Maximally-Localized Lattice Wannier Functions

Karin Rabe, Rutgers
Razvan Caracas, UCL

Electronic Structure Discussion Group

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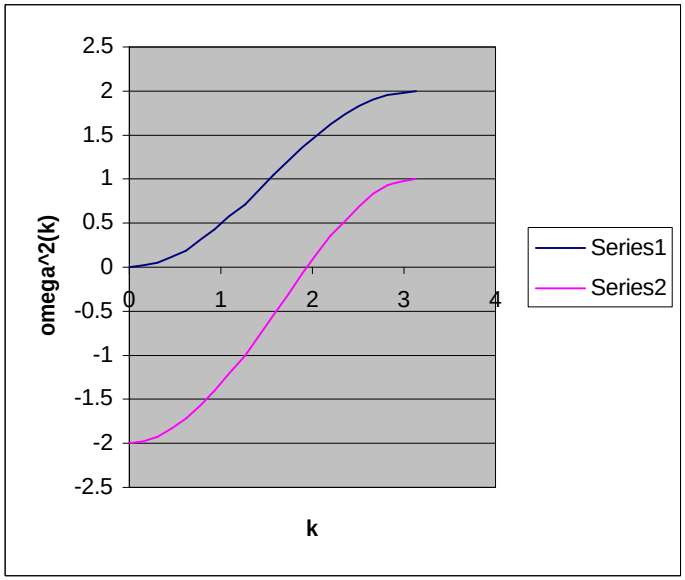
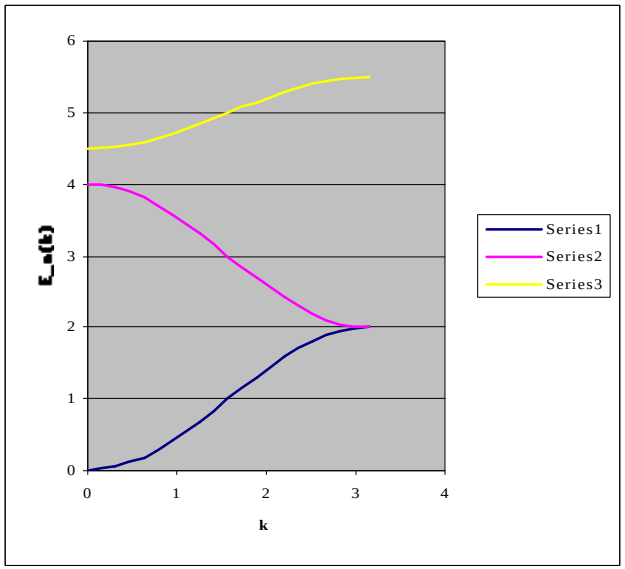
isolated band



composite band (d >1)

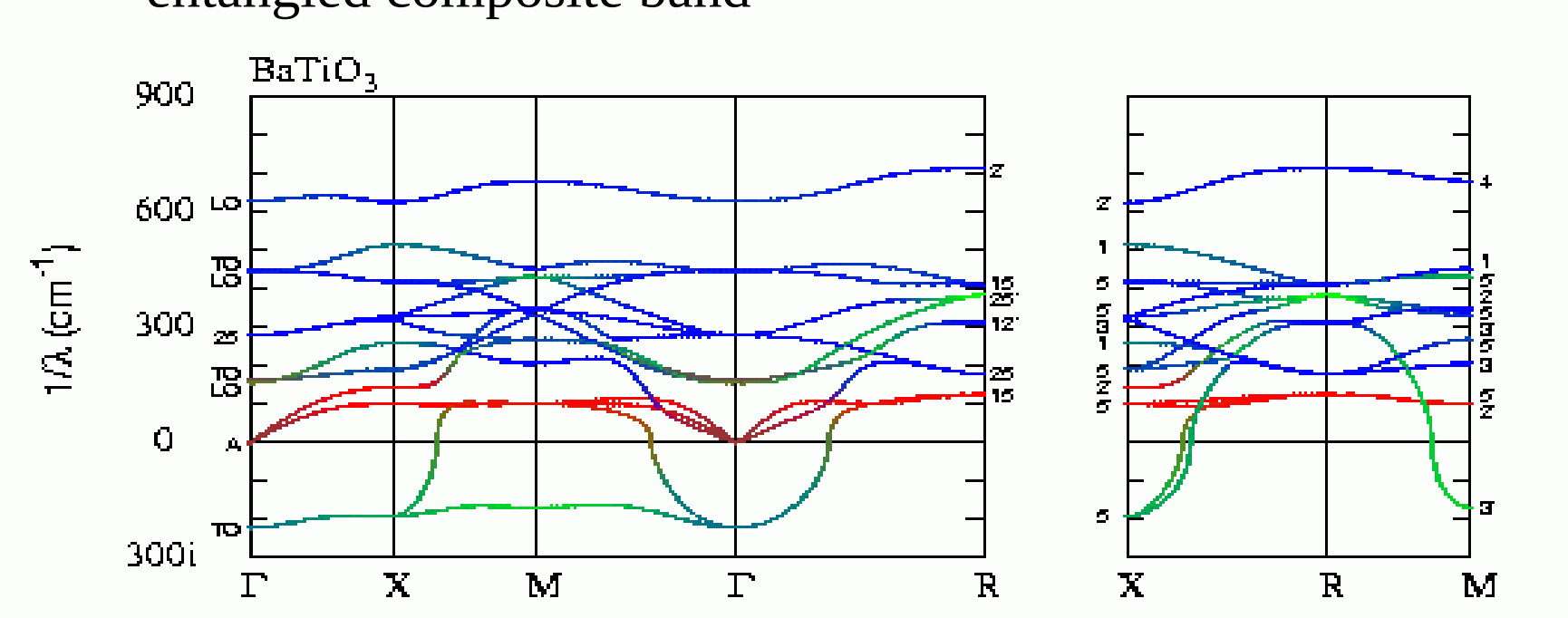


K. M. Rabe and U. V. Waghmare, “Localized basis for effective lattice Hamiltonians: Lattice Wannier functions,” PRB 52, 13246 (1995)

