THE POTENTIAL DUE TO TWO POINT CHARGES EACH AT THE CENTRE OF A SPHERICAL CAVITY AND EMBEDDED IN A DIELECTRIC MEDIUM

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Summary

A method is found for determining the electrostatic potential due to two separated spherical cavities each containing a point charge with the whole system embedded in a continuous dielectric medium. The potential is obtained as a sum involving Legendre polynomials and it is shown that the coefficients of this series can be expanded as a convergent power series in the reciprocal of the distance between the centres of the cavities. This solution is suitable for numerical calculations because there is a simple relationship between successive terms in the series and because this series is convergent even at contact separation.

I. INTRODUCTION

Ever since Bernal and Fowler (1933) discussed the nature of ions in an aqueous solution there has been a growing interest in spherical and ellipsoidal cavity models which are used to represent ions and their attached water molecules. For example, Onsager (1936), Kirkwood and Westheimer (1938, 1939), Hill (1944), Scholte (1949), Ross and Sack (1950), Abbott and Bolton (1952), Linderstrøm-Lang (1953), Buckley and Maryott (1954), Buckingham (1957), and Kober and Fitts (1966) have placed charges in an isolated cavity at appropriate points and have solved the electrostatic problem in order to develop a theory of polar liquids. Now to discuss the interaction of an ion pair in an aqueous medium we can use, as a very crude mathematical model, a pair of nonoverlapping spherical cavities each containing a point charge at its centre. Rosenthal (1967) discussed some of the applications of a two-sphere model where both cavities have the same radius but opposite charge, but he did not consider the validity of the expansions nor did he find an expression for successive terms in the series.

To date a number of problems involving separated conducting spheres have been solved by making use of spherical polar coordinates. Thus, Kottler (1927) and Mitra (1944) found a functional equation whose solution leads to a determination of the capacity of two spheres, assumed to be exterior to each other. On the other hand, Hobson (1931) and Lebedev (1965) obtained a much simpler solution for the potential in terms of dipolar coordinates. Davis (1964) extended this work to take into account the influence of a field that is uniform at infinity. The latter approach was not found useful in solving the problem under consideration here because it leads to a set of four simultaneous difference equations for which there is no known solution. Instead, we shall use two spherical polar coordinate systems and apply Hobson's

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method of transforming solid harmonics in order to satisfy the boundary conditions on the two surfaces.

Similar problems related to the present one are treated by Shail (1962), who extended Mitra's method to find a harmonic function that takes prescribed values on two nonintersecting spheres, and Snow (1949), who considered the case of overlapping conducting spheres in great detail. There are also a number of papers on inviscid flow near toroids, lenses, and overlapping spheres which are related to the problem at hand (see Stimson and Jeffrey 1926; Payne and Pell 1960; Pell and Payne 1960*a*, 1960*b*; Collins 1963; Ranger 1965).

II. EXPANSIONS FOR THE POTENTIAL

Consider two spherical cavities S_1 and S_2 which do not overlap and which are at separation $R = O_1 O_2$ where O_1 and O_2 are the centres of the cavities containing the point charges e_1 and e_2 respectively. Let P be a typical point in the vicinity such that $O_i P = r_i$, for i = 1 or 2, and let θ_1 and θ_2 be the angles $PO_1 O_2$ and $PO_2 O_1$. (In what follows the suffix i = 1 or 2 will be used to refer to the first and second cavity respectively.) These coordinates are so defined that $r_1 = r_2$ and $\theta_1 = \theta_2$ for any point P on the median plane. The spherical cavities are taken to have radius a_i and the whole system is embedded in a continuous medium of dielectric constant ϵ .

