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Research article

A generalization of the Shell Theorem.

Electric potential of charged spheres and charged vesicles surrounded by electrolyte

István P. Sugár*

Department of Neurology, Icahn School of Medicine at Mount Sinai, New York, NY 10029

* **Correspondence:** istvansugar0@gmail.com

Appendix 1

Let us do the following substitution in the integral (in Eq.8): $u = \cos(\alpha)$. Thus in Eq.8 $\sin(\alpha)\, d\alpha$ can be substituted by $-du$ and we get

$$V(Z) = \frac{k_e \cdot \rho_1 \cdot 2R_1^2 \pi}{\varepsilon} \int_{-1}^{1} \frac{1}{\sqrt{R_1^2 + Z^2 - 2ZR_1 u}} e^{-\sqrt{R_1^2 + Z^2 - 2ZR_1 u}/\lambda_D} du \tag{A1}$$

Finally, let us do this substitution in Eq.A1: $w = -\sqrt{R_1^2 + Z^2 - 2ZR_1 u}/\lambda_D$ and thus

$$dw = \frac{ZR_1}{\lambda_D \sqrt{R_1^2 + Z^2 - 2ZR_1 u}} du \text{ and we get}$$

$$V(Z) = \frac{k_e \cdot \rho_1 \cdot 2R_1^2 \pi \cdot \lambda_D}{\varepsilon \cdot Z \cdot R_1} \int_{w(u=-1)}^{w(u=1)} e^w \, dw = \frac{k_e \rho_1 2R_1^2 \pi \lambda_D}{\varepsilon Z R_1} [e^w]_{w(u=-1)}^{w(u=1)} \tag{A2}$$

where

$$w(u=-1) = -\frac{\sqrt{R_1^2 + Z^2 + 2ZR_1}}{\lambda_D} = -\frac{(Z+R_1)}{\lambda_D}, \text{ while}$$

in the case of $Z > R_1$

$$w(u=1) = -\frac{\sqrt{R_1^2+Z^2-2ZR_1}}{\lambda_D} = -\frac{\sqrt{(Z-R_1)^2}}{\lambda_D} = -\frac{(Z-R_1)}{\lambda_D}, \text{ and}$$

in the case of $Z < R_1$

$$w(u=1) = -\frac{\sqrt{R_1^2+Z^2-2ZR_1}}{\lambda_D} = -\frac{\sqrt{(R_1-Z)^2}}{\lambda_D} = -\frac{(R_1-Z)}{\lambda_D}$$

Here we mention that the square root of a positive number, $(Z-R_1)^2$ *or* $(R_1-Z)^2$ should be positive (only imaginary number's square root is negative). Thus the square root is $Z-R_1$ if $Z > R_1$ and the square root is $R_1 - Z$ if $Z < R_1$.

Thus the potential at $Z > R_1$ is

$$V(Z) = \frac{k_e \cdot \rho_1 \cdot 2R_1^2\pi \cdot \lambda_D}{\varepsilon \cdot Z \cdot R_1}\left[e^{-\frac{(Z-R_1)}{\lambda_D}} - e^{-\frac{(Z+R_1)}{\lambda_D}}\right] = \frac{k_e \cdot Q_1 \cdot \lambda_D}{\varepsilon \cdot Z \cdot R_1} \cdot e^{-\frac{Z}{\lambda_D}} \cdot sinh\left(\frac{R_1}{\lambda_D}\right) \quad \text{(A3)}$$

where $Q_1 = 4R_1^2\pi \cdot \rho_1$ is the total charge of the sphere.

Finally, the potential at $Z < R_1$ is

$$V(Z) = \frac{k_e \cdot \rho_1 \cdot 2R_1^2\pi \cdot \lambda_D}{\varepsilon \cdot Z \cdot R_1}\left[e^{-\frac{(R_1-Z)}{\lambda_D}} - e^{-\frac{(Z+R_1)}{\lambda_D}}\right] = \frac{k_e \cdot Q_1 \cdot \lambda_D}{\varepsilon \cdot Z \cdot R_1} \cdot e^{-\frac{R_1}{\lambda_D}} \cdot sinh\left(\frac{Z}{\lambda_D}\right) \quad \text{(A4)}$$