W. Kohn, “Localized basis for lattice vibrations,” PRB 7, 2285 (1973)

improve localization of LWF:
J. Iniguez, A. Garcia and J. M. Perez-Mato, “Optimized local modes for lattice dynamical applications,” PRB 61, 3127 (2000)

entangled composite band



Recent developments in ***electronic*** Wannier functions:

N. Marzari and D. Vanderbilt, “Maximally localized Wannier functions for composite energy bands,” PRB 56, 12847 (1997)

I. Souza, N. Marzari and D. Vanderbilt, “Maximally localized Wannier functions for entangled energy bands,” PRB 65, 035109 (2001)

"Lattice Wannier functions" are to phonons what Wannier functions are to Bloch states

consider an isolated band in 1D (a=1)

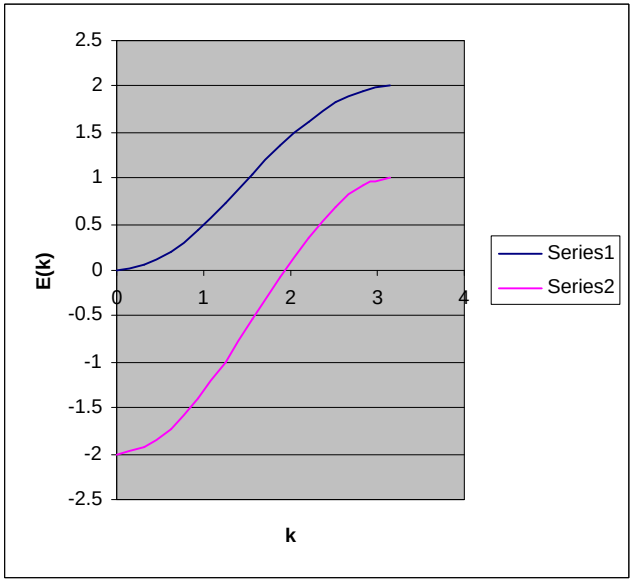
$\psi_k(x) = \exp(ikx)\, u_k(x)$

orthonormal basis set for same space

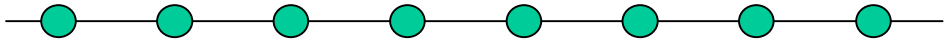
- localized around lattice site n
- related by lattice translations
- *definite point symmetry*

$\psi_k(x) \propto \Sigma_n \exp(ikn)\, w_n(x)$

(Bloch sum of localized "orbitals")

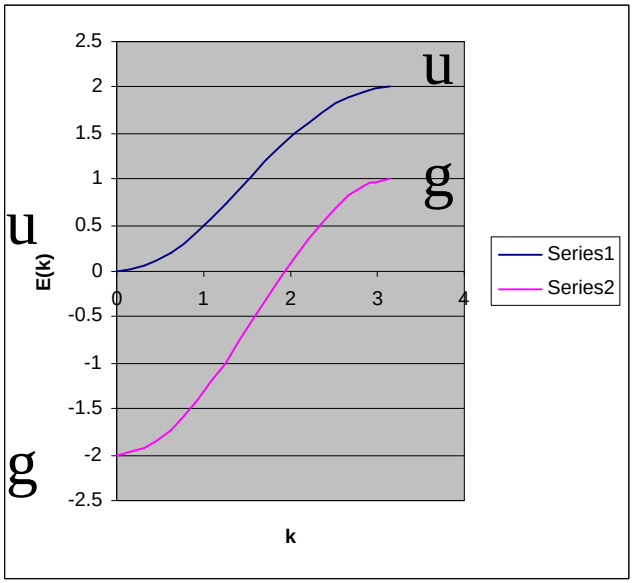


bands carry symmetry labels
(irreducible representations of space groups)



lattice translations, inversion through atom

Wannier functions can have definite
symmetry properties
consistent with symmetry labels of bands



on atoms:
"s" orbitals (even under x → -x): Γ_g, X_g
"p" orbitals (odd under x → -x): Γ_u, X_u
midway between atoms:
"s" orbitals (even under x → -x): Γ_g, X_u
"p" orbitals (odd under x → -x): Γ_u, X_g

explicit construction by transform
$w_n(x) = (1/2\pi) \int dk \exp(ikn) \psi_k(x)$

nonuniqueness: phase ambiguity of $\psi_k(x) \rightarrow \exp(i\phi(k)) \psi_k(x)$
- u_k is a smooth function of k in the extended zone scheme
- symmetry

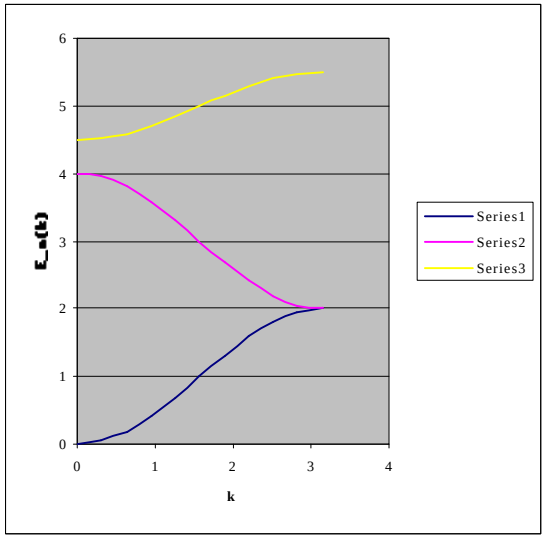
measure of localization: "spread functional" Ω
$\int dx\ (x-x_n)^2\ w_n(x)^2$ is a functional of $\phi(k)$: $\Omega[\phi(k)]$
minimize wrt $\phi(k)$

