A practical Peierls phase recipe for periodic atomistic systems under magnetic fields

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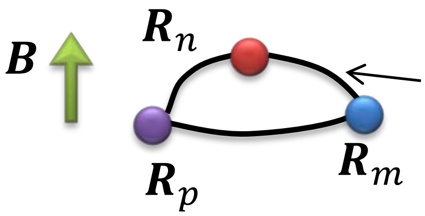
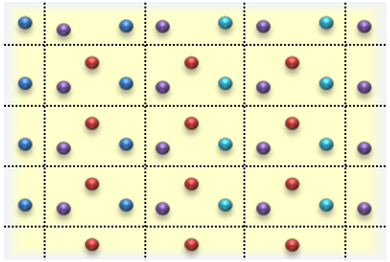
Plan of the presentation

The context: Tight-binding Hamiltonian, magnetic field and **Peierls phase**



$$\phi_{mn} = \frac{2\pi}{\Phi_0}\int_{\boldsymbol{R}_m}^{\boldsymbol{R}_n} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})$$

The problem: **Periodicity** of the Hamiltonian in quasi-1D and 2D systems



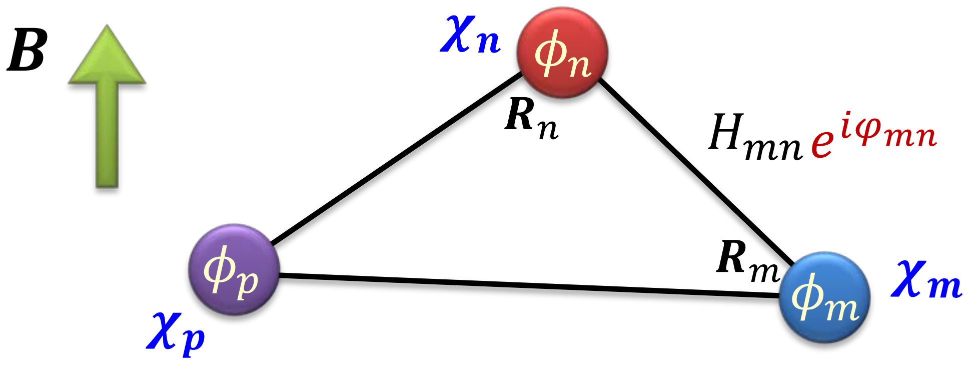
The solution: **Gauge invariance** to obtain practical and general formulas

$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$$

$$\boldsymbol{A} \rightarrow \boldsymbol{A} + \boldsymbol{\nabla}\chi$$

An example: disordered **2DEG Hall bar**

Tight-binding-like Hamiltonian and Peierls phase



Peierls phase

$$\varphi_{mn} \equiv \frac{2\pi}{\Phi_0} \int_{\mathbf{R}_m}^{\mathbf{R}_n} d\mathbf{r} \cdot \mathbf{A}(\mathbf{r})$$

R. Peierls, Z. Phys. ***80****, 763 (1933)*

$$H_{mn} \equiv \langle \phi_m | \widehat{H} | \phi_n \rangle = \int dr^3 \phi_m^*(\boldsymbol{r}) H(\boldsymbol{r}, -i\hbar\boldsymbol{\nabla}) \phi_n(\boldsymbol{r})$$

In the presence of a magnetic field $\mathbf{B}=\nabla\times\mathbf{A}(\mathbf{r})$ we operate the **minimal substitution**

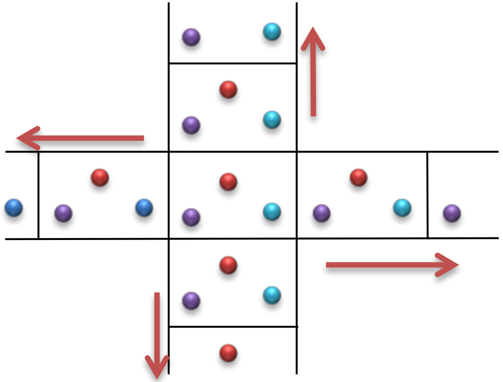
$$\widehat{\boldsymbol{\pi}} = \widehat{\boldsymbol{p}} + \frac{\mathbf{e}}{\mathbf{c}}\mathbf{A}(\widehat{\boldsymbol{r}}) \quad \rightarrow \quad -i\hbar\boldsymbol{\nabla} \rightarrow -i\hbar\boldsymbol{\nabla} + \frac{\mathbf{e}}{\mathbf{c}}\mathbf{A}(\mathbf{r})$$

