PHY 712 Electrodynamics 12-12:50 AM MWF Olin 103 Plan for Lecture 4:

Reading: Chapter 1 - 3 in JDJ

Electrostatic potentials

- 1. One, two, and three dimensions (Cartesian coordinates)
- 2. Mean value theorem for the electrostatic potential

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Colloquium: "Prediction and Inverse Design of Sustainable Energy Materials"

Dr. Ongun Ozcelik

Theoretical and Computational Chemistry

University of California, San Diego

George P. Williams, Jr. Lecture Hall, (Olin 101)

Wednesday, January 22, 2020 at 3:00 PM

There will be a reception in the Olin Lounge at approximately 4 PM following the colloquium. All interested persons are cordially invited to attend.

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PHY 712 Electrodynamics

MWF 12-12:50 PM OPL 103 http://www.wfu.edu/~natalie/s20phy712/

Instructor: Natalie Holzwarth Phone:758-5510 Office:300 OPL e-mail:natalie@wfu.edu

Course schedule for Spring 2020

Mon: 01/13/2020 Wed: 01/15/2020	Chap. 1 & Appen.	Introduction, units and Poisson equation		
Ned: 01/15/2020		introduction, units and Poisson equation	#1	01/17/2020
	Chap. 1	Electrostatic energy calculations	#2	01/22/2020
ri: 01/17/2020	Chap. 1	Electrostatic potentials and fields	#3	01/24/2020
Mon: 01/20/2020	No class	Martin Luther King Holiday		
Wed: 01/22/2020	Chap. 1 - 3	Poisson's equation in 2 and 3 dimensions	#4	01/27/2020
ri: 01/24/2020	Chap. 1 - 3	Brief introduction to numerical methods		
Mon: 01/27/2020	Chap. 2 & 3	Image charge constructions		
Ned: 01/29/2020	Chap. 2 & 3	Cylindrical and spherical geometries		
ri: 01/31/2020	Chap. 3 & 4	Spherical geometry and multipole moments		
Mon: 02/03/2020	Chap. 4	Dipoles and Dielectrics		
/	Ved: 01/22/2020 Fri: 01/24/2020 Mon: 01/27/2020 Ved: 01/29/2020 Fri: 01/31/2020	Ved: 01/22/2020 Chap. 1 - 3 rit: 01/24/2020 Chap. 1 - 3 One on 10/27/2020 Chap. 2 & 3 Ved: 01/29/2020 Chap. 2 & 3 rit: 01/31/2020 Chap. 3 & 4 Interval of the one of	Ved: 01/22/2020 Chap. 1 - 3 Poisson's equation in 2 and 3 dimensions rit: 01/24/2020 Chap. 1 - 3 Brief introduction to numerical methods Mon: 01/27/2020 Chap. 2 & 3 Image charge constructions vect: 01/29/2020 Chap. 2 & 3 Cylindrical and spherical geometries rit: 01/31/2020 Chap. 3 & 4 Spherical geometry and multipole moments don: 02/03/2020 Chap. 4 Dipoles and Dielectrics	Ved: 01/22/2020 Chap. 1 - 3 Poisson's equation in 2 and 3 dimensions #4 rit: 01/24/2020 Chap. 1 - 3 Brief introduction to numerical methods Mon: 01/27/2020 Chap. 2 & 3 Image charge constructions Ved: 01/29/2020 Chap. 2 & 3 Cylindrical and spherical geometries rit: 01/31/2020 Chap. 3 & 4 Spherical geometry and multipole moments don: 02/03/2020 Chap. 4 Dipoles and Dielectrics

Poisson Equation

$$\nabla^2 \Phi_P(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0}$$

Solution to Poisson equation using Green's function $G(\mathbf{r},\mathbf{r}')$:

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int_V d^3r' \rho(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') +$$

$$\frac{1}{4\pi}\int_{S}d^{2}r'\left[G(\mathbf{r},\mathbf{r}')\nabla'\Phi(\mathbf{r}')-\Phi(\mathbf{r}')\nabla'G(\mathbf{r},\mathbf{r}')\right]\cdot\hat{\mathbf{r}}'.$$

Poisson equation for one-dimensional system

Poisson equation for one-dimension
$$\frac{d^2\Phi_p(x)}{dx^2} = -\frac{\rho(x)}{\varepsilon_0}$$
 Example solution:

$$\Phi_{p}(x) = \frac{1}{4\pi\varepsilon_{0}} \int_{-\infty}^{\infty} G(x, x') \rho(x') dx' + C_{1} + C_{2}x$$

where $G(x, x') = 4\pi x$, where x, is the smaller of x and x'; C_1 and C_2 are constants.

