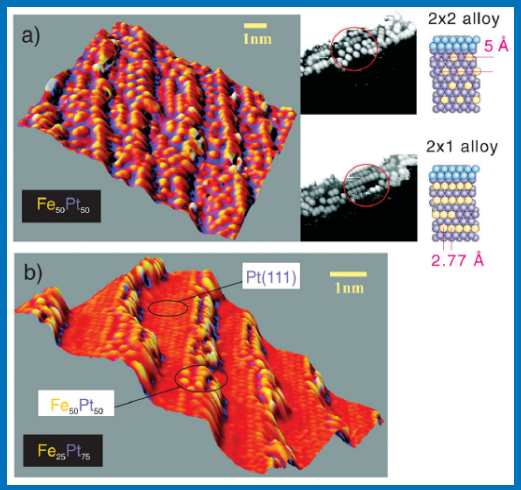
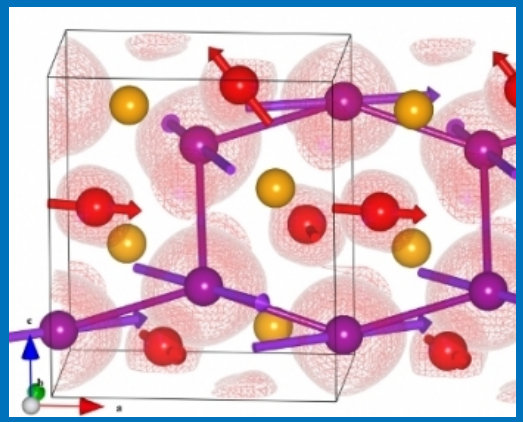
KKR and Green Functions





Julie Staunton
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Electron Density Functional Theory

- $\hat{H} = \frac{\hbar^2}{2m} \int \nabla\psi^\dagger(\mathbf{r})\nabla\psi(\mathbf{r})\, d\mathbf{r} + \frac{e^2}{2} \int\int \frac{\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}'\, d\mathbf{r} + \int V^{ext}(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\, d\mathbf{r}$

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- i.e. $\hat{H} = K.E. + V_{e-e} + V^{ext}$, $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$ are electronic creation and annihilation operators.
- $E_{V^{ext}}[n] = < \Psi|\hat{H}|\Psi >$, $n(\mathbf{r}) = < \Psi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\Psi >$. Minimum gives ground state energy.

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- $\frac{\delta E_{V^{ext}}}{\delta n(\mathbf{r})} = 0$ implies $(\frac{-\hbar^2\nabla^2}{2m} + v^{eff}(\mathbf{r};[n]))\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$. Single electron Schrodinger equation with $n(\mathbf{r}) = \sum_i^{occ.}\phi_i^*(\mathbf{r})\phi_i(\mathbf{r})$.

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- Single electron Green function $G(\mathbf{r},\mathbf{r}';\varepsilon) = \sum_i \frac{\phi_i(\mathbf{r})\phi_i^*(\mathbf{r}')}{(\varepsilon-\varepsilon_i)}$.
- $(\varepsilon - H_{KS})G(\mathbf{r},\mathbf{r}';\varepsilon) = \delta(\mathbf{r}-\mathbf{r}')$

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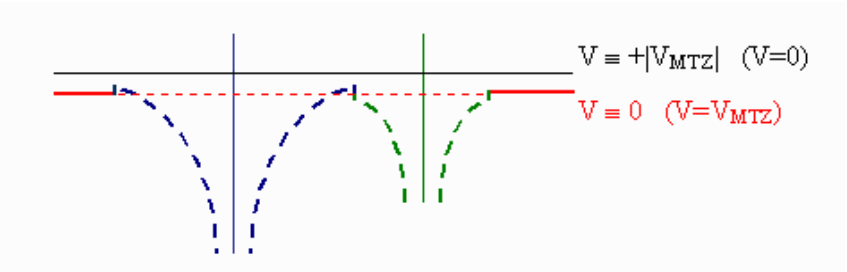
Potentials and Scattering

- Effective Kohn-Sham DFT potentials in a solid, nuclear Coulombic and electronic screening contribution.



