3. Wannier representation and gauge dependence

Conclusion: Must work in a globally fixed gauge to compute $P_{xy}^r$, $P_{y}^b$ and $Q_{xy}^q$.

4. Compute $P_{xy}^r$, $P_{y}^b$ and $Q_{xy}^q$ from ribbons

Meme: $P_{xy}^r = \sum a_i \sum n_i (0|z_i|0) = \sum n_i (0|z_i|0)$

5. How to make gauges consistent? (Projection-based construction)

Key idea:
- Project trial functions onto Wannier functions;
- Pick same trial functions ($|\psi_{trial}\rangle$) for both y-finite ribbon and x-finite ribbon;
- Cut all intracell hoppings, use eigenstates of a finite flake as trial functions;
- Easier to do in k-space

1. Fourier transform trial functions to k-space

$\langle k|\alpha\rangle = N^{-1/2} \sum_{\mathbf{x}} \psi_{\mathbf{x}}^{\alpha} |k|\alpha\rangle$

2. Calculate the overlap matrix between trial functions and Bloch functions

$B_{\alpha,\beta} = \langle k|\alpha\rangle\langle k|\beta\rangle$

3. Optimally aligned Bloch functions with trial functions by SVD

$B = V\Sigma W^\dagger$  $\tilde{B} = V\tilde{W}^\dagger |\psi_{\mathbf{x}}\rangle = \sum_{\mathbf{x}} \tilde{B}_{\mathbf{x},\alpha} |\psi_{\mathbf{x}}\rangle$

4. Transform to real space to get WFs

6. Direct calculation of the corner charge from a finite flake

Naively sum over charges in the top right region does not lead to the correct result!

1. Smoothen the charge density $\rho(r)$ by convoluting with a window function (show by the figure). The smoothed charge density $\hat{\rho}(r)$ vanishes except in corners.

2. Integrate the smoothed charge density $\hat{\rho}(r)$ over the corner region.

7. Results

<table>
<thead>
<tr>
<th></th>
<th>Naive hybrid Wannier</th>
<th>Projection-based Wannier</th>
<th>Nested Wannier</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{xy}^r$</td>
<td>0.300250</td>
<td>0.354669</td>
<td>0.300250</td>
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<tr>
<td>$P_{y}^b$</td>
<td>0.476420</td>
<td>0.446029</td>
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<tr>
<td>$Q_{xy}^q$</td>
<td>-3.756016</td>
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<td>-3.756016</td>
</tr>
<tr>
<td>$Q_{xy}$ (predict)</td>
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<td>-2.983567</td>
<td>-2.983567</td>
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<tr>
<td>$Q_{xy}$ (direct)</td>
<td>-2.983567</td>
<td>-2.983567</td>
<td>-2.983567</td>
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</tbody>
</table>

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References:
This work: Phys. Rev. B 103, 035147 (2021)