Check:

$$\Phi_{p}(x) = \frac{1}{\varepsilon_{0}} \left\{ \int_{-\infty}^{x} x' \, \rho(x') dx' + x \int_{x}^{\infty} \rho(x') dx' \right\} + C_{1} + C_{2} x$$

$$\frac{d\Phi_{p}(x)}{dx} = \frac{1}{\varepsilon_{0}} \int_{x}^{\infty} \rho(x') dx' + C_{2} \quad \Rightarrow \frac{d^{2}\Phi_{p}(x)}{dx^{2}} = -\frac{\rho(x)}{\varepsilon_{0}}$$

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General procedure for constructing Green's function for onedimensional system using 2 independent solutions of the homogeneous equations

Consider two independent solutions to the homogeneous equation

$$\nabla^2 \phi_i(x) = 0$$

where i = 1 or 2. Let

$$G(x,x') = \frac{4\pi}{W}\phi_1(x_<)\phi_2(x_>).$$

This notation means that $x_{\scriptscriptstyle <}$ should be taken as the smaller of x and x' and $x_{>}$ should be taken as the larger.

"Wronskian": $W \equiv \frac{d\phi_1(x)}{dx}\phi_2(x) - \phi_1(x)\frac{d\phi_2(x)}{dx}$.

Beautiful method; but only works in one dimension.

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Orthogonal function expansions and Green's functions

Suppose we have a "complete" set of orthogonal functions $\{u_n(x)\}$ defined in the interval $x_1 \leq x \leq x_2$ such that

$$\int_{x_1}^{x_2} u_n(x) u_m(x) \ dx = \delta_{nm}.$$

We can show that the completeness of this functions implies that

$$\sum_{n=1}^{\infty} u_n(x)u_n(x') = \delta(x - x').$$

This relation allows us to use these functions to represent a Green's function for our system. For the 1-dimensional Poisson equation, the Green's function satisfies

$$\frac{\partial^2}{\partial x^2}G(x, x') = -4\pi\delta(x - x').$$

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Orthogonal function expansion -- continued

Suppose the orthogonal functions satisfy an eigenvalue equation:

$$\frac{d^2}{dx^2}u_n(x) = -\alpha_n u_n(x)$$

where the functions $u_n(x)$ also satisfy the appropriate boundary conditions, then we can construct the Green's function:

$$G(x,x') = 4\pi \sum_{n} \frac{u_n(x)u_n(x')}{\alpha_n}$$

$$\frac{d^2}{dx^2}G(x,x') = 4\pi \sum_{n} \frac{\left(-\alpha_n u_n(x)\right) u_n(x')}{\alpha_n} = -4\pi \sum_{n} u_n(x) u_n(x')$$
$$= -4\pi \delta(x-x')$$

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Example

For example, consider the previous example in the interval $-a \le x \le a$:

$$-u \le x \le u$$
. $0 mtext{for } x < 0$

$$\rho(x) = \begin{cases} 0 & \text{for } x < -a \\ -\rho_0 & \text{for } -a < x < 0 \\ +\rho_0 & \text{for } 0 < x < a \end{cases}$$

We want to solve the Poisson equation with boundary condition $d\Phi(-a)/dx = 0$ and $d\Phi(a)/dx = 0$. We may choose

$$u_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{[2n+1]\pi x}{2a}\right)$$
 and the corresponding Green's function

$$G(x,x') = \frac{4\pi}{a} \sum_{n=0}^{\infty} \frac{\sin\left(\frac{[2n+1]\pi x}{2a}\right) \sin\left(\frac{[2n+1]\pi x'}{2a}\right)}{\left(\frac{[2n+1]\pi}{2a}\right)^{2}}.$$

Example -- continuedThis form of the one-dimensional Green's function only allows us to find a solution to the Poisson equation within the interval $-a \le x \le a$ from

$$\Phi(x) = \frac{1}{4\pi\varepsilon_0} \int_{-a}^{a} dx' \ G(x, x') \rho(x') + C_1$$

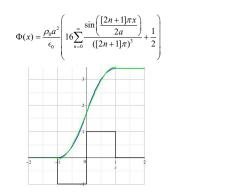
$$\Rightarrow \Phi(x) = \frac{\rho_0 a^2}{\epsilon_0} \left[16 \sum_{n=0}^{\infty} \frac{\sin\left(\frac{[2n+1]\pi x}{2a}\right)}{\left([2n+1]\pi\right)^3} + \frac{1}{2} \right]$$

choosing C_1 so that $\Phi(-a) = 0$.