Marzari and Vanderbilt, PRB 56, 12847 (1997)
discretize in k-space
numerically compute $\psi_k(x)$ (arbitrary phases)
numerically optimize $\Omega[\phi(k)]$

Composite bands (d > 1)

$\psi_{kn}(x)$, n = 1, N_b

phase ambiguity generalizes to
unitary transformation $U_{nm}(k)$
"gauge transformation"



$$\psi_{kn}(x) \rightarrow \Sigma\, U_{nm}(k)\, \psi_{km}(x)$$

Marzari and Vanderbilt covered this case as well
note: decompose $\Omega = \Omega_I + \tilde{\Omega}$
Ω_I is invariant under gauge transformation: functional of subspace
(smallest when $\{u_{kn}(x)\}$ is independent of k)
minimize $\tilde{\Omega}$

Now, for phonons

- phonon notation
- 1D example for isolated band
- entangled bands
- implementation in ABINIT

n atoms per unit cell in d dimensions

normal modes of vibration around equilibrium
assume Bloch form
for d = 1:
$u_{m\kappa}(k,j) = \mathrm{Re}[M_\kappa^{-1/2}\, u_\kappa(k,j) \exp(i(kma-\omega(k,j)t))]$

m labels lattice vector (1D)
κ labels atom in unit cell
k is a wavevector in 1st BZ
j labels the branch (j=1,…,nd)

nd x nd dynamical matrix at each k
each eigenvector: nd complex numbers $u_\kappa(k,j)$

unstable modes

If the crystal structure is an extremum but not a local minimum, then one or more of the eigenvalues of the dynamical matrix will be negative

The frequency ω (the square root of the eigenvalue) of that mode will be imaginary, and for plotting the dispersion relation, is taken as negative

The presence and nature of unstable modes shows that the structure considered is energetically unstable against certain distortions, and unstable modes are a central feature of the “soft-mode” theory of structural phase transitions. The main motivation of the present work is to construct subspaces that contain the unstable modes.

Example:
1D chain with two atoms per cell ($M_1 = M_2 = 1$)

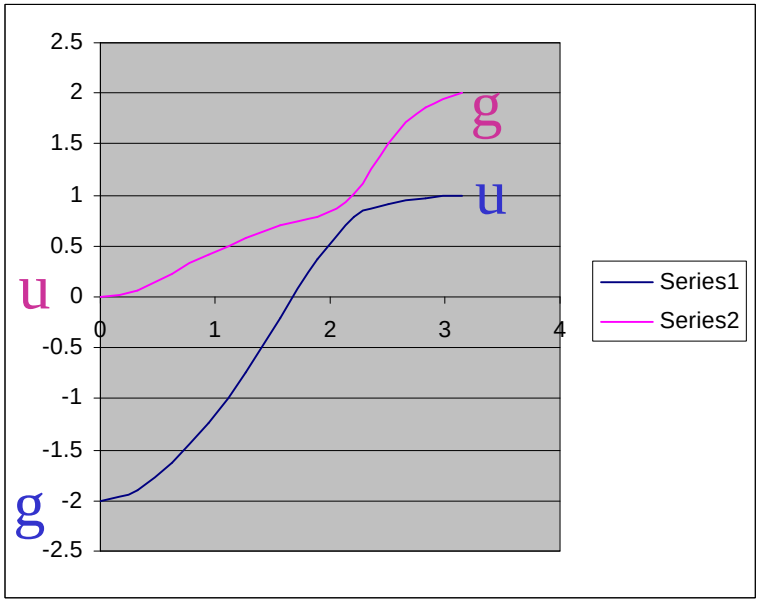
2 x 2 dynamical matrix at each k

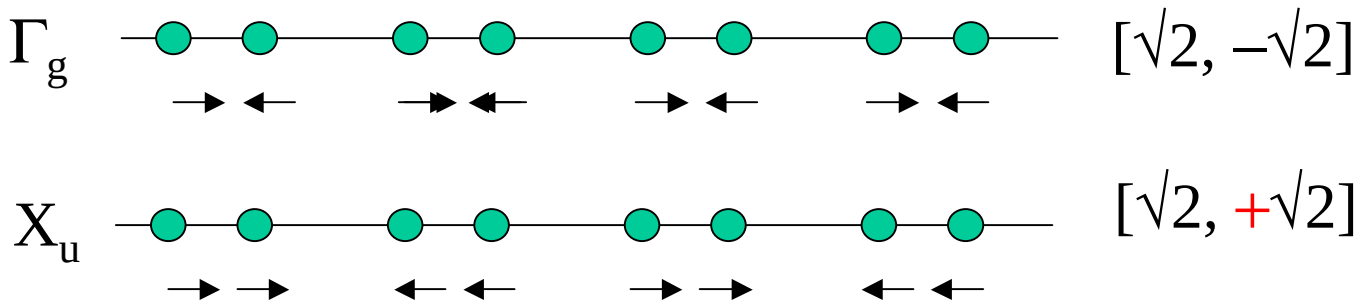
each eigenvector:

2 complex numbers $[u_1(k,j)\ u_2(k,j)]$

snapshot at t=0

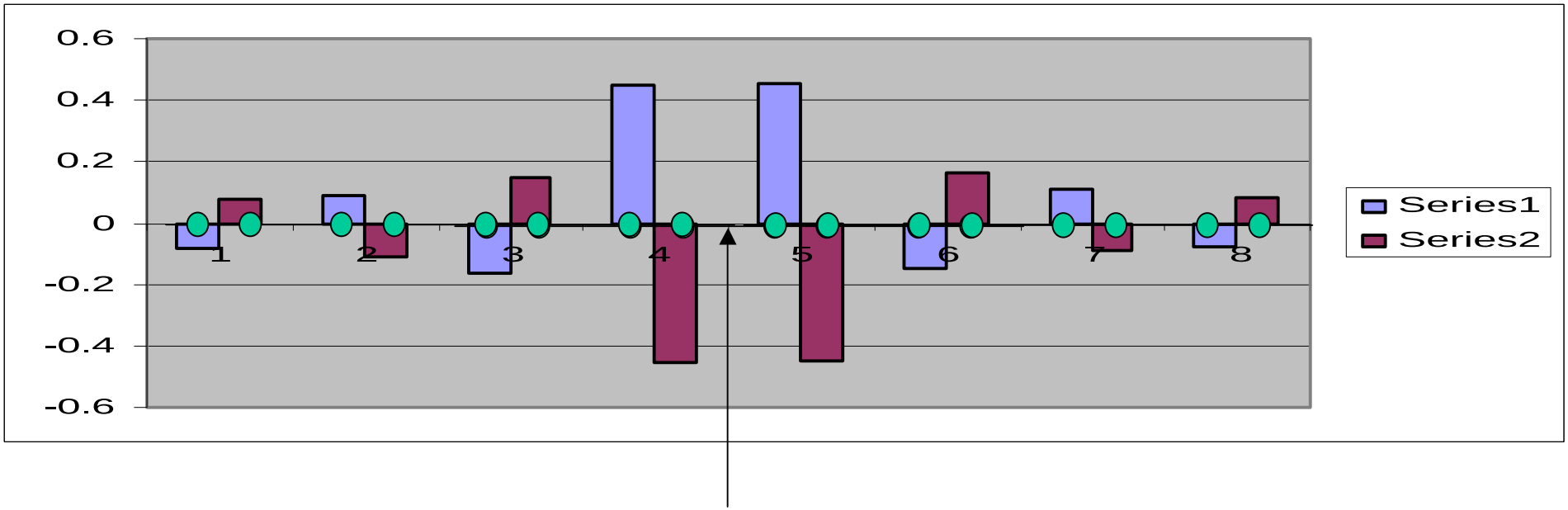
$u_{m\kappa}(k,j) = \mathrm{Re}[u_\kappa(k,j)\ \exp(i(kma))]$



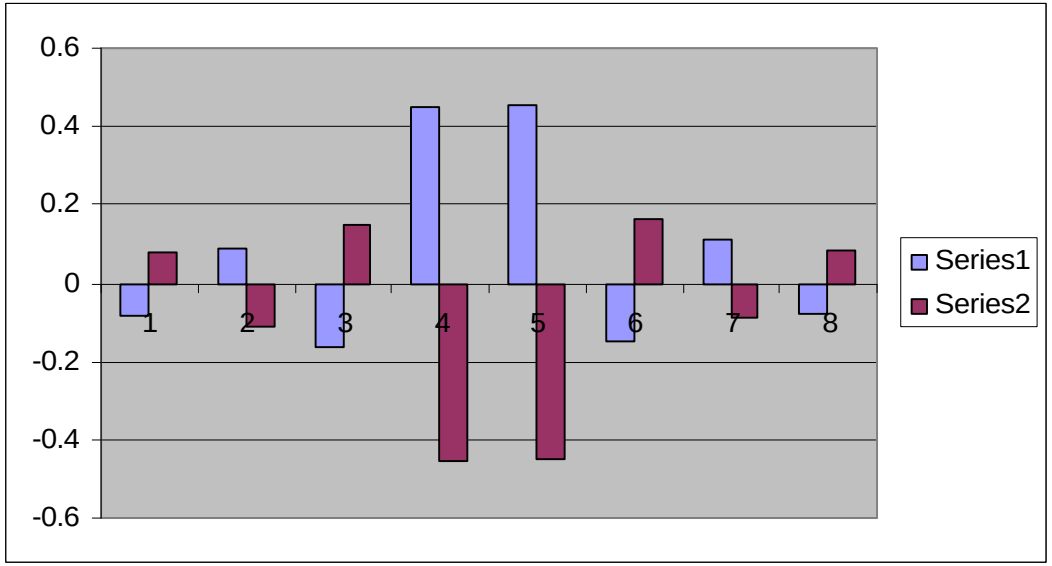


transform to lattice Wannier functions

(note: $\phi(k)$ was constrained to produce definite point symmetry;
consistency with $\Gamma_g - X_u \rightarrow$ must be even around center of long bond)



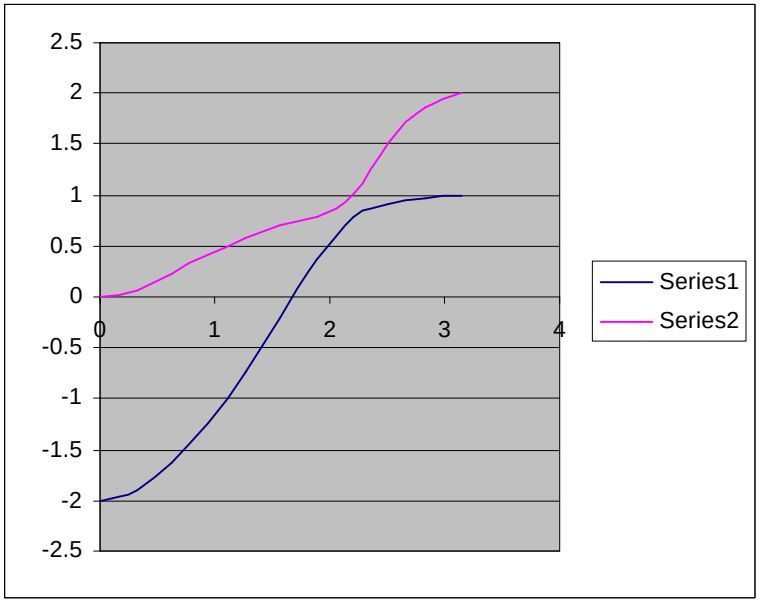
atomic displacement pattern is even around this point