$\chi(\boldsymbol{R}_n)$ $\chi(\boldsymbol{R}_m)$

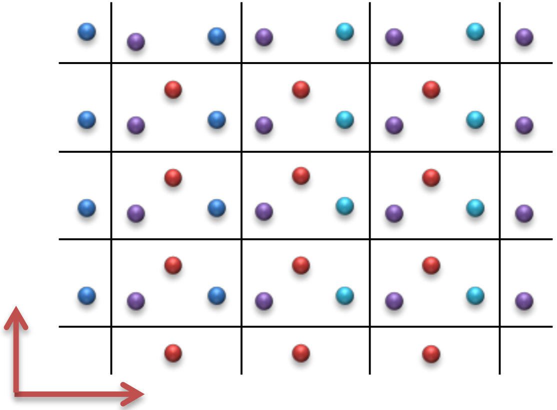
The **gauge freedom** $\mathbf{A}(\mathbf{r}) \rightarrow \mathbf{A}(\mathbf{r}) + \boldsymbol{\nabla}\chi(\boldsymbol{r})$ entails $\varphi_{mn} \rightarrow \varphi_{mn} + \frac{2\pi}{\Phi_0}(\chi_n - \chi_m)$

The problem of periodicity

quasi-1D (e.g., *multiterminal bars*)



2D



Hamiltonian periodicity

⇩

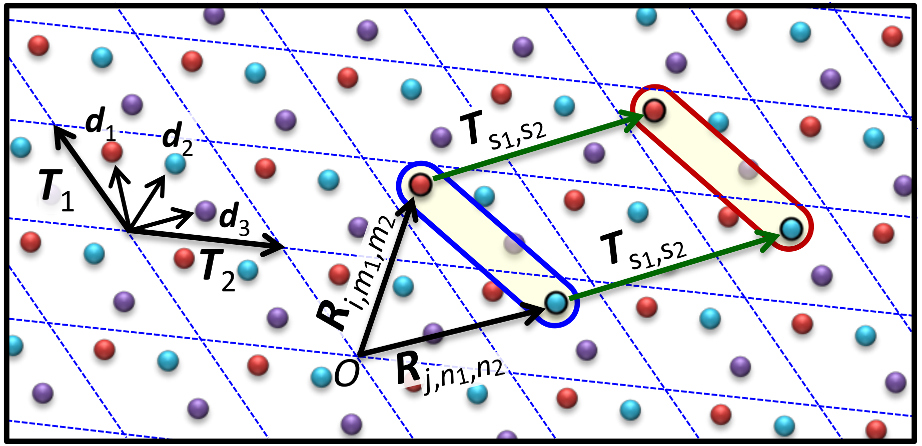
efficient numerical techniques
for electronic structure and transport

Bloch theorem (band structure)
[Zeitschrift für Physik **52**, 555 (1928)]

Sancho-Rubio algorithm (NEGF simulations)
[Phys. F: Met. Phys. **14**, 1205 (1984)]

A homogeneous magnetic field **B** is periodic
but the vector potential **A**(***r***) is not !

Periodic 2D system



Lattice vectors: $\boldsymbol{T}_1$ and $\boldsymbol{T}_2$ Basis vectors: $\boldsymbol{d}_1, \boldsymbol{d}_2 \ldots \boldsymbol{d}_n$

Site/atomic positions: $\boldsymbol{R}_{i,m_1,m_2} = m_1 \boldsymbol{T}_1 + m_2 \boldsymbol{T}_2 + \boldsymbol{d}_i$