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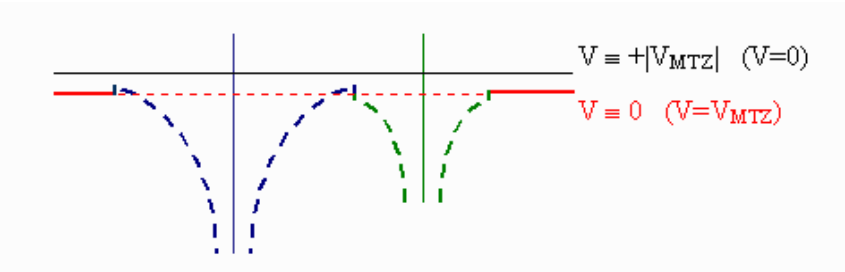
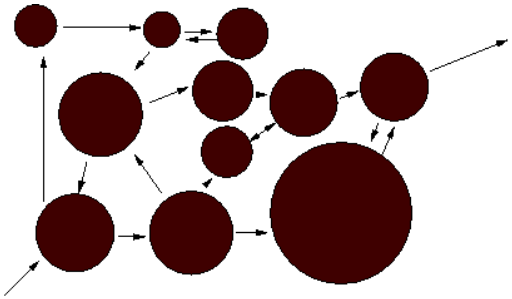


- Muffin-tin approximation



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Single site scattering

- Spherical symmetry $\left(-\bigtriangledown^2 + v\left(r\right)\right)\psi\left(\mathbf{r}\right) = E\psi\left(\mathbf{r}\right)$ $\left(\left(\frac{\hbar^2}{2m}=1, \text{a.u.}\right)\right.$
- $\psi\left(\mathbf{r}\right) = \sum_L a_L(E) R_l(E,r) Y_L(\hat{r})$ where $R_l(E,r)$ is the solution of the radial Schrödinger equation $[-\frac{1}{r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{r^2} + v(r)]R_l(E,r) = ER_l(E,r)$ and $Y_L(\hat{r})$ is a spherical harmonic.

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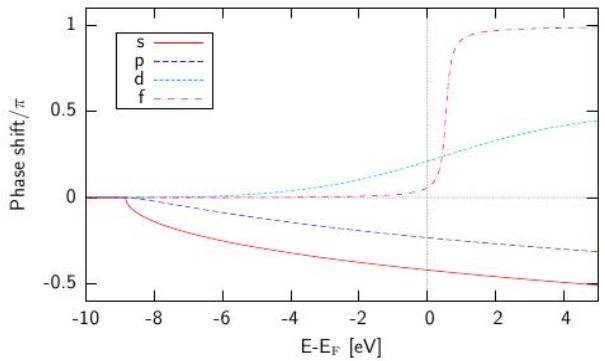

Figure 4.2: Phase shifts of electron states in Ce, obtained from LDA calculation.

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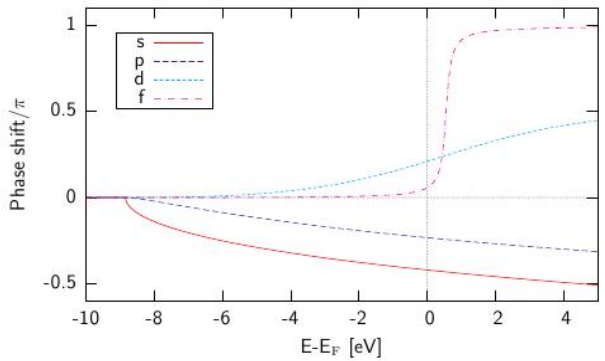

Figure 4.2: Phase shifts of electron states in Ce, obtained from LDA calculation.

- Localised electronic states are characterised by phase shifts with very sharp resonances, whereas band-like states have more slowly varying phase shifts.

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Green Functions

- $G(E) = \lim_{\epsilon \to 0}(E + i\epsilon - H)^{-1}, \cdots G(\mathbf{r}, \mathbf{r}', E) = \sum_i \frac{\phi_i(\mathbf{r})\phi_i^*(\mathbf{r}')}{E - \epsilon_i}$.

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  $t(\mathbf{r}, \mathbf{r}', E) = v(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') + \int d\mathbf{r}''\ v(\mathbf{r}) G_0(\mathbf{r}, \mathbf{r}'', E) t(\mathbf{r}'', \mathbf{r}', E)$

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- Spherical symmetric potential, $t_{L,L'} = t_L \delta_{L,L'} = -\frac{1}{\sqrt{E}} \sin\delta_l e^{i\delta_l}$, phase shifts again. $t \leftrightarrow \delta_l$.

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- $G_{0,LL'}$ are so-called *structure constants*, which depend only where the scatterers are located $\mathbf{R}_1$,$\mathbf{R}_2$, $\cdots$.

