Basic concepts on electron lattice coupling: the Peierls model

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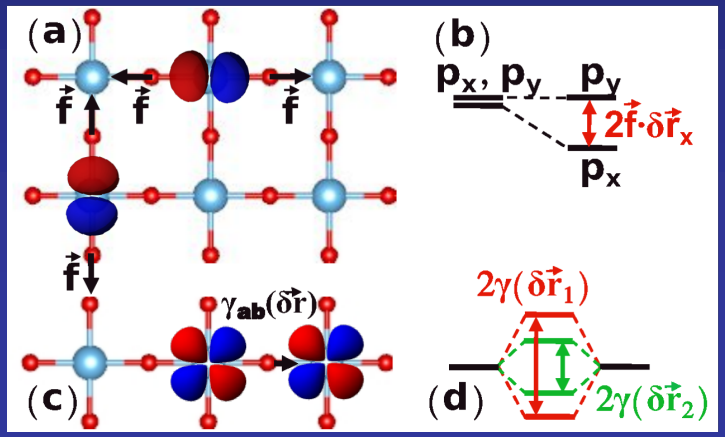
Electron-lattice coupling in SCALE-UP

The dependence of the model parameters on the atomic configuration is captured by the electron-lattice couplings



$$\gamma_{ab}^{\mathrm{sr}} = \gamma_{ab}^{\mathrm{RAG,\ sr}} + \sum_{\lambda\upsilon}\left[-\vec{f}^{T}_{ab,\lambda\upsilon}\delta\vec{r}_{\lambda\upsilon} + \right.$$

$$\left. + \sum_{\lambda'\upsilon'} \delta\vec{r}^{T}_{\lambda\upsilon} \overleftrightarrow{g}_{ab,\lambda\upsilon\lambda'\upsilon'} \delta\vec{r}_{\lambda'\upsilon'} + \cdots \right],$$

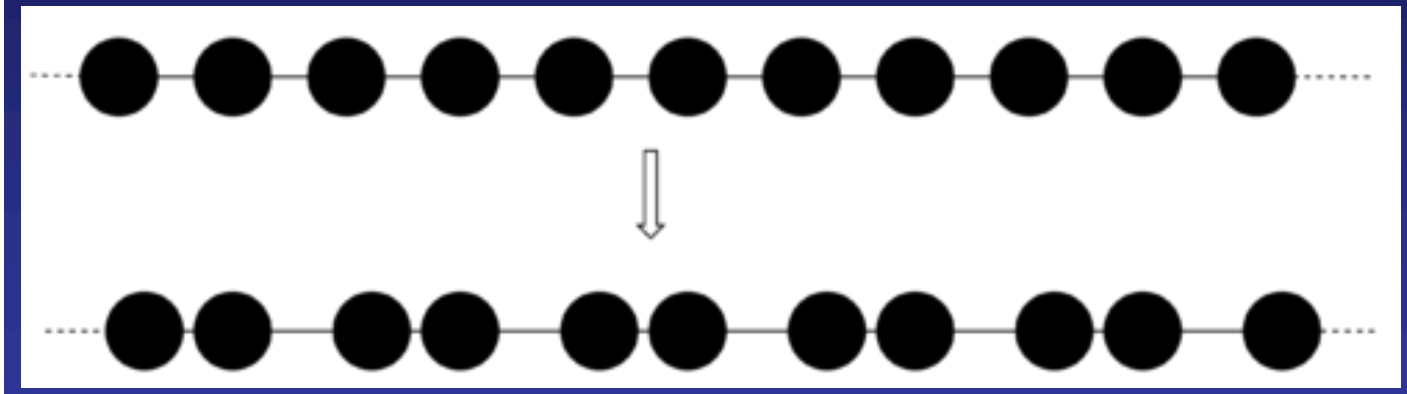
Including quadratic constants: enough to describe typical changes in γ

Physical meaning of the parameters:

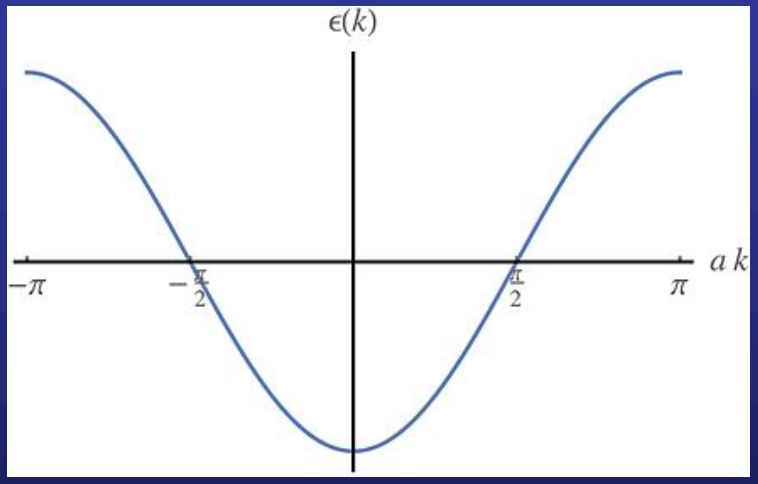
When $a = b$: it represents the force created by an electron occupying the WF χ_a over the surrounding atoms (Jahn-Teller effect in solids or polaron formation)

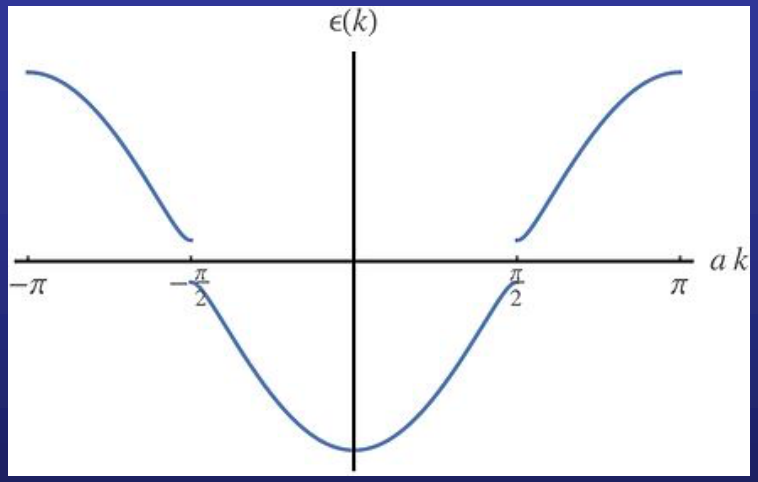
Off-diagonal terms in $\vec{f}$ describe the mixing of two WFs upon an atomic distortion, and thus quantify changes in covalency (pseudo Jahn-Teller vibronic constants and are involved in ferroelectricity).

The Peierls transition in one-dimension



Imagine a lattice distortion where every other ion moves closer to one neighbor and further away from the other





From Wikipedia

Introducing the electron-lattice coupling parameters in SCALE-UP

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      hopa="0"
      hopb="0"
      hopc="0"
      gamma="0.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
   </interaction_gm>
   <interaction_gm
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      orbital_2="1"
      hopa="0"
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      hopc="1"
      gamma="2.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
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      orbital_2="1"
      hopa="0"
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      hopc="-1"
      gamma="2.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
   </interaction_gm>
</electron_hamiltonian_one>
```

Gamma 1

Gamma 2

Gamma 2 is the one electron hamiltonian matrix element between orbital 1 in the unit cell and orbital 1 in the unit cell centered at [001]

Gamma 3

Gamma 3 is the one electron hamiltonian matrix element between orbital 1 in the unit cell and orbital 1 in the unit cell centered at [001]

Introducing the electron-lattice coupling parameters in SCALE-UP