State at site $\boldsymbol{R}_{i,m_1,m_2}$: $|\phi_{i,m_1,m_2}\rangle$

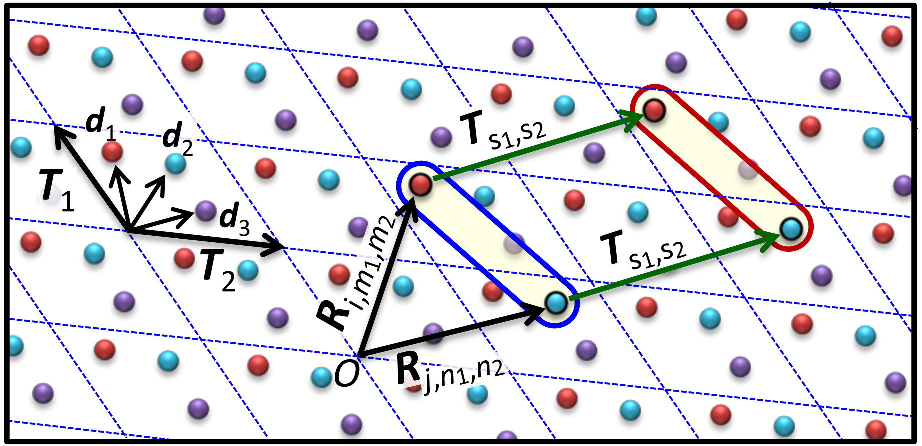
Hamiltonian elements

$$H_{i,m_1,m_2;j,n_1,n_2} = \langle\phi_{i,m_1,m_2}|\hat{H}|\phi_{j,n_1,n_2}\rangle = \int dr^3 \phi_i^*(\boldsymbol{r}-\boldsymbol{R}_{i,m_1,m_2}) H(\boldsymbol{r},-i\hbar\boldsymbol{\nabla}) \phi_j(\boldsymbol{r}-\boldsymbol{R}_{j,n_1,n_2})$$

Hamiltonian periodicity under translation by a generic lattice vector $\boldsymbol{T}_{s_1,s_2} = s_1 \boldsymbol{T}_1 + s_2 \boldsymbol{T}_2$

$$H_{i,m_1+s_1,m_2+s_2;j,n_1+s_1,n_2+s_2} = H_{i,m_1,m_2;j,n_1,n_2} = \int dr^3 \phi_i^*(\boldsymbol{r}-\boldsymbol{R}_{i,m_1,m_2}-\boldsymbol{T}_{s_1s_2}) H(\boldsymbol{r},-i\hbar\boldsymbol{\nabla}) \phi_j(\boldsymbol{r}-\boldsymbol{R}_{j,n_1,n_2}-\boldsymbol{T}_{s_1s_2})$$

Periodic 2D system



Lattice vectors: $\boldsymbol{T}_1$ and $\boldsymbol{T}_2$

Basis vectors: $\boldsymbol{d}_1, \boldsymbol{d}_2 \ldots \boldsymbol{d}_n$

Site/atomic positions: $\boldsymbol{R}_{i,m_1,m_2} = m_1\, \boldsymbol{T}_1 + m_2\, \boldsymbol{T}_2 + \boldsymbol{d}_i$

Generic vector potential: $\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r} + \boldsymbol{\nabla}\chi(\boldsymbol{r})$

Peierls phase for the Hamiltonian element $H_{i,m_1,m_2;j,n_1,n_2} \rightarrow e^{\varphi_{i,m_1,m_2;j,n_1,n_2}} H_{i,m_1,m_2;j,n_1,n_2}$

$\chi(\boldsymbol{R}_{jn_1n_2})$ $\chi(\boldsymbol{R}_{im_1m_2})$

$$\varphi_{i,m_1,m_2;j,n_1,n_2} = \frac{2\pi}{\Phi_0}\int_{\boldsymbol{R}_{i,m_1,m_2}}^{\boldsymbol{R}_{j,n_1,n_2}} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) = \frac{2\pi}{\Phi_0}\left[\frac{1}{2}\,\boldsymbol{B}\cdot\left(\boldsymbol{R}_{im_1m_2}\times\boldsymbol{R}_{jn_1n_2}\right) + \chi_{jn_1n_2} - \chi_{im_1m_2}\right]$$

Condition for **periodicity**: $\varphi_{i,m_1+s_1,m_2+s_2;j,n_1+s_1,n_2+s_2} - \varphi_{i,m_1,m_2;j,n_1,n_2} = 2\pi q$