  $G_{0,LL'}(\mathbf{R}_i - \mathbf{R}_j, E) = -4\pi i\sqrt{E} \sum_{L''} i^{l''}\, C^{L''}_{LL'}\ h^+_{l''}(\sqrt{E}\ |\ \mathbf{R}_i - \mathbf{R}_j\ |)\, Y_{L''}(\widehat{\mathbf{R}_i - \mathbf{R}_j})$

  with Gaunt numbers $C^{L''}_{LL'} = \int d\Omega\ Y^*_L(\Omega)\, Y_{L'}(\Omega)\, Y_{L''}(\Omega)$.

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- T is the scattering T-matrix for the potential array, $T = V + V\, G_0\, T$.

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Multiple Scattering - scattering path operator

- $T = \sum_{i,j} \tau^{ij}$ so that τ^{ij} gives the outgoing wave from the i site if there is an incoming wave on j
  $\tau^{ij} = t_i \delta_{ij} + \sum_{k \neq i} t_i G_0^{i,k} \tau^{kj}$
- Plane wave, *on the energy shell*, angular momentum representation
  $\tau^{ij}_{L,L'}(E) = t_{i,L}(E)\delta_{ij}\delta_{LL'} + \sum_{k \neq i} \sum_{L''} \; t_{i,L}(E) G_{0,LL'}(\mathbf{R}_i - \mathbf{R}_k, E) \tau^{kj}_{L'',L'}(E)$

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- If the array of potentials forms a periodic lattice, a Lattice Fourier transform produces
  $\tau_{L,L'}(\mathbf{k}, E) = [\underline{t}^{-1}(E) - \underline{G_0}(\mathbf{k}, E)]^{-1}$ and
  $\| \; t_L^{-1}(E)\delta_{LL'} - G_{0,LL'}(\mathbf{k}, E) \; \| = 0$
  is the KKR secular equation for the band structure of the system.

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Calculating properties from the KKR

- Green function for DFT, spectra, response functions etc.
  $G(\mathbf{r},\mathbf{r}',E) = \sum_{LL'} Z^i_L(\mathbf{r}_i,E)\tau^{ij}_{L,L'}(E)Z^j_{L'}(\mathbf{r}'_j,E) - \delta_{ij}\sum_L Z^i_L(\mathbf{r}_<,E)J^i_L(\mathbf{r}_>,E)$
  where Z^n_L and J^n_L are respectively the regular and irregular solutions to the Schrödinger equation for a single site potential v_n. $\left(\mathbf{r} = \mathbf{r}_i + \mathbf{R}_i,\ \mathbf{r}' = \mathbf{r}'_j + \mathbf{R}_j\right)$.

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- Density for DFT: $n(\mathbf{r}) = -\frac{1}{\pi}\int_{E_B}^{E_F} dE\ \mathrm{Im}G(\mathbf{r},\mathbf{r},E)$

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- Electronic structure:
  - Density of states: $n(E) = -\frac{1}{\pi}\int d\mathbf{r}\mathrm{Im}G(\mathbf{r},\mathbf{r},E)$

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Calculating properties from the KKR

- Green function for DFT, spectra, response functions etc.
  $G(\mathbf{r},\mathbf{r}',E) = \sum_{LL'} Z^i_L(\mathbf{r}_i,E)\tau^{ij}_{L,L'}(E)Z^j_{L'}(\mathbf{r}'_j,E) - \delta_{ij}\sum_L Z^i_L(\mathbf{r}_<,E)J^i_L(\mathbf{r}_>,E)$
  where Z^n_L and J^n_L are respectively the regular and irregular solutions to the Schrödinger equation for a single site potential v_n. $\left(\mathbf{r}=\mathbf{r}_i+\mathbf{R}_i,\ \mathbf{r}'=\mathbf{r}'_j+\mathbf{R}_j\right)$.
- Density for DFT: $n(\mathbf{r}) = -\frac{1}{\pi}\int_{E_B}^{E_F} dE\ \mathrm{Im}G(\mathbf{r},\mathbf{r},E)$
- Electronic structure:
  - Density of states: $n(E) = -\frac{1}{\pi}\int d\mathbf{r}\mathrm{Im}G(\mathbf{r},\mathbf{r},E)$
  - Spectral function
    $\bar{A}_B(\mathbf{k},E) = -\frac{1}{\pi}\mathrm{Im}\sum_{nm}\exp[i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{R}_m)]\int d\mathbf{r}G(\mathbf{r}+\mathbf{R}_n,\mathbf{r}+\mathbf{R}_m,E)$
    $\rightsquigarrow \bar{A}_B(\mathbf{k},E) = \sum_n \delta(E-E_n(\mathbf{k}))$.
    In disordered systems peaks broaden but their positions give an effective band structure, with their width in energy interpreted as an inverse lifetime.