```
<electron_hamiltonian_one>
   <interaction_gm
      orbital_1="1"
      orbital_2="1"
      hopa="0"
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      rz="0.000">
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      rx="0.000"
      ry="0.000"
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   <interaction_gm
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      hopa="0"
      hopb="0"
      hopc="-1"
      gamma="2.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
   </interaction_gm>
</electron_hamiltonian_one>
```

Gamma 2

```
<electron_hamiltonian_electron_lattice>
   <interaction_vb gamma="2">
      <atom_1> 1 0 0 0 </atom_1>
      <atom_2> 1 0 0 1 </atom_2>
      <linear> 0.0000 0.0000 2.0000 </linear>
      <quadratic>
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
      </quadratic>
   </interaction_vb>
   <interaction_vb gamma="3">
      <atom_1> 1 0 0 0 </atom_1>
      <atom_2> 1 0 0 -1 </atom_2>
      <linear> 0.0000 0.0000 -2.0000 </linear>
      <quadratic>
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
      </quadratic>
   </interaction_vb>
</electron_hamiltonian_electron_lattice>
```

This block will modify Gamma 2 when there is a relative displacement between atom 1 in the unit cell and atom 1 in unit cell at [001]
Only linear terms are included
Magnitude of the “force” in eV/Å

Introducing the electron-lattice coupling parameters in SCALE-UP

```
<electron_hamiltonian_one>
   <interaction_gm
      orbital_1="1"
      orbital_2="1"
      hopa="0"
      hopb="0"
      hopc="0"
      gamma="0.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
   </interaction_gm>
   <interaction_gm
      orbital_1="1"
      orbital_2="1"
      hopa="0"
      hopb="0"
      hopc="1"
      gamma="2.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
   </interaction_gm>
   <interaction_gm
      orbital_1="1"
      orbital_2="1"
      hopa="0"
      hopb="0"
      hopc="-1"
      gamma="2.0000"
      rx="0.000"
      ry="0.000"
      rz="0.000">
   </interaction_gm>
</electron_hamiltonian_one>
```

```
<electron_hamiltonian_electron_lattice>
   <interaction_vb gamma="2">
      <atom_1> 1 0 0 0 </atom_1>
      <atom_2> 1 0 0 1 </atom_2>
      <linear> 0.0000 0.0000 2.0000 </linear>
      <quadratic>
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
      </quadratic>
   </interaction_vb>
   <interaction_vb gamma="3">
      <atom_1> 1 0 0 0 </atom_1>
      <atom_2> 1 0 0 -1 </atom_2>
      <linear> 0.0000 0.0000 -2.0000 </linear>
      <quadratic>
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
         0.0000 0.0000 0.0000
      </quadratic>
   </interaction_vb>
</electron_hamiltonian_electron_lattice>
```

Gamma 3

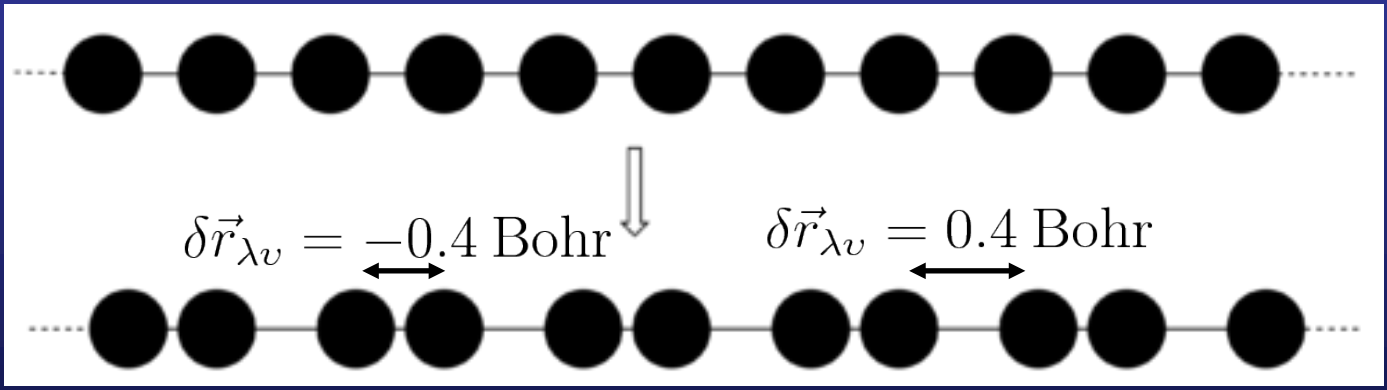
This block will modify Gamma 3 when there is a relative displacement between atom 1 in the unit cell and atom 1 in unit cell at [00-1]
Only linear terms are included
Magnitude of the “force” in eV/Å

The calculation is performed for a dimerized atomic geometry

