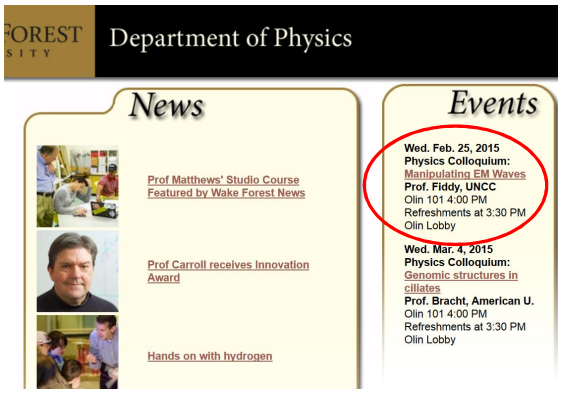
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

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

1. **Construction of and testing of pseudopotentials**

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				



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. Extracting meaningful constitutive parameters like epsilon, mu or

Construction of pseudopotential with PAW formalism

PAW transformation:

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

pseudo wavefunction; atom centered basis functions; projector function

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

All-electron Kohn-Sham equations for atom a:

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

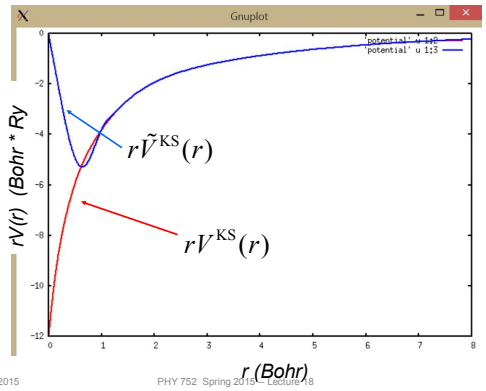
$$\mathscr{H}^{\text{KS}}(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V^{\text{KS}}(\mathbf{r})$$

Pseudo Kohn-Sham equations for atom a:

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

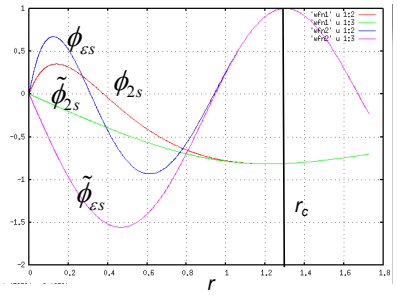
$$\tilde{\mathscr{H}}^{\text{KS}}(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2 + \tilde{V}^{\text{KS}}(\mathbf{r})$$

Example for C



Construction of atom centered basis and projector functions:

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



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

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

Construct auxiliary function:

$\chi_i(r)=\left(\varepsilon_i-\tilde{\mathcal{H}}^{\mathrm{KS}}\right)\tilde{\phi}_i(r)$

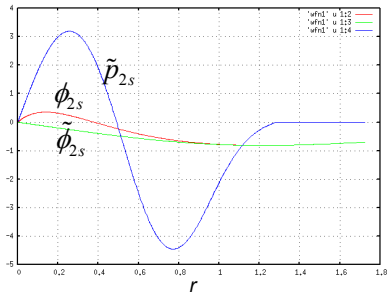
Calculate overlap matrix: $B_{ij}\equiv\langle\chi_i|\chi_j\rangle$

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

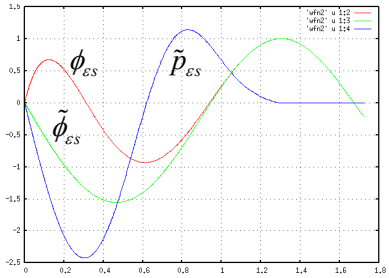
This construction ensures that

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

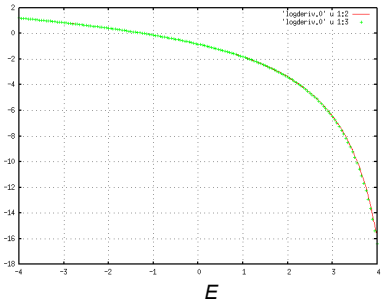
Example for C



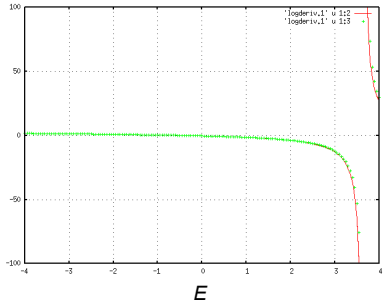
Example for C -- continued



Example for C -- continued
log derivatives for *l=0*



Example for C -- continued
log derivatives for *l=1*



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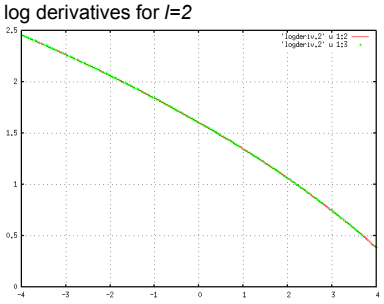
Example for C -- continued
log derivatives for *l=2*



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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.

input file for atompaw