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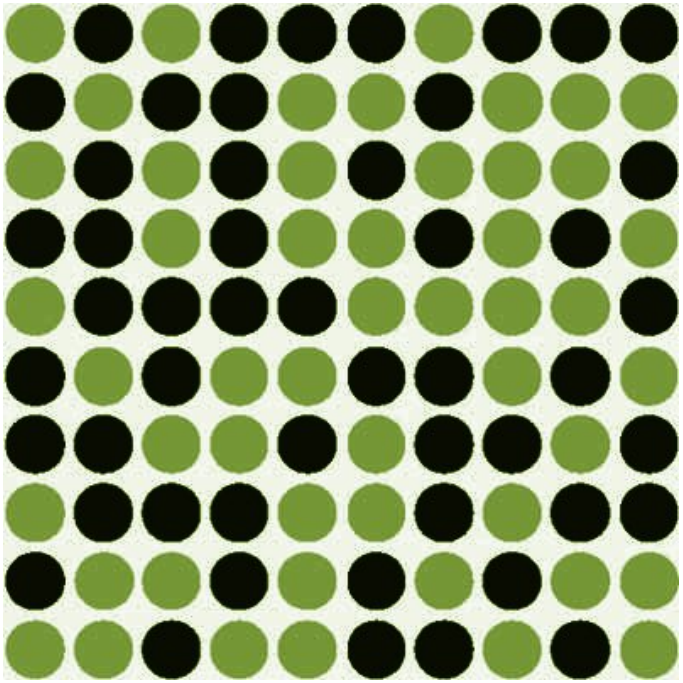
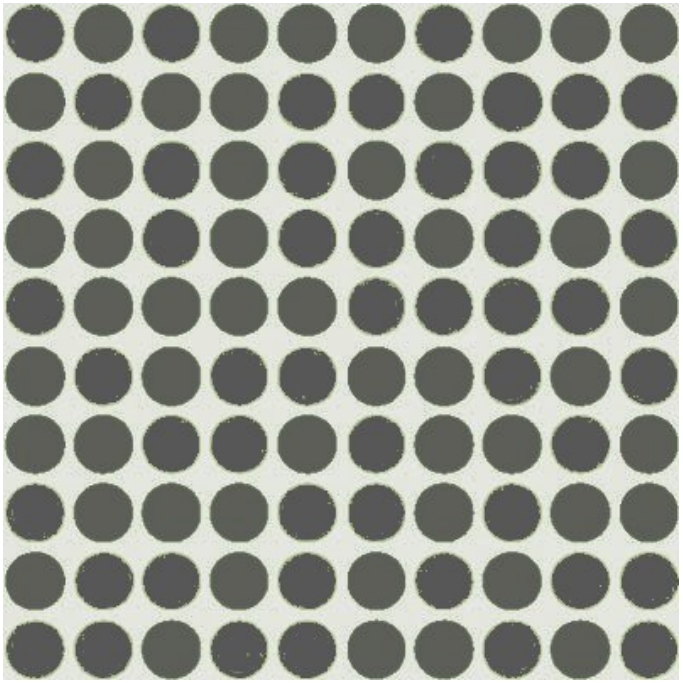
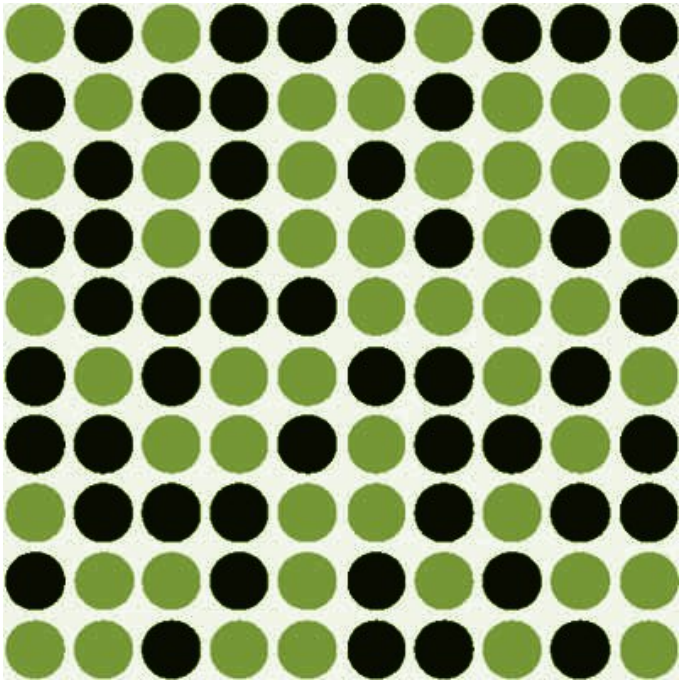
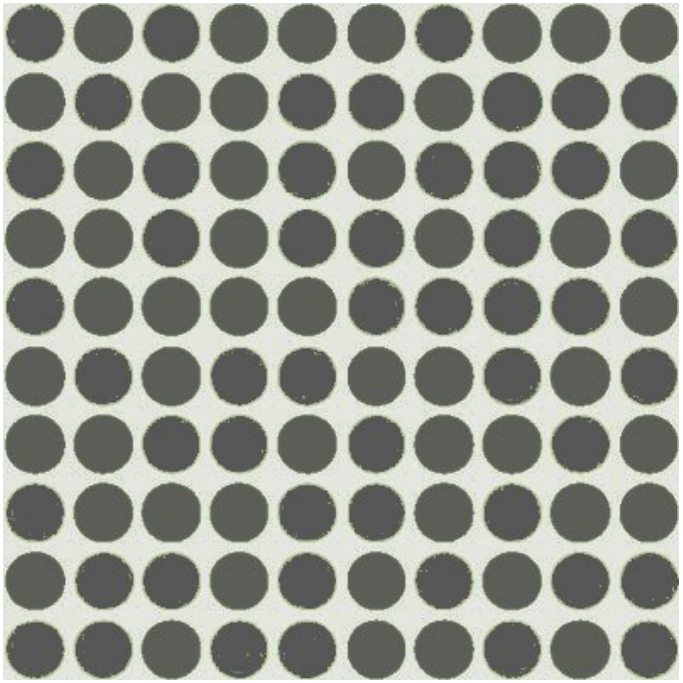
Electrons and Disorder - An Effective Lattice





