

PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 18:
Reading: Chapter 10 in MPM
Ingredients of electronic structure calculations

1. Construction of and testing of pseudopotentials

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9	Wed: 02/04/2015	Chap. 8	Electronic structure, LCAO and tight binding	#9	02/06/2015
10	Fri: 02/06/2015	Chap. 8	Band structure examples	#10	02/09/2015
11	Mon: 02/09/2015	Chap. 9	Electron-electron interactions	#11	02/11/2015
12	Wed: 02/11/2015	Chap. 9	Electron-electron interactions	#12	02/13/2015
13	Fri: 02/13/2015	Chap. 9	Electron-electron interactions	#13	02/16/2015
14	Mon: 02/16/2015	Chap. 10	Electronic structure calculation methods	#14	02/18/2015
15	Wed: 02/18/2015	Chap. 10	Electronic structure calculation methods	#15	02/20/2015
16	Fri: 02/20/2015	Chap. 10	Electronic structure calculation methods	#16	02/23/2015
17	Mon: 02/23/2015	Chap. 10	Electronic structure calculation methods	#17	02/25/2015
18	Wed: 02/25/2015	Chap. 10	Electronic structure calculation methods	#18	02/27/2015
19	Fri: 02/27/2015	Chap. 1-3,7-10	Review; Take-home exam distributed		
	Mon: 03/02/2015	APS Meeting	Take-home exam (no class meeting)		
	Wed: 03/04/2015	APS Meeting	Take-home exam (no class meeting)		
	Fri: 03/06/2015	APS Meeting	Take-home exam (no class meeting)		
	Mon: 03/09/2015	Spring break			
	Wed: 03/11/2015	Spring break			
	Fri: 03/13/2015	Spring break			
20	Mon: 03/16/2015				

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Department of Physics

News

[Prof. Matthews' Studio Course](#)
Featured by Wake Forest News

[Prof. Carroll receives Innovation Award](#)

[Hands on with hydrogen](#)

Events

Wed. Feb. 25, 2015
Physics Colloquium:
Manipulating EM Waves
Prof. Fiddy, UNCC
 Olin 101 4:00 PM
 Refreshments at 3:30 PM
 Olin Lobby

Wed. Mar. 4, 2015
Physics Colloquium:
Genomic structures in ciliates
Prof. Bracht, American U.
 Olin 101 4:00 PM
 Refreshments at 3:30 PM
 Olin Lobby

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WFU Physics Colloquium

TITLE: Manipulating Electromagnetic Waves with Engineered Materials

SPEAKER: Dr. Mike Fiddy,
*Optoelectronics Center
 University of North Carolina, Charlotte*

TIME: Wednesday February 25, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Engineered materials or metamaterials offer the promise of extreme refractive index properties (e.g. very large, zero or negative values) that do not arise in nature. The field has attracted a lot of attention because of promised of superresolved imaging and cloaking. One physical mechanism that is exploited to achieve these properties relies on the combined effect of many subwavelength-sized (high Q) circuits or meta-atoms operating close to resonance. Extrinsic meaningful constitutive parameters like anisotropic μ or

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Construction of pseudopotential with PAW formalism

PAW transformation:

$$\Psi_v(\mathbf{r}) = \tilde{\Psi}_v(\mathbf{r}) + \sum_a (\Phi_i^a(\mathbf{r} - \mathbf{R}^a) - \tilde{\Phi}_i^a(\mathbf{r} - \mathbf{R}^a)) \langle \tilde{P}_i^a | \tilde{\Psi}_v \rangle$$

↑
↑
↑

pseudo wavefunction atom centered basis functions projector function

$$E_{\text{vale}} = \underbrace{\tilde{E}_{\text{vale}}}_{\text{pseudo-energy}} + \sum_a \underbrace{(E_{\text{vale}}^a - \tilde{E}_{\text{vale}}^a)}_{\text{atom-centered corrections}}$$

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All-electron Kohn-Sham equations for atom a :

$$(\mathcal{H}^{\text{KS}}(\mathbf{r}) - \varepsilon_i^a) \Phi_i^a(\mathbf{r}) = 0$$