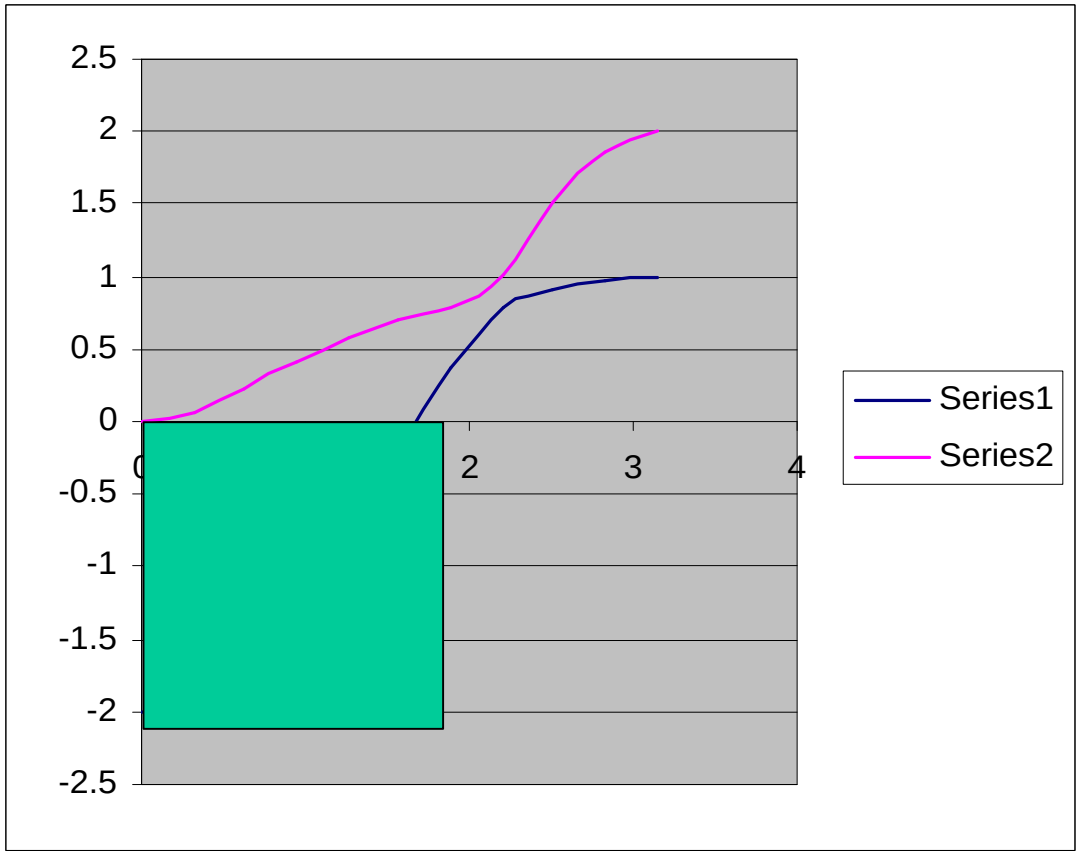
terrible localization

this is inevitable given the change of character

entangled bands



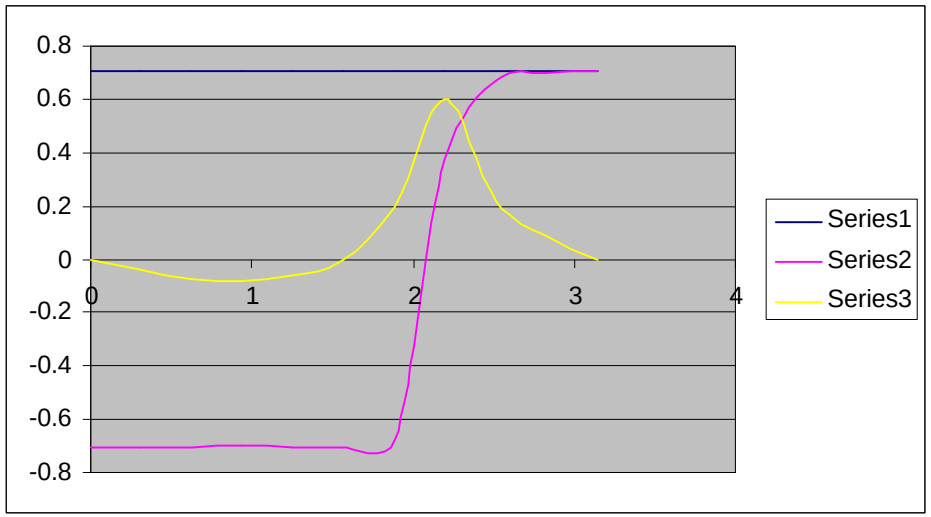
Souza, Marzari and Vanderbilt PRB 65, 035109 (2001)
single band = linear combination of bands in energy window
(e.g. containing the two bands shown)
optimize Ω_I

