Dispersion-theory approach to multipole, finite-mass, and energy-dependent corrections in long-range Coulombic interactions

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(Received 13 July 1989)

Simple expressions are derived for all multipole, finite-mass, and energy-dependent corrections to the long-range effective potential due to two-Coulomb-photon exchange between Coulombic systems by using dispersion-theory methods. The effective potential is obtained as the Fourier transform in the momentum transfer of the scattering amplitude, which is in turn obtained from its discontinuity via a dispersion relation. The contribution to this potential from each intermediate state can be expressed in closed form in terms of the Struve and Neuman functions.

In an earlier paper,[1] all multipole, nonadiabatic, and finite-nuclear-mass corrections to the long-range effective potential due to two-Coulomb-photon exchange were treated on an equal footing. Simple expressions were derived for these corrections at threshold energy and also first order in energy corrections for the scattering between a spinless point charged particle and a spinless Coulombic complex and between two spinless Coulombic complexes. The results were expressed, respectively, in terms of single-center and London-analog two-center atomic multipole spectral sums.

The effective potential is obtained as the Fourier transform of the scattering amplitude in the momentum transfer $\mathbf{Q}$ with respect to the distance vector $\mathbf{R}$ between the mass centers of the scattering systems. In calculations where, due to a change in the order of integrations, the Fourier transform in $\mathbf{Q}$ is carried out before the calculation of the scattering amplitude is completed, the effective potential may contain momentum-dependent terms[2,3] which violate Hermiticity. This happens because the scattering amplitude is expressed as a function of $\mathbf{Q}^2$, $\mathbf{p}\cdot\mathbf{Q}$, and $\mathbf{p}^2$ where $\mathbf{p}$ is the relative momentum of the scattering systems. Overall energy conservation demands that $\mathbf{p}^2=(\mathbf{p}+\mathbf{Q})^2$. Thus the scattering amplitude can only be a function of two independent scalars $\mathbf{p}^2$ and $\mathbf{Q}^2$ and the effective potential should be a function of R and p^2. Hence, momentum-dependent terms in the effective potential are mathematical artifacts. A procedure to undo such artifacts and to reobtain the correct effective potential has been given[4] and successfully applied in the analysis of long-range forces between Coulombic systems.[1,5] Nevertheless, this procedure requires the inversion of a system of equations and the complexity increases drastically with the order of p^2 corrections. It is for this reason that only corrections up to first order in p^2 were obtained in closed form in the earlier work.[1]

In the present Brief Report the corrections are obtained for all orders in p^2 in closed form through the use of a dispersion-theory approach where the energy-conserving scattering amplitude $T(p^2,Q^2)$ is obtained via a dispersion relation in the square of the momentum transfer $t=-\mathbf{Q}^2$:

$$T(p^2,Q^2)=\frac{1}{\pi}\int_0^\infty \frac{\rho(p^2,t')}{t'-t}dt' , \tag{1}$$

where

$$\rho(p^2,t)\equiv\frac{1}{2i}[T(p^2,t+i\epsilon)-T(p^2,t-i\epsilon)] \tag{2}$$

is the spectral function in the t channel. The effective potential, defined as the Fourier transform of T in $\mathbf{Q}$, can then be obtained as a Laplace transform in $\sqrt{t}$ on reversing the order of integration:

$$V(p^2,R)=\frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{i\mathbf{Q}\cdot\mathbf{R}}\int_0^\infty \frac{dt'}{\pi}\frac{\rho(p^2,t')}{t'-t} , \tag{3a}$$

$$=\frac{1}{4\pi^2 R}\int_0^\infty dt\, \rho(p^2,t)\exp(-\sqrt{t}R) . \tag{3b}$$

Thus, the computation of V reduces to a computation of ρ.

Here I would like to use the same notations as in the earlier analysis.[1] To make the present paper self-contained, I restate these here collectively as Eq. (4). Let $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$, and $\mathbf{r}_4$ be the coordinate vectors of particles 1, 2, 3, and 4, with masses m_1, m_2, m_3, and m_4 and charges Z_1e, Z_2e, Z_3e, and Z_4e, such that particles 1 and 2 form a spinless complex A and particles 3 and 4 form another spinless complex B. I define the following:

$$m_A\equiv m_1+m_2 , \tag{4a}$$

$$m_B\equiv m_3+m_4 , \tag{4b}$$

$$\alpha\equiv m_2/m_A , \tag{4c}$$

$$\beta\equiv m_4/m_B , \tag{4d}$$

$$m\equiv m_A+m_B , \tag{4e}$$

$$\gamma_i=m_i/m, \quad i=1,2,3,4 \tag{4f}$$

$$\mathbf{x}\equiv\mathbf{r}_1-\mathbf{r}_2 , \tag{4g}$$

$$\mathbf{y}\equiv\mathbf{r}_3-\mathbf{r}_4 , \tag{4h}$$

$$\mathbf{X}\equiv(1-\alpha)\mathbf{r}_1+\alpha\mathbf{r}_2 , \tag{4i}$$

$$\mathbf{Y}\equiv(1-\beta)\mathbf{r}_3+\beta\mathbf{r}_4 , \tag{4j}$$

$$\mathbf{R}\equiv\mathbf{Y}-\mathbf{X} , \tag{4k}$$

$$\mathbf{S}\equiv\sum_i \gamma_i\mathbf{r}_i , \tag{4l}$$

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and

$$\mu \equiv m_A m_B / m \ . \tag{4m}$$

Then, in terms the Jacobi coordinates **x**, **y**, **R**, and **S**, the total Hamiltonian is cyclic in **S** and the kinetic energy of the center of mass of the entire system is a conserved quantity and can be dropped. The Hamiltonian can thus be expressed in the form

$$H = h_{0A} + h_{0B} + T + H_1 \ , \tag{4n}$$

where

$$h_{0A} \equiv -\frac{\nabla_x^2}{2\alpha m_1} + \frac{Z_1 Z_2 e^2}{|x|} \ , \tag{4o}$$

$$h_{0B} \equiv -\frac{\nabla_y^2}{2\beta m_3} + \frac{Z_3 Z_4 e^2}{|y|} \ , \tag{4p}$$

$$T \equiv \frac{-\nabla_R^2}{2\mu} \ , \tag{4q}$$

and

$$H_1 \equiv e^2 \left[\frac{Z_1 Z_3}{|\mathbf{R}+\beta\mathbf{y}-\alpha\mathbf{x}|} + \frac{Z_2 Z_4}{|\mathbf{R}+(1-\alpha)\mathbf{x}-(1-\beta)\mathbf{y}|} + \frac{Z_2 Z_3}{|\mathbf{R}+(1-\alpha)\mathbf{x}+\beta y|} + \frac{Z_1 Z_4}{|\mathbf{R}-\alpha\mathbf{x}-(1-\beta)y|} \right] \tag{4r}$$

$$= e^2 \int \frac{d^3k}{k^2} e^{i\mathbf{k}\cdot\mathbf{R}} (Z_1 e^{-i\alpha\mathbf{k}\cdot\mathbf{x}} + Z_2 e^{i(1-\alpha)\mathbf{k}\cdot\mathbf{x}})(Z_3 e^{i\beta\mathbf{k}\cdot\mathbf{y}} + Z_4 e^{-i(1-\beta)\mathbf{k}\cdot\mathbf{x}})/(2\pi^2) \tag{4s}$$

$$= \sum_{L_A L_B = 0}^{\infty} h_1^{L_A L_B} \ , \tag{4t}$$

where

$$h_1^{L_A L_B} \equiv e^2 \int \frac{d^3k}{k^2} [Z_1(-\alpha)^{L_A} + Z_2(1-\alpha)^{L_A}] \frac{(i\mathbf{k}\cdot\mathbf{x})^{L_A}}{L_A!} \times [Z_3 \beta^{L_B} + Z_4(\beta-1)^{L_B}] \frac{(i\mathbf{k}\cdot\mathbf{y})^{L_B}}{L_B!} \frac{e^{i\mathbf{k}\cdot\mathbf{R}}}{2\pi^2} \ . \tag{4u}$$

The quantities in the square brackets in Eq. (4u) act as multipole modification factors. Let $|0_A\rangle$ and $|0_B\rangle$ be the initial zero angular momentum states of the complexes A and B and E_{n_A} and E_{n_B} be the energy eigenvalues of the states $|n_A\rangle$ and $|n_B\rangle$. I define

$$\Delta_{n_A n_B} \equiv 2\mu(E_{n_A} - E_{0_A} + E_{n_B} - E_{0_B}) \tag{4v}$$

and the two-center correlated multipole matrix element

$$B_{n_A n_B}^{L_A L_B} \equiv 2\mu e^2 [Z_1(-\alpha)^{L_A} + Z_2(1-\alpha)^{L_A}]^2 \times [Z_3 \beta^{L_B} + Z_4(\beta-1)^{L_B}]^2 \times |\langle 0_A | x^{L_A} P_{L_A} | n_A \rangle|^2 |\langle 0_B | y^{L_B} P_{L_B} | n_B \rangle|^2 \ , \tag{4w}$$

where P_L is the Legendre polynomial.