An expansion for the potential at P inside S_i can be obtained by applying Green's theorem. Now the potential inside the cavity S_i may be written

$$V_{i}(\mathbf{P}) = e_{i}/r_{i} + U_{i}(\mathbf{P}), \qquad (1)$$

where $U_i(\mathbf{P})$ is harmonic inside S_i . Let Q_i be any point on the boundary of S_i with coordinates $(a_i, \theta_i^*, \phi_i^*)$ then

$$U_{i}(\mathbf{P}) = \frac{1}{4\pi} \int \left\{ U(\mathbf{Q}_{i}) \frac{\partial}{\partial n} \left(\frac{1}{\rho_{i}} \right) - \frac{1}{\rho_{i}} \frac{\partial U(\mathbf{Q}_{i})}{\partial n} \right\} d\mathbf{S}_{i}, \qquad (2)$$

where $\rho_i = PQ_i$, $U(Q_i)$ is the potential on the boundary of S_i , and $\partial/\partial n$ denotes differentiation along the outward normal n. An expression for $U_i(P)$ can then be found by integrating the above equation with respect to ϕ_i^* , remembering that the potential is independent of the azimuthal angle, and using the identities

$$\rho_i^2 = a_i^2 + r_i^2 - 2a_i r_i \cos \gamma_i \tag{3}$$

and

$$\cos \gamma_i = \cos \theta_i \cos \theta_i^* + \sin \theta_i \sin \theta_i^* \cos(\phi_i - \phi_i^*), \qquad (4)$$

together with the addition formula

$$\mathbf{P}_{n}(\cos\gamma_{i}) = \mathbf{P}_{n}(\cos\theta_{i}) \mathbf{P}_{n}(\cos\theta_{i}^{*}) + 2\sum_{m=1}^{n} \frac{(n-m)!}{(n+m)!} \mathbf{P}_{n}^{m}(\cos\theta_{i}) \mathbf{P}_{n}^{m}(\cos\theta_{i}^{*}) \cos\{m(\phi_{i}-\phi_{i}^{*})\},$$
(5)

where the $P_n^m(x)$ are the associated Legendre functions as defined in Hobson (1931).

Finally, we obtain

$$V_i(\mathbf{P}) = e_i/r_i + (e_i/a_i) \sum_{s=0}^{\infty} d_s^i (r_i/a_i)^s \mathbf{P}_s(\cos\theta_i), \qquad (6)$$

where the unknown coefficients d_s^i will be determined from the boundary conditions and

$$d_s^i = -(a_i/2e_i) \int_0^{\pi} W(\mathbf{Q}_i) \mathbf{P}_s(\cos\theta_i^*) \sin\theta_i^* \,\mathrm{d}\theta_i^*, \qquad (7)$$

with

$$W(\mathbf{Q}_i) = a_i \,\partial U(\mathbf{Q}_i) / \partial n + (s+1)U(\mathbf{Q}_i) \,. \tag{8}$$

By Schwarz's inequality (Titchmarsh 1950) it follows that

$$(d_s^i)^2 \leqslant (a_i/2e_i)^2 \int_0^{\pi} W^2(\mathbf{Q}_i) \sin \theta_i^* \, \mathrm{d}\theta_i^* \int_0^{\pi} \mathbf{P}_s^2(\cos \theta_i^*) \sin \theta_i^* \, \mathrm{d}\theta_i^* \\ = \{a_i^2/2e_i(2s+1)\} \int_0^{\pi} W^2(\mathbf{Q}_i) \sin \theta_i^* \, \mathrm{d}\theta_i^*.$$
(9)

From equations (7) and (8) and the integrability of the potential and its gradient normal to the boundary S_i we obtain the result that $|s^{-\frac{1}{2}}d_s^i|$ is bounded for all s. Thus the series in (6) is absolutely and uniformly convergent within S_i and convergent on the boundary of S_i , except perhaps at the points $\theta_i = 0$ or π (see Hobson 1931).

In much the same way we can find an expression for the potential outside the two cavities. Thus,

$$V_{0}(\mathbf{P}) = \frac{1}{\epsilon} \left(\frac{e_{1}}{r_{1}} + \frac{e_{2}}{r_{2}} \right) + \frac{1}{\epsilon} \sum_{s=1}^{\infty} \left(\frac{e_{1}}{a_{1}} g_{s}^{1} \left(\frac{a_{1}}{r_{1}} \right)^{s+1} \mathbf{P}_{s}(\cos \theta_{1}) + \frac{e_{2}}{a_{2}} g_{s}^{2} \left(\frac{a_{2}}{r_{2}} \right)^{s+1} \mathbf{P}_{s}(\cos \theta_{2}) \right\},$$
(10)

where

$$g_s^i = (\epsilon a_i/2e_i) \int_0^{\pi} X(\mathbf{Q}_i) \mathbf{P}_s(\cos\theta_i^*) \sin\theta_i^* \,\mathrm{d}\theta_i^* \tag{11}$$

and

$$X(\mathbf{Q}_i) = a_i \,\partial U(\mathbf{Q}_i) / \partial n - sU(\mathbf{Q}_i) \,. \tag{12}$$

In this way we find that the series in (10) are absolutely and uniformly convergent outside the two cavities and convergent on the boundaries, except possibly at the points where $\theta = 0$ or π .