Exact result:
$$\Phi(x) = \begin{cases} 0 & \text{for } x < -a \\ \frac{\rho_0}{2\varepsilon_0}(x+a)^2 & \text{for } -a < x < 0 \\ -\frac{\rho_0}{2\varepsilon_0}(x-a)^2 + \frac{\rho_0 a^2}{\varepsilon_0} & \text{for } 0 < x < a \\ \frac{\rho_0}{\varepsilon_0} a^2 & \text{for } x > a \end{cases}$$

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Example -- continued



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Orthogonal function expansions in 2 and 3 dimensions

$$\nabla^2 \Phi(\mathbf{r}) \equiv \frac{\partial^2 \Phi(\mathbf{r})}{\partial x^2} + \frac{\partial^2 \Phi(\mathbf{r})}{\partial y^2} + \frac{\partial^2 \Phi(\mathbf{r})}{\partial z^2} = -\rho(\mathbf{r}) / \epsilon_0.$$

Let $\{u_n(x)\}, \{v_n(y)\}, \{w_n(z)\}\$ denote complete orthogonal function sets in the x, y, and z dimensions, respectively. The Green's function construction becomes:

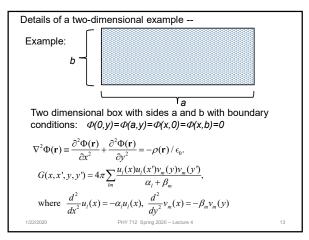
$$G(x,x',y,y',z,z') = 4\pi \sum_{lmn} \frac{u_l(x)u_l(x')v_m(y)v_m(y')w_n(z)w_n(z')}{\alpha_l + \beta_m + \gamma_n},$$

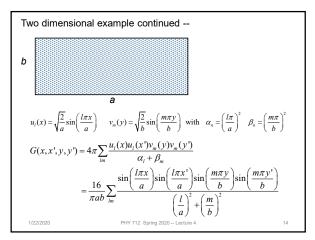
$$\frac{d^2}{dx^2}u_l(x) = -\alpha_l u_l(x), \ \frac{d^2}{dy^2}v_m(y) = -\beta_m v_m(y), \text{ and } \frac{d^2}{dz^2}w_n(z) = -\gamma_n w_n(z).$$

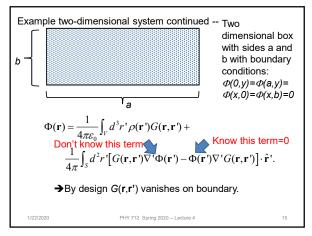
(See Eq. 3.167 in Jackson for example.)

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Example #1:
$$\rho(x,y) = \rho_0 \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{b}\right)$$

Example #2: $\rho(x, y) = \rho_0$

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int_V d^3 r' \rho(\mathbf{r}') G(\mathbf{r}, \mathbf{r}')$$

$$G(x,x',y,y') = \frac{16}{\pi ab} \sum_{lm} \frac{\sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{l\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \sin\left(\frac{m\pi y'}{b}\right)}{\left(\frac{l}{a}\right)^2 + \left(\frac{m}{b}\right)^2}$$

For example #1:
$$\Phi(x, y) = \frac{\rho_0 a^2 b^2}{\epsilon_0 \pi^2 (a^2 + b^2)} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{b}\right)$$

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Combined orthogonal function expansion and homogeneous solution construction of Green's function in 2 and 3 dimensions.

An alternative method of finding Green's functions for a second order ordinary differential equations (in 1 dimension) is based on a product of two independent solutions of the homogeneous equation, $\phi_1(x)$ and $\phi_2(x)$

$$G(x, x') = K\phi_1(x_<)\phi_2(x_>)$$
, where $K = \frac{4\pi}{\frac{d\phi_1}{dx}\phi_2 - \phi_1}\frac{d\phi_2}{dx}$,

where x_{\cdot} denotes the smaller of x and x'.

For the two and three dimensional cases, we can use this technique in one of the dimensions in order to reduce the number of summation terms. These ideas are discussed in Section 3.11 of Jackson.