```
Geometry_restart initial_geom.restart
```

```
    1    1    2
    1    1
cation
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00
    0    0    0    1    1    0.00000000E+00    0.00000000E+00    0.20000000E+00
    0    0    1    1    1    0.00000000E+00    0.00000000E+00   -0.20000000E+00
```

One of the atoms in the unit cell is displaced towards the right 0.2 Bohrs, while the other is displaced towards the left 0.2 Bohrs

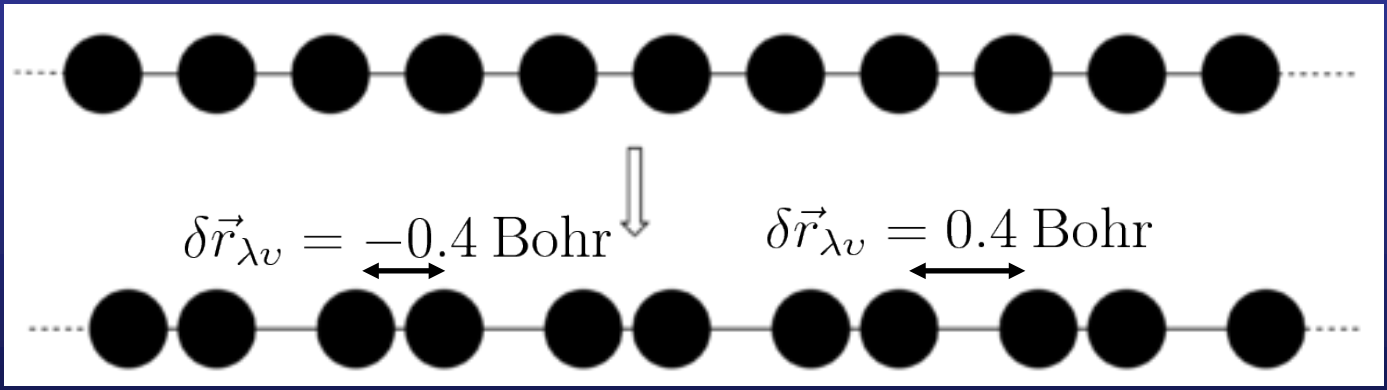


The calculation is performed for a dimerized atomic geometry