III. FORMULATION OF DIFFERENCE EQUATION

The boundary conditions that must be satisfied at the surfaces of the two spheres $r_i = a_i$ are

$$V_i = V_0, \qquad \partial V_i / \partial r_i = \epsilon \, \partial V_0 / \partial r_i \tag{13}$$

and these will be used to obtain two difference equations for the coefficients g_{s}^{i} .

In what follows we shall use the formula of zonal harmonics

$$\frac{\mathbf{P}_n(\cos\theta_2)}{r_2^{n+1}} = \frac{1}{R^{n+1}} \sum_{m=0}^{\infty} \binom{m+n}{n} \binom{r_1}{R}^m \mathbf{P}_m(\cos\theta_1), \qquad (14)$$

when $|r_1| < R$ and a similar expression with the suffixes 1 and 2 interchanged. These formulae were obtained by Hobson (1931) but he defined the angles θ_i in a slightly different way.

To begin, both boundary conditions will be applied on the surface $r_1 = a_1$ and then an interchange of the suffixes will give the equations appropriate to the surface $r_2 = a_2$. From the first of the conditions in (13) we obtain, after substituting (14) into (10), rearranging the absolutely (and uniformly) convergent series, multiplying by $P_s(\cos \theta_i) \sin \theta_i$, and integrating from 0 to π ,

$$\frac{e_1}{a_1}d_0^1 = -\frac{e_1}{a_1}\left(1 - \frac{1}{\epsilon}\right) + \frac{e_2}{\epsilon R}\left(1 + \sum_{m=1}^{\infty} g_m^2 t_2^m\right)$$
(15)

and

$$\frac{e_1}{a_1}d_n^1 = -\frac{e_1}{\epsilon a_1}g_n^1 + \frac{e_2}{\epsilon R} \left(1 + \sum_{m=1}^{\infty} {\binom{m+n}{n}}g_m^2 t_2^m\right) t_1^n,$$
(16)

for $n = 1, 2, 3, \ldots$, where $t_i = a_i/R$. Similarly, the second boundary condition in (13) leads to

$$\frac{e_1}{\epsilon a_1} d_n^1 = -\frac{e_1}{\epsilon a_1} \left(1 + \frac{1}{n} \right) g_n^1 + \frac{e_2}{\epsilon R} \left(1 + \sum_{m=1}^{\infty} {m+n \choose n} g_m^2 t_2^m \right) t_1^n,$$
(17)

for $n = 1, 2, 3, \ldots$ Since the last terms in (16) and (17) are identical it follows that

$$n(\epsilon - 1)d_n^1 = (2n+1)g_n^1 \tag{18}$$

and hence, on substituting back into (16) or (17), we get

$$(e_2/e_1)\alpha_n t_1^{n+1} t_2 = g_n^1 t_2 - (e_2/e_1) \sum_{m=1}^{\infty} \alpha_n P_{n,m} g_m^2, \qquad (19)$$

for n = 1, 2, 3, ..., where

$$P_{n,m} = \binom{m+n}{n} t_2^{m+1} t_1^{n+1} \tag{20}$$

and

$$\alpha_n = (\epsilon - 1) / \{ \epsilon (1 + 1/n) + 1 \}.$$

$$(21)$$

The two boundary conditions are now applied on the second surface $r_2 = a_2$ in which case we obtain the relation

$$(e_1/e_2)\alpha_n t_2^{n+1} t_1 = g_n^2 t_1 - (e_1/e_2) \sum_{m=1}^{\infty} \alpha_n P_{m,n} g_m^1, \qquad (22)$$

for $n = 1, 2, 3, \ldots$

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IV. EXISTENCE AND UNIQUENESS OF SOLUTION

The problem that remains is to solve equations (19) and (22) for the sets of coefficients g_n^i . Since this involves an infinite number of equations it is important to determine the condition under which a solution exists and then to devise a method of finding it.