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Green's function construction -- continued For the two dimensional case, for example, we can assume that the Green's function can be written in the form:

$$G(x,x',y,y') = \sum_{n} u_n(x)u_n(x')g_n(y,y')$$
 where $\frac{d^2}{dx^2}u_n(x) = -\alpha_n u_n(x)$

The y dependence of this equation will have the required

behavior, if we choose:
$$\left[-\alpha_{n} + \frac{\partial^{2}}{\partial y^{2}}\right] g_{n}(y, y') = -4\pi\delta(y - y'),$$

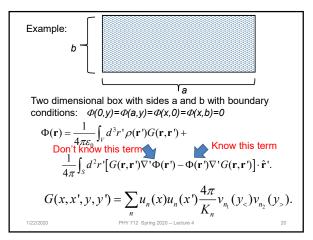
which in turn can be expressed in terms of the two independent solutions $v_{n_i}(y)$ and $v_{n_j}(y)$ of the homogeneous equation:

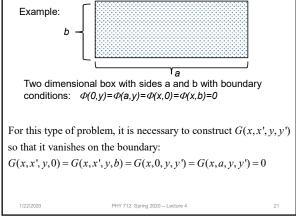
$$\left[\frac{d^2}{dy^2} - \alpha_n\right] v_{n_i}(y) = 0,$$

and the Wronskian constant: $K_n \equiv \frac{dv_{n_1}}{dy}v_{n_2} - v_{n_1}\frac{dv_{n_2}}{dy}$

$$\begin{bmatrix} -\alpha_n + \frac{\partial^2}{\partial y^2} \end{bmatrix} g_n(y, y') = -4\pi\delta(y - y'),$$

$$g_n(y, y') = \frac{4\pi}{K_n} v_{n_1}(y_<) v_{n_2}(y_>)$$
where:
$$\left[\frac{d^2}{dy^2} - \alpha_n \right] v_{n_1}(y) = 0,$$
and
$$K_n \equiv \frac{dv_{n_1}}{dy} v_{n_2} - v_{n_1} \frac{dv_{n_2}}{dy}$$
For example, choose
$$v_{n_1}(y) = \sinh(\sqrt{\alpha_n}y) \quad \text{and} \quad v_{n_2}(y) = \sinh(\sqrt{\alpha_n}(b - y))$$
where
$$K_n = \sqrt{\alpha_n} \sinh(\sqrt{\alpha_n}b)$$
using the identity:
$$\cosh(r) \sinh(s) + \sinh(r) \cosh(s) = \sinh(r + s)$$





$$G(x,x',y,y') = \sum_{n} u_{n}(x)u_{n}(x')\frac{4\pi}{K_{n}}v_{n_{1}}(y_{<})v_{n_{2}}(y_{>}).$$

$$\frac{d^{2}}{dx^{2}}u_{n}(x) = -\alpha_{n}u_{n}(x) \quad \text{where} \quad u_{n}(0) = u_{n}(a) = 0$$

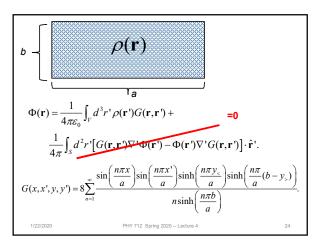
$$\Rightarrow u_{n}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad \alpha_{n} = \left(\frac{n\pi}{a}\right)^{2}$$

$$\left[\frac{d^{2}}{dy^{2}} - \left(\frac{n\pi}{a}\right)^{2}\right]v_{n_{1}}(y) = 0$$

$$v_{n_{1}}(y) = \sinh\left(\frac{n\pi}{a}y\right) \qquad v_{n_{2}}(y) = \sinh\left(\frac{n\pi}{a}(b-y)\right)$$

$$K_{n} = \frac{n\pi}{a}\sinh\left(\frac{n\pi b}{a}\right)$$
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Green's function construction — continued $G(x,x',y,y') = \sum_n u_n(x)u_n(x')K_nv_{n_1}(y_<)v_{n_2}(y_>).$ For example, a Green's function for a two-dimensional rectangular system with $0 \le x \le a$ and $0 \le y \le b$, which vanishes on the rectangular boundaries: $G(x,x',y,y') = 8\sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n\pi x'}{a}\right)\sinh\left(\frac{n\pi y_<}{a}\right)\sinh\left(\frac{n\pi}{a}(b-y_>)\right)}{n\sinh\left(\frac{n\pi b}{a}\right)}.$



$$G(x,x',y,y') = 8 \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{n\pi x'}{a}\right) \sinh\left(\frac{n\pi y_{s}}{a}\right) \sinh\left(\frac{n\pi}{a}(b-y_{s})\right)}{n \sinh\left(\frac{n\pi b}{a}\right)}.$$
Example:
$$\rho(x,y) = \rho_{0} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{b}\right)$$