```
Geometry_restart initial_geom.restart
```

```
    1    1    2
    1    1
cation
    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00
    0    0    0    1    1    0.00000000E+00    0.00000000E+00    0.20000000E+00
    0    0    1    1    1    0.00000000E+00    0.00000000E+00   -0.20000000E+00
```

One of the atoms in the unit cell is displaced towards the right 0.2 Bohrs, while the other is displaced towards the left 0.2 Bohrs



Change in the one-body hamiltonian matrix elements

$$\gamma_{ab}^{\mathrm{sr}} = \gamma_{ab}^{\mathrm{RAG,\ sr}} + \sum_{\lambda\upsilon} \Big[-\vec{f}^{T}_{ab,\lambda\upsilon} \delta\vec{r}_{\lambda\upsilon} + \sum_{\lambda'\upsilon'} \delta\vec{r}^{T}_{\lambda\upsilon} \overleftrightarrow{g}_{ab,\lambda\upsilon\lambda'\upsilon'} \delta\vec{r}_{\lambda'\upsilon'} + \ldots \Big] ,$$

With the above considerations, we can estimate the change in the one particle hamiltonian matrix elements

$$0.4\ \mathrm{Bohr} \times \frac{0.529177\ \text{Å}}{1.0\ \mathrm{Bohr}} \times 2.0 \frac{\mathrm{eV}}{\text{Å}} = 0.423341\ \mathrm{eV}$$

As can be seen in the _FINAL.rham file

```
Geometry_restart initial_geom.restart

!spin   hopa   hopb   hopc   orb1   orb2         real_ham         imag_ham
    1      0      0      0      1      1       -0.0000000        0.0000000
    1      0      0      0      1      2        2.4233418        0.0000000
    1      0      0     -1      1      2        1.5766582        0.0000000
    1      0      0      0      2      2       -0.0000000        0.0000000
    1      0      0      1      2      1        1.5766582        0.0000000
    1      0      0      0      2      1        2.4233418        0.0000000
```

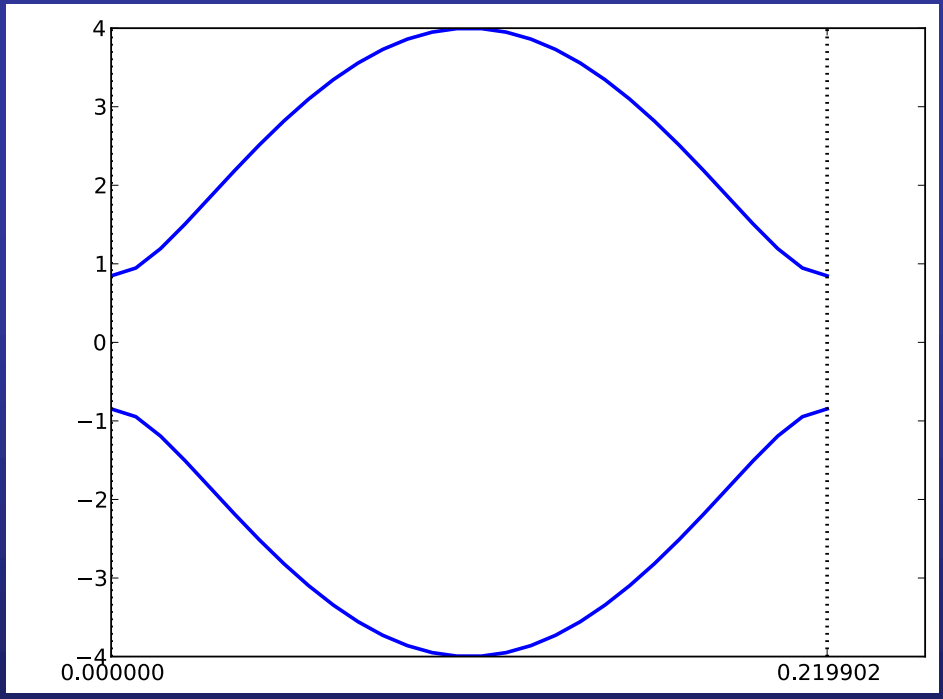
Metal-insulator phase transition

```
$ python  <your_path_to_scale_up_dir>/bin/scaleup.x < peierls.fdf > peierls.out