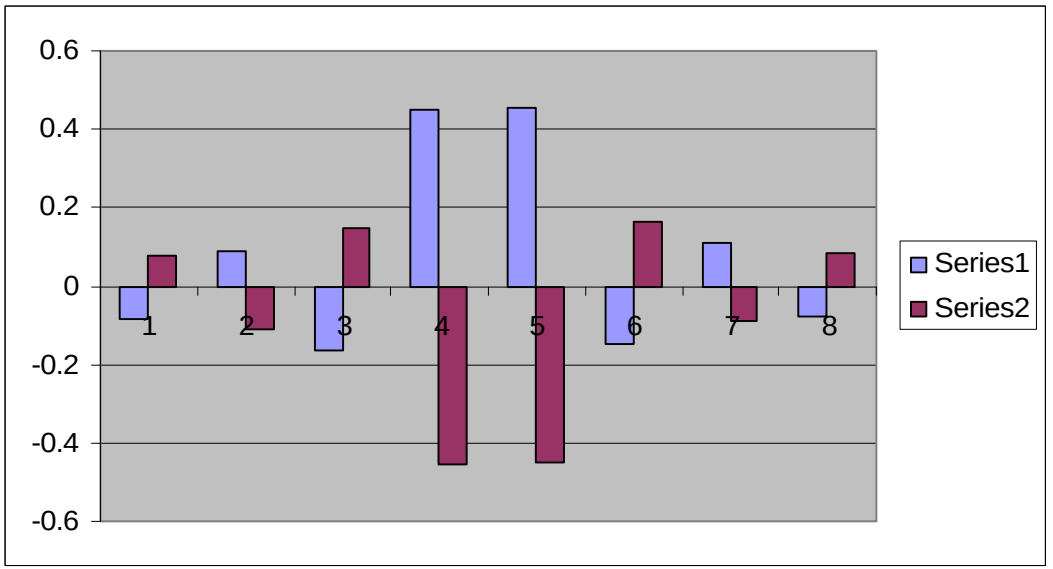


suppose we want to reproduce part of a band exactly

inner window: subspace at those k is fixed

$$[u_1, u_{2r} + I\, u_{2i}]$$


0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
1
2
3
4
Series1
Series2
Series3


0.6
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-0.4
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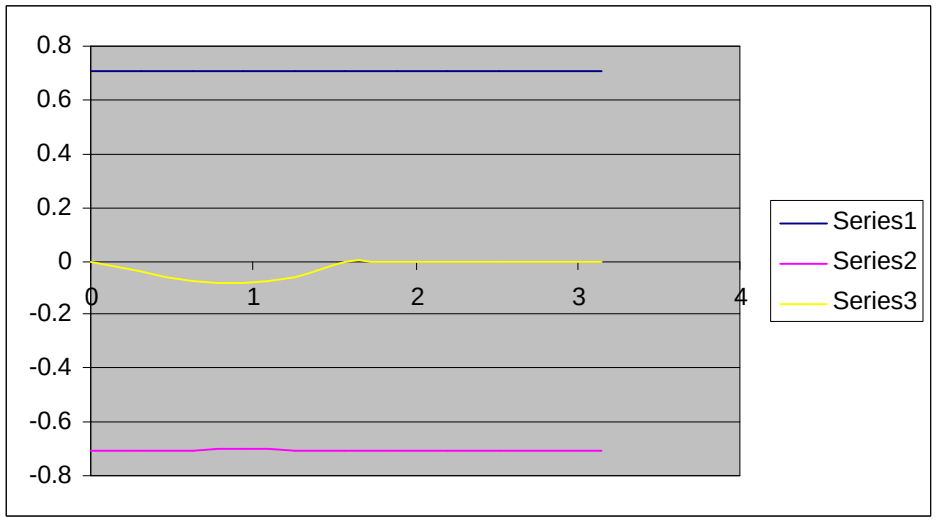
6
7
8
Series1
Series2