At this point, it is convenient to decompose the spectral function ρ in Eq. (2) into its multipole and atomic intermediate state contributions:

$$\rho(p^2,t) = \sum_{L_A, L_B, n_A, n_B} \rho_{n_A n_B}^{L_A L_B}(p^2,t) \ . \tag{5}$$

The evaluation of the dipole-dipole part ($L_A = L_B = 1$) has been carried out in detail by Feinberg and Sucher.[6] As we are dealing with the nondegenerate and low-energy situation here, the calculation leading to Eq. (20b) of Ref. 6 applies. The essence of the factors that determine the t discontinuity of the scattering amplitude T remains the same, being determined by identical denominators which owe their origins strictly to kinematics. One may regard the parametric vector **k** in Eq. (4u) as the "momentum" of the virtual Coulomb photon. Our earlier analysis[1,5] indicates that terms proportional to powers of the square of this virtual momentum which arise in the calculation of the atomic excitation dynamics due to the interaction $h_1^{L_A L_B}$ in Eq. (4u) lead only to a δ function or derivatives of δ-function-type short-ranged terms. In the spirit of a dispersion calculation, this is equivalent to saying that such terms do not contribute to the t discontinuity of T around $t=0$, and is the reason for neglecting the second term of Eq. (13) of Ref. 6 in the computation of the spectral function ρ. Using this property and the same procedure that I have used recently[1,7] to handle the multipolar transition dynamics, one can proceed to handle the kinematics in a manner completely analogous to that used in Ref. 6 to obtain $\rho_{n_A n_B}^{L_A L_B}$. Since the calculational techniques are already reported in the literature[1,6,7] I simply state the results here:

$$\rho_{n_A n_B}^{L_A L_B}(p^2,t) = \frac{-2\pi^2 e^2 t^{L_A + L_B}}{(2L_A)!(2L_B)!\Delta_{n_A n_B}} B_{n_A n_B}^{L_A L_B} \left[\frac{t_0}{t(t+t_0)} \right]^{1/2} \ , \tag{6}$$

where $B_{n_A n_B}^{L_A L_B}$ and $\Delta_{n_A n_B}$ are defined in Eqs. (4w) and (4v), and t_0 is given by

$$t_0 = \frac{\Delta_{n_A n_B}^2}{\Delta_{n_A n_B} - p^2} \ . \tag{7}$$

The corresponding effective potential can be obtained as the Laplace transform in Eq. (3.2). After a change of variable from t to y^2, one obtains

$$V_{n_A n_b}^{L_A L_B}(p^2,R)=\frac{-e^2 B_{n_A n_B}^{L_A L_B}}{(2L_A)!(2L_B)!R\,\Delta_{n_A n_B}} \times \int_0^\infty dy\, y^{2(L_A+L_B)}\left[1+\frac{y^2}{t_0}\right]^{-1/2} e^{-yR} . \tag{8}$$

Below the excitation threshold, i.e., for $p^2<\Delta_{n_A n_B}$, Eq. (8) can be integrated in closed form to give

$$V_{n_A n_B}^{L_A L_B}(p^2,R) = \frac{-e^2 B_{n_A n_B}^{L_A L_B} t_0 \pi}{2(2L_A)!(2L_B)!R\,\Delta_{n_A n_B}}(-\partial_R)^{2L_A+2L_B-1} \times[\mathcal{H}_1(\sqrt{t_0}R)-N_1(\sqrt{t_0}R)] , \tag{8'}$$

where $\mathcal{H}_1$ is the Struve function and N_1 is the Neuman function. I remind the reader that t_0 is a function of n_A and n_B. With a little algebraic manipulation, one can write

$$\left[1+\frac{y^2}{t_0}\right]^{-1/2} = \sum_{M,J=0}^{\infty}(-1)^M \frac{(2M+2J)!}{2^{2(M+J)}(M+J)!J!M!} \times \frac{y^{2M+2J}p^{2J}}{\Delta_{n_A n_B}^{M+2J}} . \tag{9}$$

When one uses Eq. (9) in Eq. (8) and retains the same dummy indices M and J, one obtains

$$V_{n_A n_B}^{L_A L_B} \equiv \sum_{MJ} V_{MJ}^{L_A L_B}(n_A,n_B)p^{2J} . \tag{10}$$