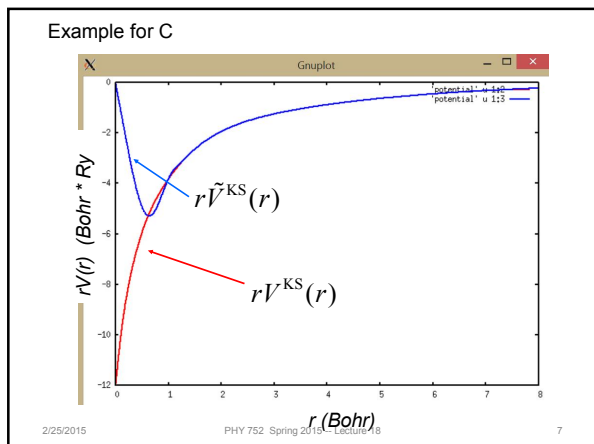
$$\mathcal{H}^{\text{KS}}(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V^{\text{KS}}(\mathbf{r})$$

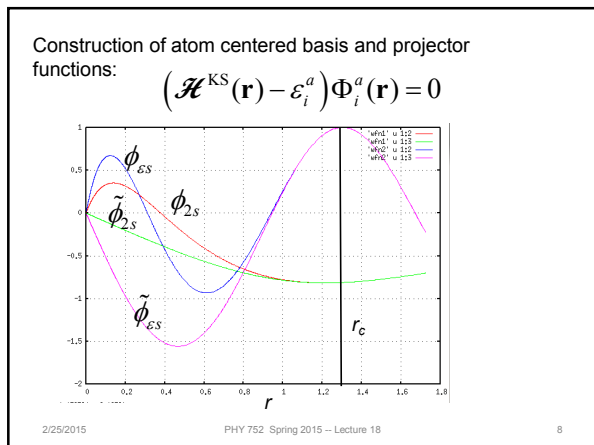
Pseudo Kohn-Sham equations for atom a :

$$(\tilde{\mathcal{H}}^{\text{KS}}(\mathbf{r}) - \varepsilon_i^a) \tilde{\Phi}_i^a(\mathbf{r}) = \sum_j \tilde{P}_j^a(\mathbf{r}) \langle \tilde{\Phi}_j^a | \tilde{\mathcal{H}}^{\text{KS}} - \varepsilon_i^a | \tilde{\Phi}_i^a \rangle$$

$$\tilde{\mathcal{H}}^{\text{KS}}(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + \tilde{V}^{\text{KS}}(\mathbf{r})$$

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Construction of atom centered basis and projector functions – continued (scheme developed by David Vanderbilt for ultra-soft pseudopotentials; for each l channel at a time):

Let
$$\tilde{\phi}_l(r) = \begin{cases} r^{l+1} \sum_{m=1}^4 C_m r^{2m} & r < r_c \\ \phi_l(r) & r > r_c \end{cases}$$

Construct auxiliary function:

$$\chi_l(r) = (\varepsilon_l - \tilde{\mathcal{H}}^{\text{KS}}) \tilde{\phi}_l(r)$$

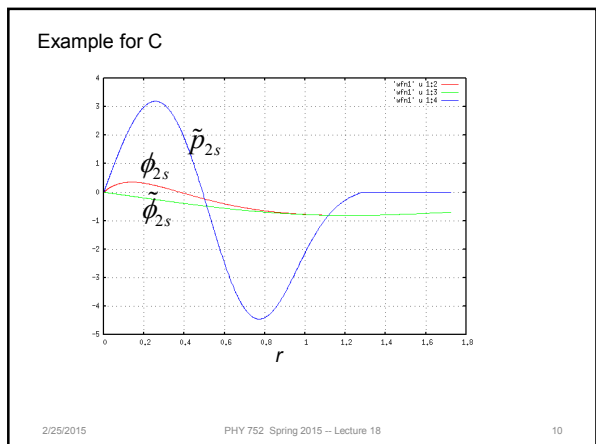
Calculate overlap matrix: $B_{ij} \equiv \langle \chi_i | \chi_j \rangle$

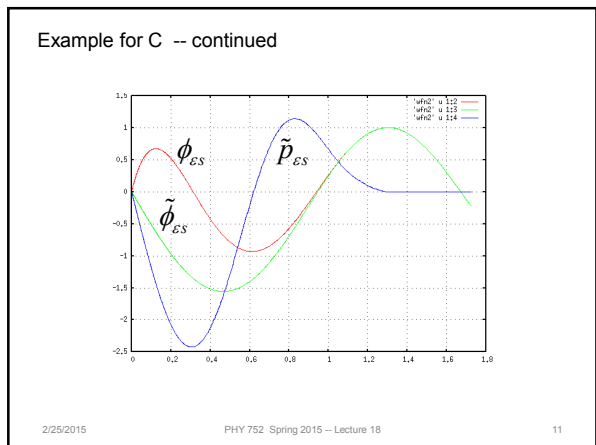
Form projector function: $p_i(r) = \sum_j \chi_j(r) (\mathbf{B}^{-1})_{ji}$