Periodic 2D system

Condition for **periodicity**: $\varphi_{i,m_1+s_1,m_2+s_2;j,n_1+s_1,n_2+s_2} - \varphi_{i,m_1,m_2;j,n_1,n_2} = 2\pi q \ \forall \ s_1, s_2 \in \mathbb{Z}$

only depends on $\boldsymbol{R}_{j,n_1,n_2}$

$$\chi_{j,n_1+s_1,n_2+s_2} - \chi_{j,n_1,n_2} - \frac{1}{2}\boldsymbol{R}_{j,n_1,n_2} \cdot \left(\boldsymbol{T}_{s_1,s_2} \times \boldsymbol{B}\right) +$$

multiple of the quantum magnetic flux

only depends on $\boldsymbol{R}_{i,m_1,m_2}$

$$-\chi_{i,m_1+s_1,m_2+s_2} + \chi_{i,m_1,m_2} + \frac{1}{2}\boldsymbol{R}_{i,m_1,m_2} \cdot \left(\boldsymbol{T}_{s_1,s_2} \times \boldsymbol{B}\right) = q\Phi_0$$

If we write the translated gauge as

$$\chi_{i,m_1+s_1,m_2+s_2} = \chi_{i,m_1,m_2} + \frac{1}{2}\boldsymbol{B} \cdot \left(\boldsymbol{R}_{i,m_1,m_2} \times \boldsymbol{T}_{s_1,s_2}\right) + f(i, m_1, m_2, s_1, s_2)$$

then the condition is $f(j, n_1, n_2, s_1, s_2) - f(i, m_1, m_2, s_1, s_2) = q\Phi_0 \ \ \forall \ \ i, j, m_1, m_2, n_1, n_2, s_1, s_2$

and then $f(i, m_1, m_2, s_1, s_2) \ \rightarrow \ f(s_1, s_2)$

Periodic 2D system

$$\chi_{i,m_1+s_1,m_2+s_2} = \chi_{i,m_1,m_2} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{R}_{i,m_1,m_2}\times\boldsymbol{T}_{s_1,s_2}\right) + f(s_1,s_2)$$

$$= \chi_{i,m_1,m_2} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{d}_i\times\boldsymbol{T}_{s_1,s_2}\right) + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{T}_{m_1,m_2}\times\boldsymbol{T}_{s_1,s_2}\right) + f(s_1,s_2)$$

$s_1 = m_1$, $m_1 = 0$ $\qquad$ $s_2 = m_2$, $m_2 = 0$

$$\chi_{i,m_1,m_2} = \chi_{i,0,0} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{d}_i\times\boldsymbol{T}_{m_1,m_2}\right) + f(m_1,m_2)$$

$m_1 = m_1 + s_1$ $\qquad$ $m_2 = m_2 + s_2$

$$\chi_{i,m_1+s_1,m_2+s_2} = \underbrace{\chi_{i,0,0} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{d}_i\times\boldsymbol{T}_{m_1,m_2}\right)} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{d}_i\times\boldsymbol{T}_{s_1,s_2}\right) + f(m_1+s_1,m_2+s_2)$$

$$= \overbrace{\chi_{i,m_1,m_2} - f(m_1,m_2)} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{d}_i\times\boldsymbol{T}_{s_1,s_2}\right) + f(m_1+s_1,m_2+s_2)$$

$$\Rightarrow \quad f(m_1+s_1,m_2+s_2) = f(m_1,m_2) + f(s_1,s_2) + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{T}_{m_1,m_2}\times\boldsymbol{T}_{s_1,s_2}\right)$$