Electrons and Disorder - An Effective Lattice





- $< G^{ij} >= G_0^{ij} + \sum_{kl} G_0^{ik} \, \Xi^{kl} \, < G^{lj} >$
- $\bar{G}(\mathbf{k}) = \frac{1}{N} \sum_j < G^{ij} > e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} = (G_0^{-1}(\mathbf{k}) - \Xi(\mathbf{k}))^{-1}$
- $\Xi(\mathbf{k})$ is a *self energy*.

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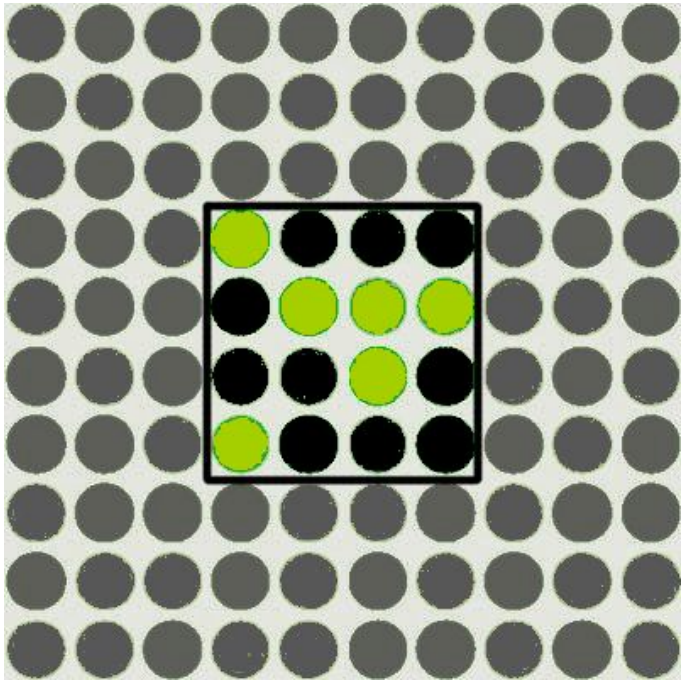
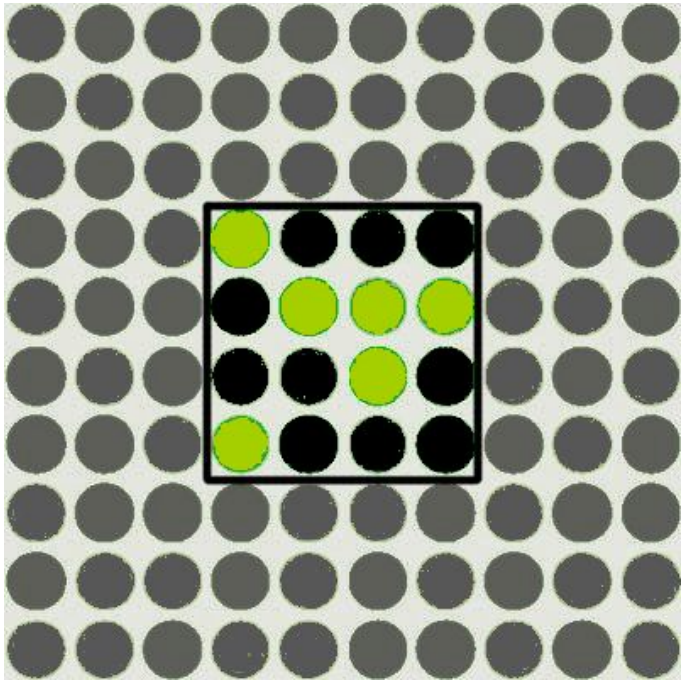
Cluster Approximation