The effective potential is given by the sum over intermediate state contributions and one can suitably define

$$V_{MJ}^{L_A L_B}(R) \equiv \sum_{n_A n_B} V_{MJ}^{L_A L_B}(n_A,n_B) . \tag{11}$$

On putting all this together, one has the final result:

$$V(p^2,R)=\sum_{L_A,L_B,M,J} V_{MJ}^{L_A L_B}(R)p^{2J} , \tag{12}$$

$$V_{MJ}^{L_A L_B}(R)=(-1)^{M+1}e^2 D_{M+2J+1}^{L_A L_B}\frac{(2M+2J)![2(L_A+L_B+M+J)]!R^{-2(L_A+L_B+M+J+1)}}{(2L_A)!(2L_B)!(M+J)!J!M!2^{2(M+J)}} , \tag{13}$$

where

$$D_N^{L_A L_B} \equiv \sum_{n_A,n_B} B_{n_A n_B}^{L_A L_B}/\Delta_{n_A n_B}^N \tag{14}$$

is the two-center London-analog correlated multipole spectral sum introduced in Ref. 1. For $J=0$ and 1, Eq. (13) reduces to Eqs. (3.28) and (3.29) of Ref. 1. This serves as a very important check on the validity of the mathematical procedure developed earlier[4] to remove the non-Hermitian momentum-dependent terms in the effective potential. In addition, Eqs. (12) and (13) give low-energy corrections to all orders in p^2.

If B is a point charged particle of charge $Z_B e$, all one has to do to obtain the effective potential is to set $L_B=0$, $L_A=L$, and replace $D_N^{L_A L_B}$ by $Z_B^2 A_N^L$ where the single-center atomic sum is defined by

$$A_N^L \equiv 2\mu e^2[Z_1\alpha^L+Z_2(\alpha-1)^L]^2\sum_n \frac{|\langle 0|x^L P_L|n\rangle|^2}{\Delta_n^N} . \tag{15}$$

The atom-point charge potential is found to be

$$V(p^2,R)=\sum_{L,M,J} V_{MJ}^L p^{2J} \tag{16}$$

where

$$V_{MJ}^L(R)=(-1)^{M+1}e^2 A_{M+2J+1}^L Z_B^2 \frac{(2M+2J)![2L+M+J)]!R^{-2(L+M+J+1)}}{(2L)!(M+J)!J!M!2^{2(M+J)}} . \tag{17}$$

Again, for $J=0$ and 1, Eq. (17) reduces to Eqs. (2.34)–(2.37) of Ref. 1. For the potential arising from only one atomic intermediate state $|n\rangle$, the effective potential can be written in terms of the Struve and Neuman functions as

$$V_n^L(p^2,R)=\frac{-e^2 C_n^L t_0' \pi Z_B^2}{2(2L)!R\,\Delta_n}(-\partial_R)^{2L-1} \times[\mathcal{H}_1((t_0')^{1/2}R)-N_1((t_0')^{1/2}R)] , \tag{18}$$

where

$$C_n^L \equiv 2\mu e^2[Z_1\alpha^L + Z_2(\alpha-1)^L]^2|\langle 0|x^L P_L|n\rangle|^2 \quad (19)$$

and

$$t_0' \equiv \frac{\Delta_n^2}{\Delta_n - p^2} \ . \quad (20)$$

In terms of the per intermediate state contribution to the effective potential [Eqs. (8′) and (18)], the pseudostate method probably is a reliable and easy to use method to calculate the total effective potential. This has proven to be quite successful in the computation of $V_{MJ}^{L_A L_B}$ [Eq. (13)] for a pair of hydrogenic atoms for $J=0$, and low values of M.[3,6] Our analysis[8] has shown that the method should work reliably for all values of L_A, L_B, M, and J. Hence it is quite reasonable to conjecture that this method works well with Eqs. (8′) and (18), as the representation of the per state effective potential in terms of the special Bessel functions is just equivalent to a summation over the M and J indices. Expressing the effective potential as a sum over intermediate states including the continuum appears formidable. But the pseudostate method reduces it to a finite number of terms.

This work is supported by the National Science Foundation under Grant No. PHY-87-10118. I thank Professor G. Feinberg and Professor J. Sucher for providing me with great details of unpublished background calculations of Ref. 6 during our earlier collaborations. These details provide important guides in the present calculation.

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