Appendix 2

First we calculate the potential within the membrane induced by the charges located at the intra-vesicular membrane surface, $V_1(Z)$ (see Figure 2A) where $R_1 < Z < R_2$:

$$V_1(Z) = \int_0^{\alpha_1} V_1(\alpha, Z)d\alpha = \int_0^{\alpha_1} \frac{k_e \cdot \rho_1 \cdot 2 \cdot R_1 \cdot \sin(\alpha) \cdot \pi \cdot R_1 \cdot d\alpha}{\varepsilon_m R(\alpha, Z, R_1)} \quad \text{(A5)}$$

Note, that at $\alpha > \alpha_1$ the line between point P1 and any one charge of the intra-vesicular membrane surface partially goes through the intra-vesicular electrolyte. The electrolyte's ion concentration is assumed to be so high that the screening reduces the potential of any one of those charges to zero. α_1 is defined in Figure 2A and its cosine is: $\cos(\alpha_1) = R_1/Z$. However at $0 < \alpha < \alpha_1$ the entire line between any of those charges and point P1 is in the membrane and the potential is not screened at all (see Eq.A5). After substituting Eq.7 into Eq.A5 and doing substitution $u = \cos(\alpha)$ we get:

$$V_1(Z) = \frac{k_e \cdot \rho_1 \cdot 2R_1^2\pi}{\varepsilon_m}\int_{R_1/Z}^{1} \frac{1}{\sqrt{R_1^2+Z^2-2ZR_1 u}}du = \frac{k_e \cdot \rho_1 \cdot 2R_1^2\pi}{\varepsilon_m} \cdot \frac{\left[\sqrt{R_1^2+Z^2-2ZR_1 u}\right]_{\frac{R_1}{Z}}^{1}}{-R_1 Z} =$$

$$\frac{k_e \cdot Q_1}{2 \cdot \varepsilon_m \cdot R_1 \cdot Z} \cdot \left[\sqrt{(Z-R_1)(Z+R_1)} - (Z-R_1)\right] \qquad (A6)$$

$V_2(Z)$ is the potential at point P1 generated by the charges located at the extra-vesicular surface of the membrane. In this case charges located within $0 < \alpha < \alpha_1 + \alpha_2$ generate potential without any screening, while charges located at $\alpha > \alpha_1 + \alpha_2$ are screened out completely. Note that α_2 is defined in Figure 2B and its cosine is $\cos(\alpha_2) = R_1/R_2$. Thus

$$V_2(Z) = \int_0^{\alpha_1+\alpha_2} \frac{k_e \cdot \rho_2 \cdot 2 \cdot R_2 \cdot \sin(\alpha) \cdot \pi \cdot R_2 \cdot d\alpha}{\varepsilon_m R(\alpha, Z, R_2)} =$$

$$\frac{k_e \cdot Q_2}{2 \cdot \varepsilon_m} \int_{\cos(\alpha_1+\alpha_2)}^{1} \frac{1}{\sqrt{R_2^2+Z^2-2ZR_2u}} du = \frac{k_e \cdot Q_2}{2 \cdot \varepsilon_m} \cdot \frac{\left[\sqrt{R_2^2+Z^2-2ZR_2u}\right]_{\cos(\alpha_1+\alpha_2)}^{1}}{-R_2 Z} =$$

$$\frac{k_e \cdot Q_2}{2 \cdot \varepsilon_m \cdot R_2 \cdot Z} \cdot \left[\sqrt{Z^2 + R_2^2 - 2R_1^2 + 2\sqrt{(Z^2-R_1^2)(R_2^2-R_1^2)}} - (R_2 - Z)\right] \qquad (A7)$$

where we used

$$\cos(\alpha_1+\alpha_2) = \cos(\alpha_1)\cos(\alpha_2) - \sin(\alpha_1)\sin(\alpha_2) =$$

$$\cos(\alpha_1)\cos(\alpha_2) - \sqrt{1-cos^2(\alpha_1)} \cdot \sqrt{1-cos^2(\alpha_2)} =$$

$$\frac{R_1}{Z} \cdot \frac{R_1}{R_2} - \sqrt{1-(R_1/Z)^2} \cdot \sqrt{1-(R_1/R_2)^2} = \frac{R_1^2 - \sqrt{(Z^2-R_1^2)(R_2^2-R_1^2)}}{Z \cdot R_2} \qquad (A8)$$