Cluster Approximation



- $G^{\eta}_{IJ} = [\underline{G}^{0,-1} + \underline{\Xi} - \underline{V}^{\eta}]^{-1}_{IJ}$
- $\sum_{\eta} P(\eta) G^{\eta}_{IJ} = \hat{G}_{IJ} \approx < G_{IJ} >$

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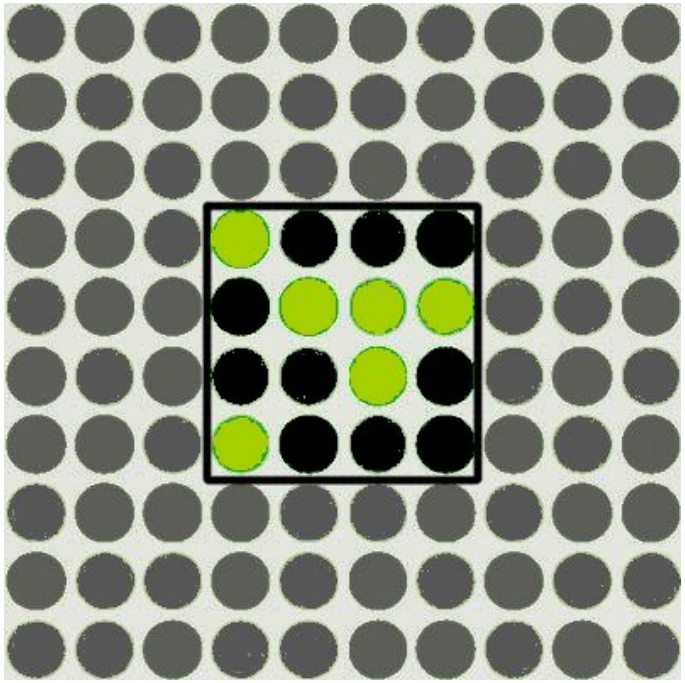
Cluster Approximation



- $G^{\eta}_{IJ} = [\underline{G}^{0,-1} + \underline{\Xi} - \underline{V}^{\eta}]^{-1}_{IJ}$
- $\sum_{\eta} P(\eta) G^{\eta}_{IJ} = \hat{G}_{IJ} \approx < G_{IJ} >$
- $\hat{G}_{IJ} = \frac{1}{\Omega_{BZ}} \sum_{\mathbf{K}_n} \int [G^0(\mathbf{k}) - \Xi(\mathbf{K}_n]^{-1} e^{i\mathbf{K}_n \cdot (\mathbf{R}_I - \mathbf{R}_J)} d\mathbf{k}_n.$