0.8
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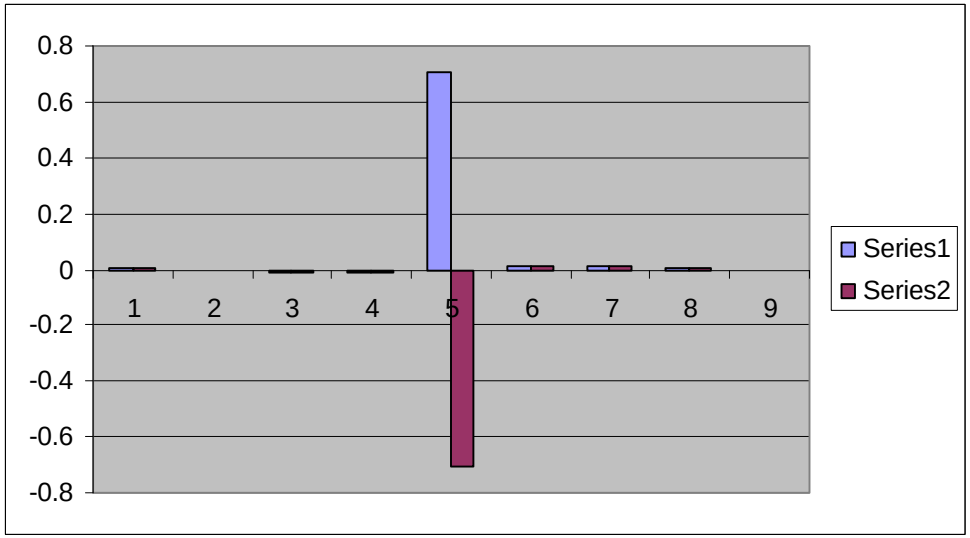
Series1
Series2
Series3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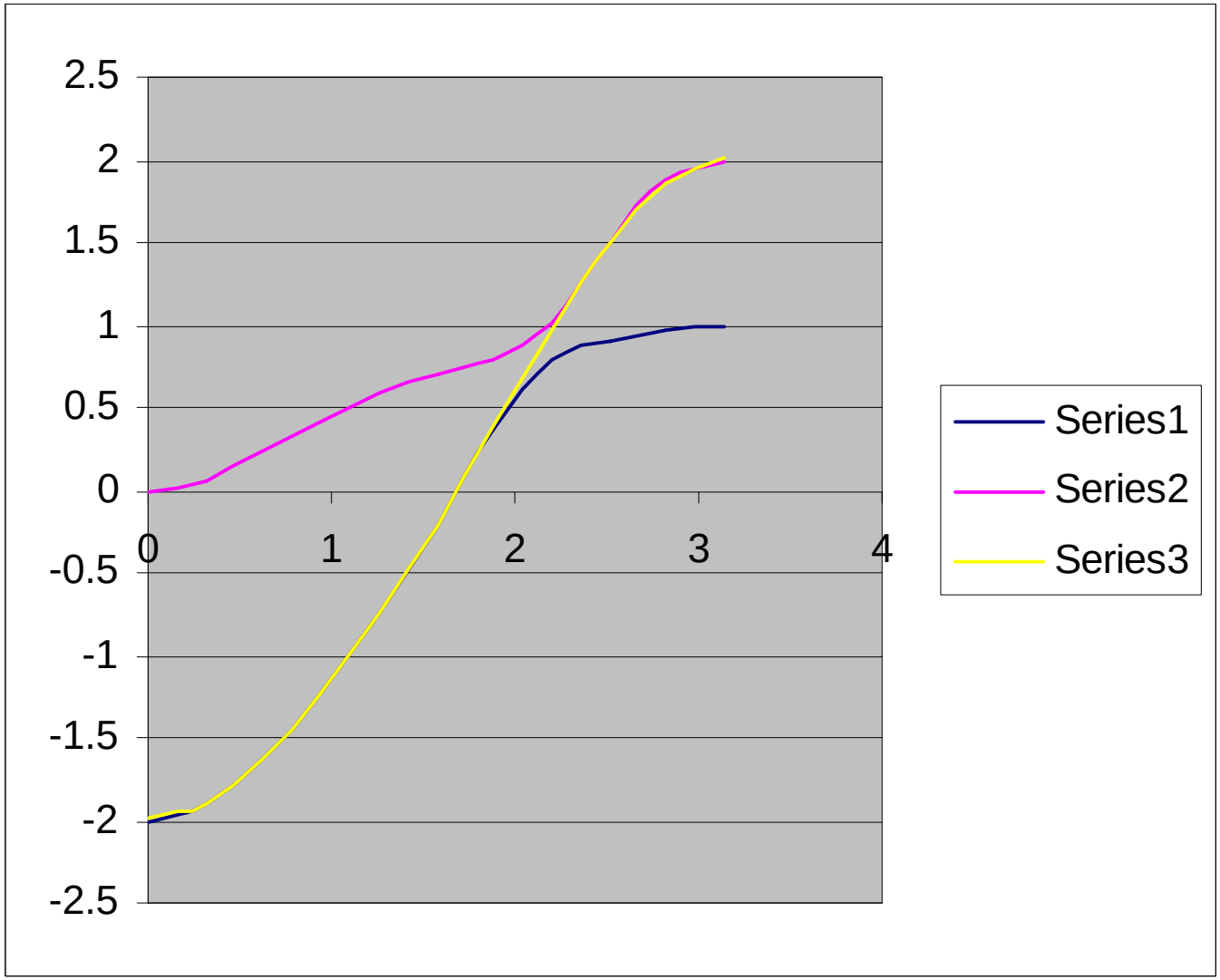
Series1
Series2


2.5
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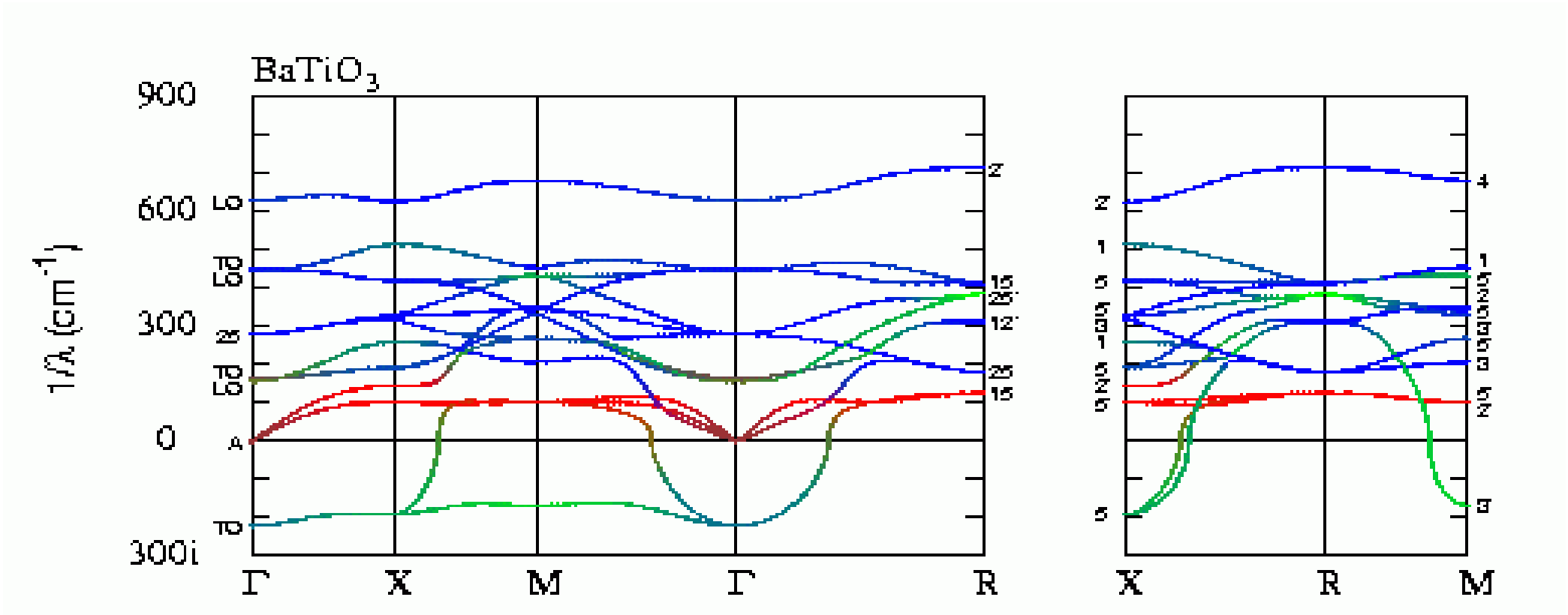
Series1
Series2
Series3