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_{0}} \int_{V} d^{3}r' \rho(\mathbf{r}') G(\mathbf{r},\mathbf{r}')$$
In this example, only n=1 contributes because
$$\int_{0}^{a} dx' \sin\left(\frac{\pi x'}{a}\right) \sin\left(\frac{n\pi x'}{a}\right) = \frac{a}{2} \delta_{1s}$$

$$\Phi(x,y) = \frac{8\rho_{0}}{4\pi\varepsilon_{0}} \frac{a}{2\sinh(\pi a/b)} \sin\left(\frac{\pi x}{a}\right) \times \left(\sinh\left(\frac{\pi y'}{a}\right) \int_{0}^{b} dy' \sin\left(\frac{\pi y'}{a}\right) \sinh\left(\frac{\pi y'}{a}\right)\right)$$

$$\left(\sinh\left(\frac{\pi(b-y)}{a}\right) \int_{0}^{y} dy' \sin\left(\frac{\pi y'}{a}\right) \sinh\left(\frac{\pi y'}{a}\right) + \sinh\left(\frac{\pi y}{a}\right) \int_{y}^{b} dy' \sin\left(\frac{\pi y'}{b}\right) \sinh\left(\frac{\pi(b-y')}{a}\right)\right)$$
When the dust clears:
$$\Phi(x,y) = \frac{\rho_{0}}{\varepsilon_{0}} \frac{a^{2}b^{2}}{\pi^{2}(a^{2}+b^{2})} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{b}\right)$$

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A useful theorem for electrostatics The mean value theorem (Problem 1.10 in Jackson)

The "mean value theorem" value theorem (problem 1.10 of your textbook) states that the value of $\Phi({\bf r})$ at the arbitrary (charge-free) point ${\bf r}$ is equal to the average of $\Phi({\bf r}')$ over the surface of any sphere centered on the point r (see Jackson problem #1.10). One way to prove this theorem is the following. Consider a point $\mathbf{r}' = \mathbf{r} + \mathbf{u}$, where \mathbf{u} will describe a sphere of radius R about the fixed point ${\bf r}$. We can make a Taylor series expansion of the electrostatic potential $\Phi(\mathbf{r}')$ about the fixed point $\mathbf{r}:$

$$\Phi(\mathbf{r}+\mathbf{u}) = \Phi(\mathbf{r}) + \mathbf{u} \cdot \nabla \Phi(\mathbf{r}) + \frac{1}{2!} (\mathbf{u} \cdot \nabla)^2 \Phi(\mathbf{r}) + \frac{1}{3!} (\mathbf{u} \cdot \nabla)^3 \Phi(\mathbf{r}) + \frac{1}{4!} (\mathbf{u} \cdot \nabla)^4 \Phi(\mathbf{r}) + \cdots$$
 (1

According to the premise of the theorem, we want to integrate both sides of the equation 1 over a sphere of radius R in the variable ${\bf u}$:

$$\int_{\text{sphere}} dS_u = R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u). \tag{2}$$

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Mean value theorem - continued

We note that
$$\begin{split} R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) 1 &= 4\pi R^2, \\ R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) \mathbf{u} \cdot \nabla &= 0, \\ R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) (\mathbf{u} \cdot \nabla)^2 &= \frac{4\pi R^4}{3} \nabla^2, \\ R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) (\mathbf{u} \cdot \nabla)^3 &= 0, \end{split}$$
 and
$$R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) (\mathbf{u} \cdot \nabla)^3 &= \frac{4\pi R^6}{5} \nabla^4. \end{split}$$
 Since $\nabla^2 \Phi(\mathbf{r}) = 0$, the only non-zero term of the average is thus the first term:
$$R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) \Phi(\mathbf{r} \cdot \nabla)^4 &= \frac{4\pi R^6}{5} \nabla^4. \end{split}$$

or $\Phi(\mathbf{r}) = \frac{1}{4\pi R^2} \ R^2 \int_0^{2\pi} d\phi_u \int_{-1}^{+1} d\cos(\theta_u) \Phi(\mathbf{r}+\mathbf{u}) \equiv \frac{1}{4\pi R^2} \int_{\text{sphere}} dS_u \Phi(\mathbf{r}+\mathbf{u}).$ Since this result is independent of the radius R, we see that we have the theorem.

Summary: Mean value theorem	
$\Phi(\mathbf{r}) = \frac{1}{4\pi R^2} \int R^2 d\Omega_u \ \Phi(\mathbf{r} + \mathbf{u})$	
r	