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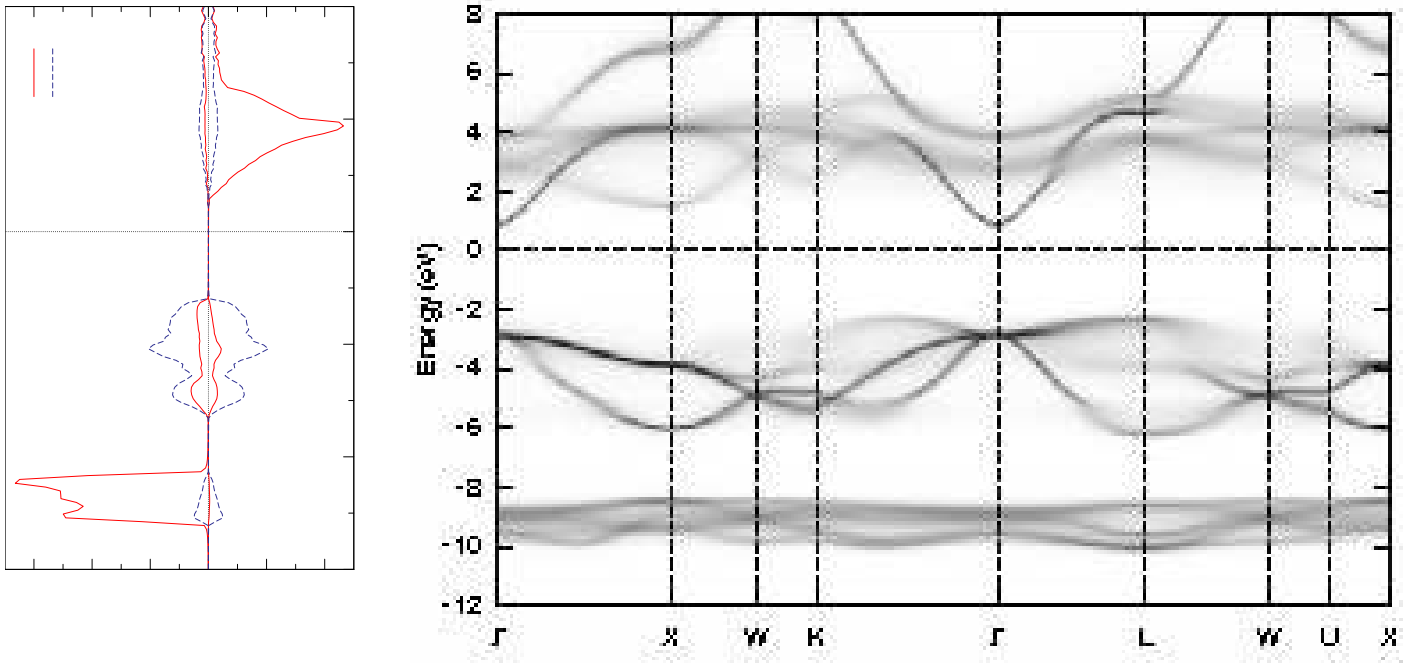
The paramagnetic state of transition metal oxides

The electronic structure for MnO in its paramagnetic (DLM) state. The loci of the peaks of the Bloch spectral function with the shading showing the spin fluctuation disorder broadening of these quasi-particle peaks.



DOS for MnO on Mn and O sites (dashed). The left (right) panel shows the DOS associated with electrons with spins parallel (anti-parallel) to the local moment on the site. Note the sizeable gap of the paramagnetic state.

I.D.Hughes *et al.*, New .J.Phys.10, 063010, (2008)

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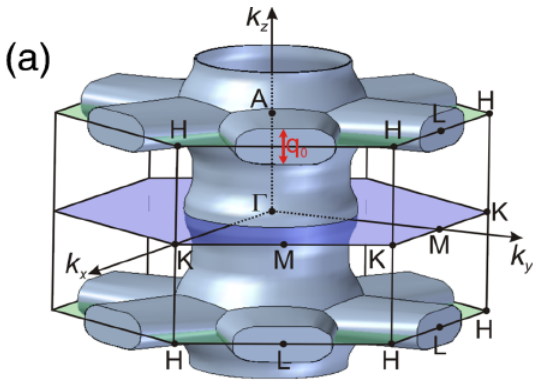
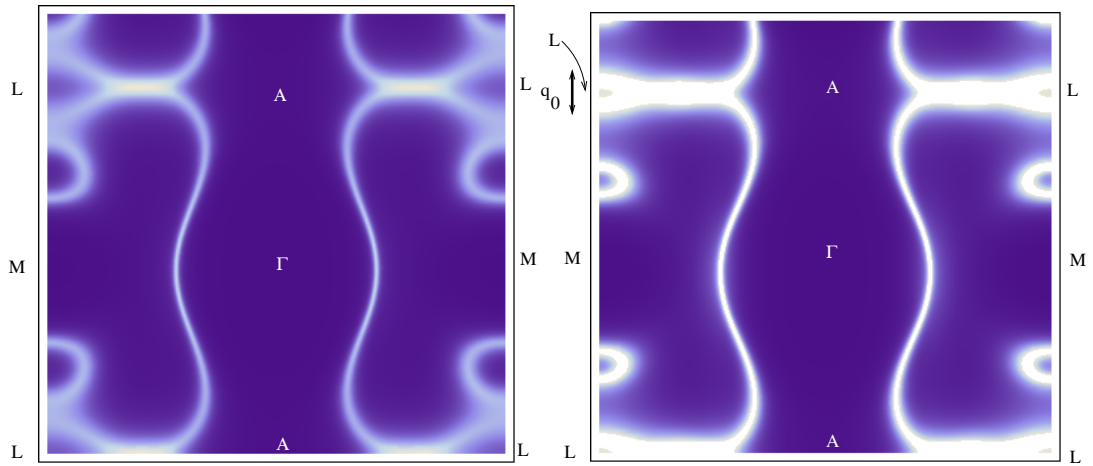
Transition from HAFM to FM - Fermi surface nesting





Theoretical FS for paramagnetic Gd and Dy.