The sum by rows and columns of the matrix $P_{n,m}$ are given by

$$R_n = \sum_{m=1}^{\infty} P_{n,m} = t_2 [\{t_1/(1-t_2)\}^{n+1} - t_1^{n+1}]$$
(23)

and

$$C_m = \sum_{n=1}^{\infty} P_{n,m} = t_1 [\{t_2/(1-t_1)\}^{m+1} - t_2^{m+1}].$$
(24)

Clearly both R_n and C_m are bounded functions since, for nonoverlapping cavities, we have $0 \leq t_1+t_2 < 1$. Hence

$$0 < R_n < t_2$$
 and $0 < C_m < t_1$. (25)

If we now eliminate g_n^2 between equations (19) and (22) we obtain

$$(e_2/e_1)\alpha_n t_1^{n+1} + \sum_{m=1}^{\infty} \alpha_m \alpha_n P_{n,m} t_2^m = \sum_{s=1}^{\infty} (\delta_{n,s} - Q_{n,s}) g_s^1, \qquad (26)$$

where $\delta_{n,s}$ is the Kronecker delta and

$$Q_{n,s} = \sum_{m=1}^{\infty} \alpha_n \alpha_m P_{n,m} P_{s,m} / (t_1 t_2).$$
 (27)

Since $0 < \alpha_k < 1$ the inequalities in (25) imply that $Q_{n,s}$ has row and column bounds less than unity and hence, from theorem 2.4.I on page 30 of Cooke (1950), it follows that $(\delta_{n,s}-Q_{n,s})$ has the unique and two-sided reciprocal

$$\mathbf{I} + \sum_{p=1}^{\infty} \mathbf{Q}^p, \qquad (28)$$

where $\mathbf{Q} = (Q_{n,s})$ and \mathbf{I} is the unit matrix. The coefficients g_s^i can therefore be expressed as a double power series in t_1 and t_2 provided that $0 \leq t_1+t_2 < 1$.

V. ITERATIVE SOLUTION

The double power series expansion for the unknown coefficients can be obtained more easily by a direct substitution into equations (19) and (22). Let

$$g_n^i = \alpha_n t_i^{n+1} \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} a_n^i(r,s) t_i^r t_{(3-i)}^s, \qquad i = 1 \text{ or } 2,$$
(29)

and substitute into equations (19) and (22). On equating the coefficients of powers

of t_1 and t_2 we obtain

$$a_n^i(0,0) = 1$$
, $a_n^i(r,s) = \sum_{m=1}^{\lfloor \frac{i}{2}(s-1) \rfloor} {\binom{m+n}{n}} \alpha_m a_m^{(3-i)}(r,s-2m-1)$, (30)

if r and s are not both zero. This is a difference equation from which it is a straightforward matter to calculate successive values of $a_n^i(r,s)$. Thus, after a considerable amount of algebra, we find that

$$g_{n}^{1} = \alpha_{n} t_{1}^{n+1} \left\{ 1 + \left(\frac{e_{2}}{e_{1}}\right) \binom{n+1}{1} \alpha_{1} t_{2}^{3} + \left(\frac{e_{2}}{e_{1}}\right) \binom{n+2}{2} \alpha_{2} t_{2}^{5} + 2\binom{n+1}{1} \alpha_{1}^{2} t_{1}^{3} t_{2}^{3} + \left(\frac{e_{2}}{e_{1}}\right) \binom{n+3}{3} \alpha_{3} t_{2}^{7} + 3\binom{n+2}{2} \alpha_{1} \alpha_{2} t_{1}^{3} t_{2}^{5} + 2\binom{n+1}{1} \alpha_{1}^{2} t_{1}^{5} t_{2}^{3} + \ldots \right\},$$
(31)

with a similar expression for g_n^2 . The above equation is consistent with the result given by Rosenthal (1967), who was concerned only with the case $e_1 = -e_2$ and $t_1 = t_2$.

This method of determining an expansion for the coefficients g_n^i is very easily carried out and is particularly suitable for numerical computations, some of which were carried out in an earlier paper (see Rosenthal 1967 for further discussion).

VI. References

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