$ are neglected.

Finally, our expression for the interior contribution to the screened phase shift is similarly modified in the case of arbitrary energy shift. We find, through third order in λ, the result

$$\delta(k,l)=\phi(k_c)+\delta_c(k_c,l)-\lambda^2(V_2/16T_c)\nu[7\nu^2+l(l+3)-4d_2]-\lambda^3(aV_3/32T_c^2)\nu[-(l+1)(5l+6)+\tfrac{1}{3}(29-37\nu^2)-4ad_3/\nu^2], \tag{15}$$

where $\delta_c(k_c,l)$ is the point Coulomb phase shift of shifted energy and $\phi(k_c)$, the interior contribution to the phase, is as defined in Ref. 1 [cf. Eqs. (88) and (89)].

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[1]J. McEnnan, L. Kissel, and R. H. Pratt, Phys. Rev. A 13, 532 (1976); 13, 2325(E) (1976).

[2]This assumption is not particularly restrictive. For most applications of our theory this value of T_1 is the correct physical choice. In any case, one may construct analytic screened wave functions using our perturbation theory for arbitrary values of T_1. However, the resulting expressions will be somewhat more complicated.

[3]This additional term, which at large distances gives a contribution involving both regular and irregular confluent hypergeometric functions, would seem to bring our work into closer contact with the quantum-defect method [see, for example, M. J. Seaton, Mon. Not. R. Astron. Soc. 118, 504 (1958)] and with the model potential approach of E. J. McGuire [Phys. Rev. 161, 51 (1967); 175, 20 (1968)]. The precise correspondence between these approaches and our own, however, is not yet fully understood.

[4]Theorem of Poincaré: If a differential equation depends holomorphically on a parameter and the boundary conditions are independent of that parameter, then the solutions of the equation are holomorphic functions of the parameter.