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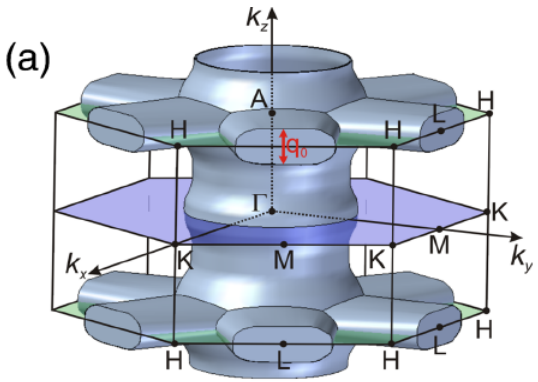
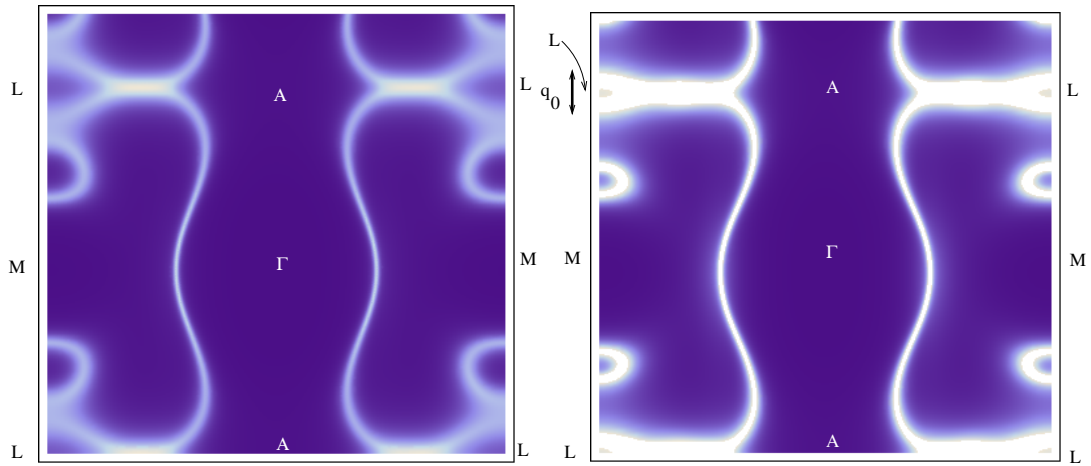
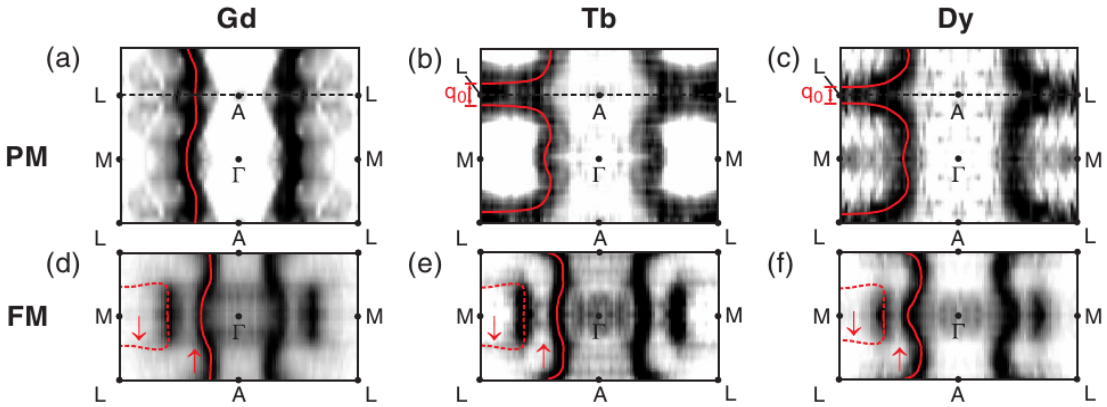
Transition from HAFM to FM - Fermi surface nesting





Theoretical FS for paramagnetic Gd and Dy.



K.M.Dobrich et al., Phys.Rev.Lett. **104**, 246401, (2010)

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