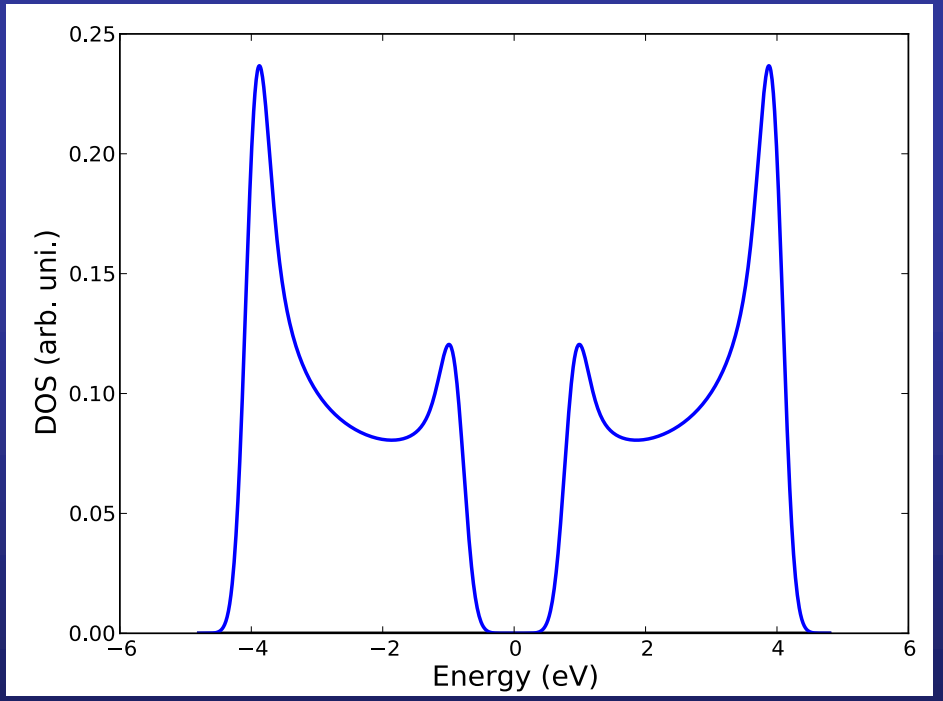
$ python  <your_path_to_scale_up_dir>/scripts/scaleup_utils.py -bands -file _peierls_model_FINAL.bands

$ python  <your_path_to_scale_up_dir>/scripts/scaleup_utils.py -dos -file _peierls_model_FINAL.ener
```

Bands



DOS



Metal-insulator phase transition

The dimerized atomic configuration is energetically more stable (if we do not consider the elastic terms)

With electron-lattice coupling

```
Energy decomposition:
  Reference Energy      :   0.0000000E+00 eV
  Total Delta           :  -0.5374383E+01 eV
    Delta Lattice       :   0.0000000E+00 eV
      Harmonic          :   0.0000000E+00 eV
      Anharmonic        :   0.0000000E+00 eV
      Elastic           :   0.0000000E+00 eV
      Electrostatic     :   0.0000000E+00 eV
    Delta electron      :  -0.5374383E+01 eV
      One-electron      :  -0.4919125E+01 eV
      Two-electron      :   0.0000000E+00 eV
      Electron-lattice  :  -0.4552588E+00 eV
      Electrostatic     :  -0.1147079E-22 eV
  Total Energy          :  -0.5374383E+01 eV
```

Without electron-lattice coupling

```
Energy decomposition:
  Reference Energy      :   0.0000000E+00 eV
  Total Delta           :  -0.5091865E+01 eV
    Delta Lattice       :   0.0000000E+00 eV
      Harmonic          :   0.0000000E+00 eV
      Anharmonic        :   0.0000000E+00 eV
      Elastic           :   0.0000000E+00 eV
      Electrostatic     :   0.0000000E+00 eV
    Delta electron      :  -0.5091865E+01 eV
      One-electron      :  -0.5091865E+01 eV
      Two-electron      :   0.0000000E+00 eV
      Electron-lattice  :   0.0000000E+00 eV
      Electrostatic     :  -0.1072636E-22 eV
  Total Energy          :  -0.5091865E+01 eV
```