Appendix 3

Here we calculate the length of the chord, r_2 shown in Figure A1. The equation of the red line is:

$$y = tg(\gamma) \cdot (x+Z) \qquad (A9)$$

and the equation of the circle of radius R_2 is:

$$x^2 + y^2 = R_2^2 \qquad (A10)$$

The solutions of Eqs.A9,A10 results in the coordinates of the two intersections between the straight line and the circle. The solutions are:

$$x_{2/1} = \frac{-Z \cdot tg^2(\gamma) \pm \sqrt{R_2^2 \cdot [tg^2(\gamma)+1] - tg^2(\gamma) \cdot Z^2}}{tg^2(\gamma)+1} \qquad (A11)$$

$$y_{2/1} = tg(\gamma) \cdot [x_{2/1} + Z] \qquad (A12)$$

From Eqs.A11,A12 we get the length of the chord:

$$r_2 = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} = 2 \cdot \sqrt{\frac{R_2^2 \cdot [tg^2(\gamma)+1] - tg^2(\gamma) \cdot Z^2}{tg^2(\gamma)+1}} \qquad \text{(A13)}$$

and based on Figure A1 $tg(\gamma)$ depends on α as follows:

$$tg(\gamma) = \frac{R_2 \cdot \sin(\alpha)}{Z - R_2 \cdot \cos(\alpha)} \qquad \text{(A14)}$$

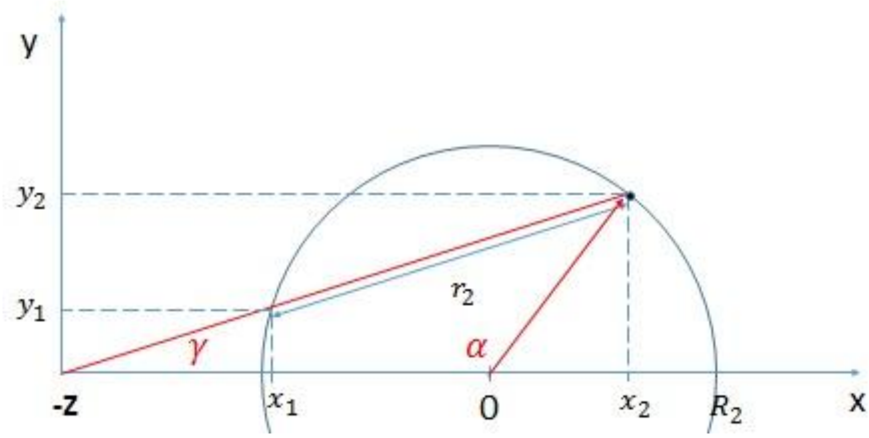


Figure A1. Calculating the length of the chord, r_2.

If the straight line intersects the circle with radius R_1 the length of the chord, r_1 is:

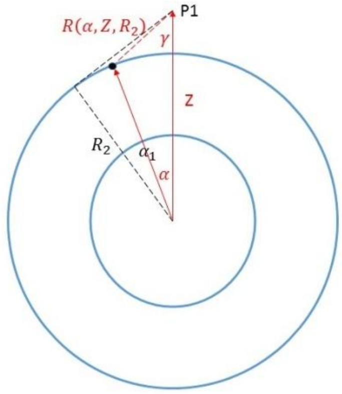
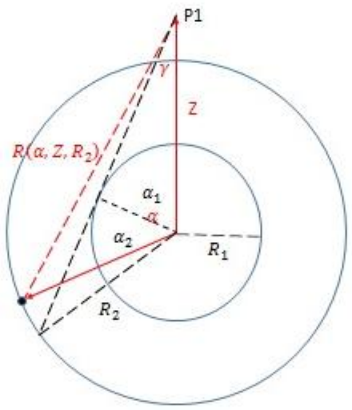
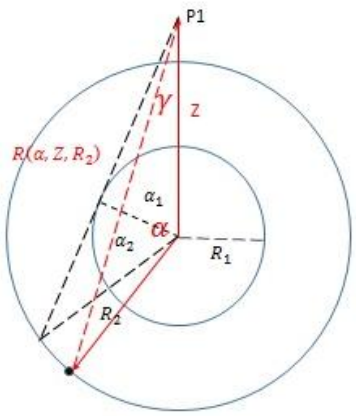
$$r_1 = 2 \cdot \sqrt{\frac{R_1^2 \cdot [tg^2(\gamma)+1] - tg^2(\gamma) \cdot Z^2}{tg^2(\gamma)+1}} \qquad \text{(A15)}$$

and $tg(\gamma)$ depends on α as follows:

$$tg(\gamma) = \frac{R_1 \cdot \sin(\alpha)}{Z - R_1 \cdot \cos(\alpha)} \qquad \text{(A16)}$$