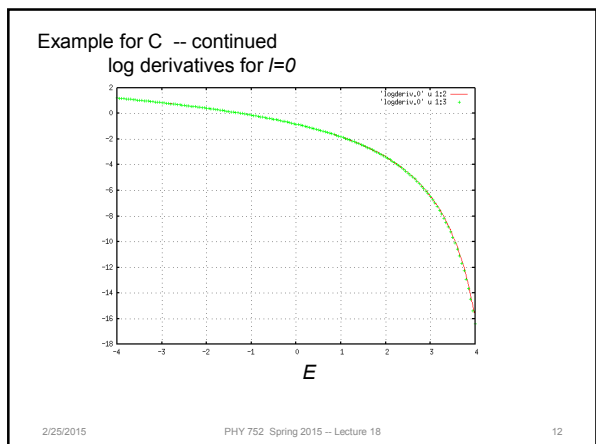
This construction ensures that

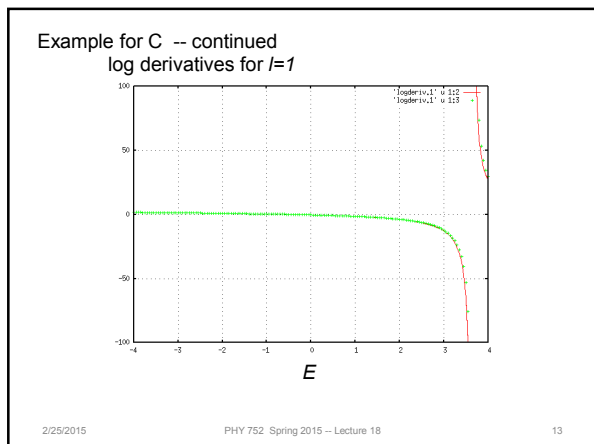
$$\langle \tilde{P}_j^a(\mathbf{r}) | \tilde{\Phi}_i^a \rangle = \delta_{ij}$$

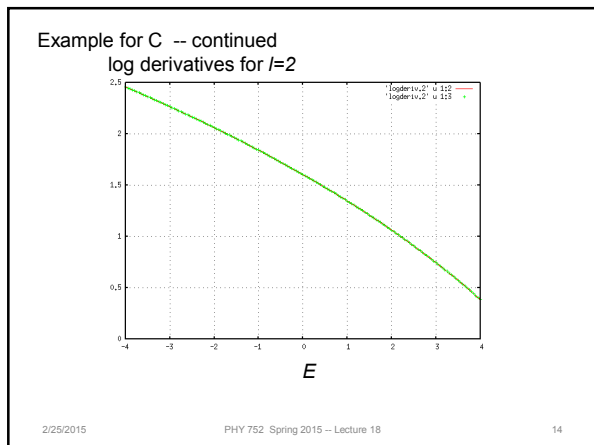
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Instructions for running atompaw pgm

- Log into cluster
- `cd /wfurc1/classes/phy752/login`
- `mkdir [directory name]`
- `cd [directory name]`
- `cp /wfurc1/classes/phys752/natalie/Examples/Atompaw-C/C.in [atom].in`
- `gedit [atom].in`
- `~natalie/EL6/Coursematerials/s15phy752/pgms/runatompaw<C.in>&out&`

Output:

- `wfn1, wfn2, ...` for each basis and projector function
- `logderiv.0, logderiv.1, logderiv.2 ...` for each l channel
- `[atom]` lists energies and basis functions
- input files for QE, abinit, etc.

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input file for atompaw

```

1 C 6
2 LDA-PW loggrid 2001
3 2 0 0 0
4 2 1 2
5 0 0 0
6 c
7 v
8 v
9 1
10 1.3 1.1 1.3 1.3
11 y
12 16
13 n
14 y
15 12
16 n
17 VANDERBILT VANDERBILTORTHO BESSELSHAPE
18 2 0 VITROULLIER
19 1.3
20 1.3
21 1.3
22 1.3
23 ABINITOUT
24 default
25 XMLOUT
26 default
27 PWSCFOUT
28 UPFDX 0.0125d0 UPFXMIN -7.d0 UPFZMESH 6.d0
29 PWPANOUT
30 END
    
```

Annotations:

- Lines 2-5: same as in graphatom
- Lines 6-10: set core (c) and valence (v) maximum / for projectors r_c values (bohr units)
- Lines 12-16: add basis states
- Lines 17-22: options for local potential matching radius for pseudo basis functions
- Lines 23-30: inputs for electronic structure codes

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