Periodic 2D system

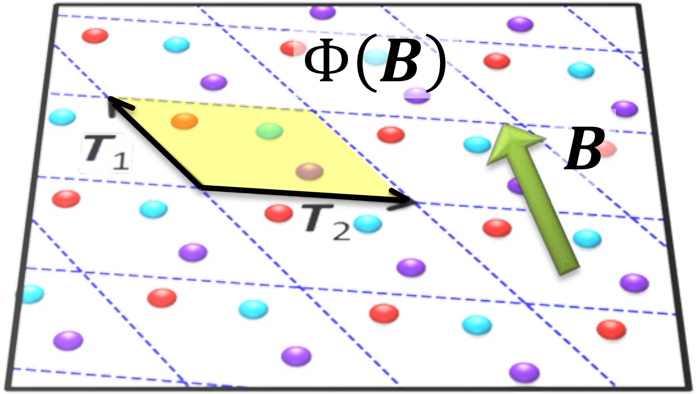
$$\chi_{i,m_1,m_2} = \chi_{i,0,0} + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{d}_i \times \boldsymbol{T}_{m_1,m_2}\right) + f(m_1,m_2)$$

$$f(m_1+s_1, m_2+s_2) = f(m_1,m_2) + f(s_1,s_2) + \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{T}_{m_1,m_2} \times \boldsymbol{T}_{s_1,s_2}\right)$$

$$f(s_1+m_1, s_2+m_2) = f(s_1,s_2) + f(m_1,m_2) - \frac{1}{2}\boldsymbol{B}\cdot\left(\boldsymbol{T}_{m_1,m_2} \times \boldsymbol{T}_{s_1,s_2}\right)$$

They must be the same modulo Φ_0

$$\boldsymbol{B}\cdot\left(\boldsymbol{T}_{m_1,m_2} \times \boldsymbol{T}_{s_1,s_2}\right) = q\Phi_0 \ \forall \ \ m_1, m_2, s_1, s_2 \in \mathbb{Z}$$



Condition on the magnetic field

$$\Rightarrow \quad \boldsymbol{B}\cdot(\boldsymbol{T}_1 \times \boldsymbol{T}_2) = \Phi(B) = q\Phi_0$$

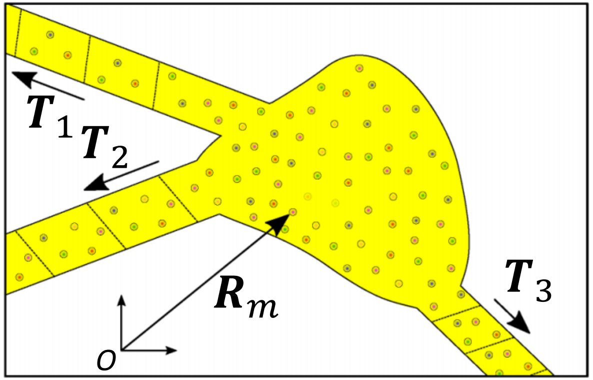
quantized flux through the unite cell

Periodic 2D system

A simple choice is: $f(m_1, m_2) = \pm\frac{1}{2}\boldsymbol{B}\cdot(m_1\boldsymbol{T}_1 \times m_2\boldsymbol{T}_2) = \pm\frac{m_1 m_2}{2}q\Phi_0$

General expression for the Peierls phase

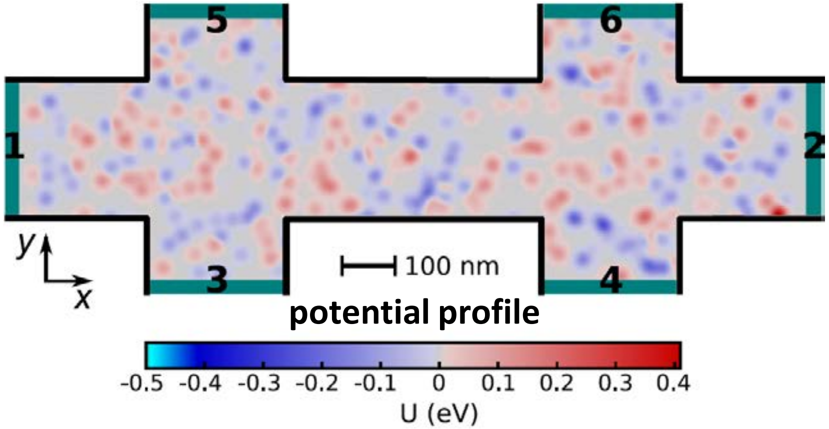
$$\varphi_{i,m_1,m_2;j,n_1,n_2} = \frac{\pi}{\Phi_0}\boldsymbol{B}\cdot\left[\begin{array}{r}\boldsymbol{d}_i \times \boldsymbol{d}_j + \left(\boldsymbol{d}_i + \boldsymbol{d}_j\right)\times[(n_1 - m_1)\boldsymbol{T}_1 + (n_2 - m_2)\boldsymbol{T}_2] \\ +(m_1 n_2 - n_1 m_2 \pm n_1 n_2 \mp m_1 m_2)\boldsymbol{T}_1 \times \boldsymbol{T}_2\end{array}\right]$$