Appendix 4

Table A1. Eleven cases for calculating the $R_{(e1)}(\alpha, Z)$ and $R_{(e2)}(\alpha, Z)$ functions.

	Figures showing the eleven different cases	Equations for calculating $R^{i}_{(e1)}$ or $R^{i}_{(e2)}$	Limits of angle α
I $(Z > R_2)$ Considered charge is on the outer sphere		$R^{I}_{(e2)}(\alpha, Z) = R(\alpha, Z, R_2)$	$\alpha^{I}_{min} = 0 < \alpha < \alpha_1 = \alpha^{I}_{max}$ $\cos(\alpha_1) = R_2/Z$
II $(Z > R_2)$ Considered charge is on the outer sphere		$R^{II}_{(e2)}(\alpha, Z) = R(\alpha, Z, R_2) - r_2$ r_2 is the length of the chord (at the intersections of the outer circle and the red dashed line) and calculated by Eq.A13	$\alpha^{II}_{min} = \alpha_1 < \alpha < \alpha_1 + \alpha_2 = \alpha^{II}_{max}$ $\cos(\alpha_1 + \alpha_2)$ is at Eq.A8
III $(Z > R_2)$ Considered charge is on the outer sphere		$R^{III}_{(e2)}(\alpha, Z) = R(\alpha, Z, R_2) - (r_2 - r_1)$ r_1 is the length of the chord (at the intersections of the inner circle and the red dashed line) and calculated by Eq.A15	$\alpha^{III}_{min} = \alpha_1 + \alpha_2 < \alpha < \pi = \alpha^{III}_{max}$ $\cos(\alpha_1 + \alpha_2)$ is at Eq.A8

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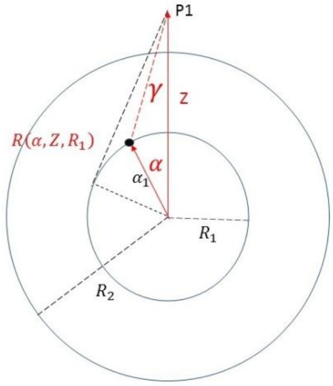
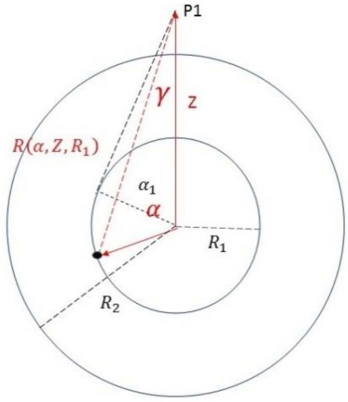
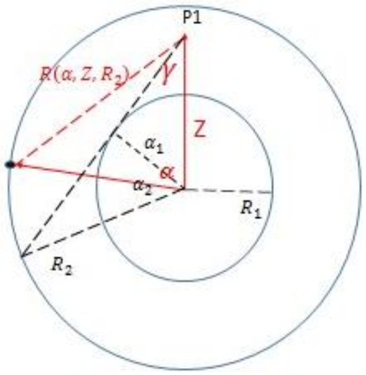
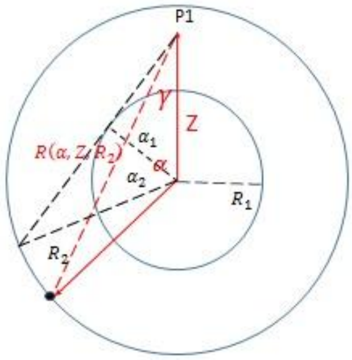
	Figures showing the eleven different cases	Equations for calculating $R^{i}_{(e1)}$ or $R^{i}_{(e2)}$	Limits of angle α
IV $(Z > R_2)$ Considered charge is on the inner sphere		$R^{IV}_{(e1)}(\alpha, Z) =$ $R(\alpha, Z, R_1) -$ $0.5 \cdot (r_2 - r_1)$	$\alpha^{IV}_{min} = 0 < \alpha <$ $\alpha_1 = \alpha^{IV}_{max}$ $\cos(\alpha_1) = R_1/Z$
V $(Z > R_2)$ Considered charge is on the inner sphere		$R^{V}_{(e1)}(\alpha, Z) =$ $R(\alpha, Z, R_1) -$ $0.5 \cdot (r_2 - r_1)$	$\alpha^{V}_{min} = \alpha_1 < \alpha <$ $\pi = \alpha^{V}_{max}$ $\cos(\alpha_1) = R_1/Z$
VI $(R_1 < Z < R_2)$ Considered charge is on the outer sphere		$R^{VI}_{(e2)}(\alpha, Z) = 0$	$\alpha^{VI}_{min} = 0 < \alpha <$ $\alpha_1 + \alpha_2 = \alpha^{VI}_{max}$ $\cos(\alpha_1 + \alpha_2)$ is at Eq.A8
VII $(R_1 < Z < R_2)$ Considered charge is on the outer sphere		$R^{VII}_{(e2)}(\alpha, Z) = r_1$	$\alpha^{VII}_{min} = \alpha_1 + \alpha_2 < \alpha <$ $\pi = \alpha^{VII}_{max}$ $\cos(\alpha_1 + \alpha_2)$ is at Eq.A8