ferroelectric perovskites



LO-TO splitting: constraint just on TO bands

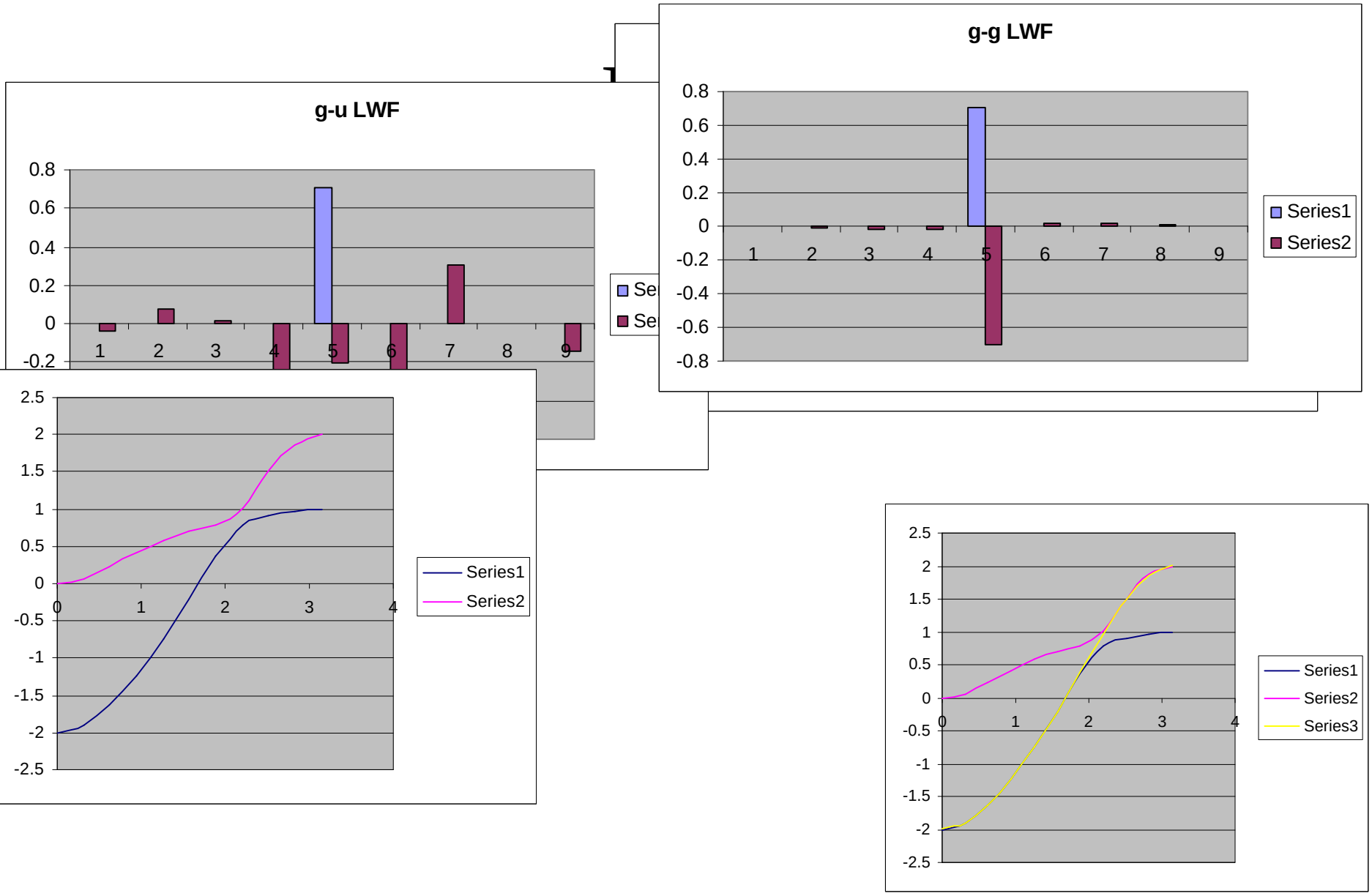
Implementation in ABINIT

uses output of IFC, crystal structure info

user chooses symmetry type of LWF
outer energy window (default: whole space)
inner energy window (or other constraints)

compute quadratic terms in effective Hamiltonian

generality? (nonsymmorphic space groups…)
more automation (consider all symmetry types…)
other measures of localization more relevant?
release orthonormality of LWFs?
efficiency?


g-g LWF
0.8
0.6
0.4
0.2
0
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-0.6
-0.8
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2
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7
8
9
Series1
Series2
g-u LWF
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Series1
Series2
Series3