Generalization to quasi 1D systems with periodic terminals oriented along different directions

→ see [Phys. Rev. B **103**, 045402 (2021)]

Example of a quasi 1D system: a 2DEG Hall bar

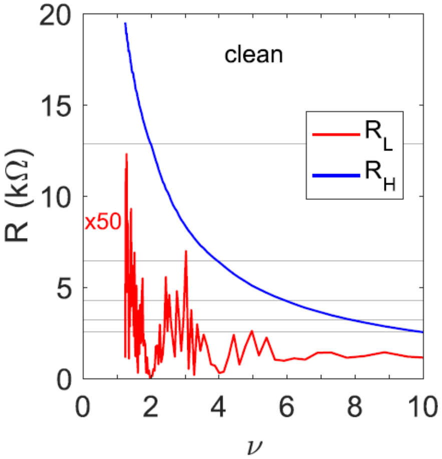


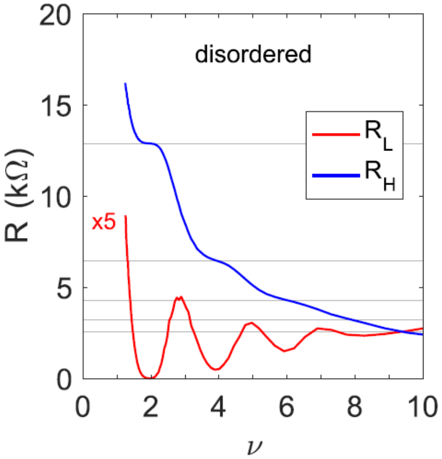
2DEG - $m^* = 0.067\ m_e$ - $\sigma = 3 \times 10^{13}\ e/\mathrm{cm}^2$ @ $T = 77.36$ K

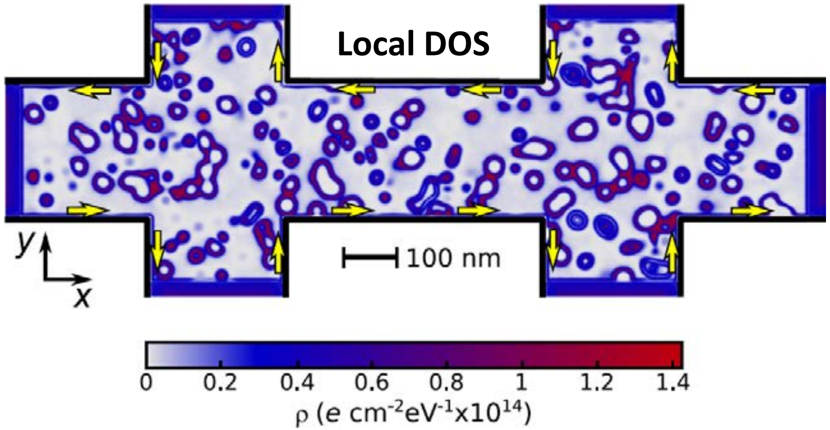
Six terminal Hall bar **pristine** or with **moderate disorder**

Simulation technique:

- discretized effective mass Hamiltonian
- Green's function approach
- complex plane integration for equilibrium charge
  [D.A. Areshkin and B.K. Nikolić, PRB **81**, 155450 (2010)]







Conclusion

- The obtained formulas for the **Peierls phase factor** that **preserve the translation symmetry of the Hamiltonian** for periodic systems under homogeneous magnetic fields.
- They allow the use of **efficient** numerical techniques for **electronic structure and transport simulation**.
- This approach is **simple, general and ready to use**.

For more details and examples → Phys. Rev. B **103**, 045402 (2021)

Thank you for your kind attention!