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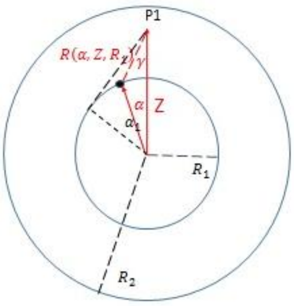
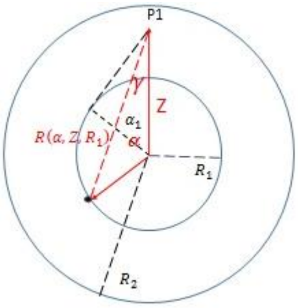
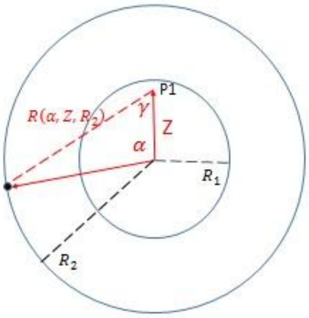
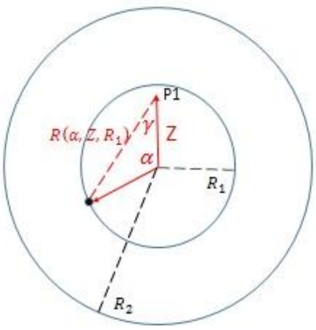
	Figures showing the eleven different cases	Equations for calculating $R^i_{(e1)}$ or $R^i_{(e2)}$	Limits of angle α
VIII ($R_1 < Z < R_2$) Considered charge is on the inner sphere		$R^{VIII}_{(e1)}(\alpha, Z) = 0$	$\alpha^{VIII}_{min} = 0 < \alpha < \alpha_1 = \alpha^{VIII}_{max}$ $\cos(\alpha_1) = R_1/Z$
IX ($R_1 < Z < R_2$) Considered charge is on the inner sphere		$R^{IX}_{(e1)}(\alpha, Z) = r_1$	$\alpha^{IX}_{min} = \alpha_1 < \alpha < \pi = \alpha^{IX}_{max}$ $\cos(\alpha_1) = R_1/Z$
X ($Z < R_1$) Considered charge is on the outer sphere		$R^{X}_{(e2)}(\alpha, Z) = R(\alpha, Z, R_2) - 0.5 \cdot (r_2 - r_1)$	$\alpha^{X}_{min} = 0 < \alpha < \pi = \alpha^{X}_{max}$
XI ($Z < R_1$) Considered charge is on the inner sphere		$R^{XI}_{(e1)}(\alpha, Z) = 0$	$\alpha^{XI}_{min} = 0 < \alpha < \pi = \alpha^{XI}_{max}$