Interlayer coupling matrix elements in twisted bilayers

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1 Tunnelling matrix element between two twisted layers

In order to describe a twisted bilayer, we use approach described in [1] which requires knowledge of the 2D Fourier transform of $t(\boldsymbol{r}) \equiv t(\boldsymbol{r}_{\mathrm{2D}}, z)$. We write

$$t(\boldsymbol{k}, z) \equiv t(k, z) = \frac{1}{A_{\mathrm{uc}}} \int d\boldsymbol{r}_{\mathrm{2D}}\, t(\boldsymbol{r}_{\mathrm{2D}}, z) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_{\mathrm{2D}}}, \tag{1}$$

$$t(\boldsymbol{r}_{\mathrm{2D}}, z) = \frac{A_{\mathrm{uc}}}{(2\pi)^2} \int d\boldsymbol{k}\, t(\boldsymbol{k}, z) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{\mathrm{2D}}}, \tag{2}$$

where $\boldsymbol{r}_{\mathrm{2D}}$ and $\boldsymbol{k}$ are two-dimensional and A_{uc} is the (in-plane) area of the unit cell. As defined, t in both real and reciprocal space is in the units of energy. For a Bloch state constructed in the usual fashion ($\boldsymbol{k}$ is the wave vector, j labels the sublattice and l keeps track of the layer, N_l is the number of unit cells in layer l),

$$|\boldsymbol{k}, j, l\rangle = \frac{1}{\sqrt{N_l}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\tau}_j)} \phi_j(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_j, z - z_l), \tag{3}$$

we have

$$\langle \boldsymbol{k'}, j', l'|\boldsymbol{\delta\hat{H}}|\boldsymbol{k}, j, l\rangle = \frac{1}{\sqrt{N_l N_{l'}}} \sum_{\boldsymbol{R},\boldsymbol{R'}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\tau}_j)} e^{-i\boldsymbol{k'}\cdot(\boldsymbol{R'}+\boldsymbol{\tau}_{j'})} \times$$
$$\langle \phi_{j'}(\boldsymbol{r} - \boldsymbol{R'} - \boldsymbol{\tau}_{j'}, z - z_{l'})|\boldsymbol{\delta\hat{H}}|\phi_j(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_j, z - z_l)\rangle =$$
$$\frac{1}{\sqrt{N_l N_{l'}}} \sum_{\boldsymbol{R},\boldsymbol{R'}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\tau}_j)} e^{-i\boldsymbol{k'}\cdot(\boldsymbol{R'}+\boldsymbol{\tau}_{j'})} t(\boldsymbol{R'} - \boldsymbol{R} + \boldsymbol{\tau}_{j'} - \boldsymbol{\tau}_j, z_{l'} - z_l),$$

where we used two-centre approximation (hopping between the two sites depends only on their distance) and assumed that the hopping $t(\boldsymbol{r}_{\mathrm{2D}}, z)$ does not depend on the direction of $\boldsymbol{r}_{\mathrm{2D}}$, that is, $t(\boldsymbol{r}_{\mathrm{2D}}, z) \equiv t(r_{\mathrm{2D}}, z)$.

We now use Eq. (2) to move from the real into reciprocal space,

$$\langle \boldsymbol{k'}, j', l'|\boldsymbol{\delta\hat{H}}|\boldsymbol{k}, j, l\rangle = \frac{A_{\mathrm{uc}}}{(2\pi)^2\sqrt{N_l N_{l'}}} \sum_{\boldsymbol{R},\boldsymbol{R'}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\tau}_j)} e^{-i\boldsymbol{k'}\cdot(\boldsymbol{R'}+\boldsymbol{\tau}_{j'})} \int d\boldsymbol{q}\, t(\boldsymbol{q}, z) e^{i\boldsymbol{q}\cdot(\boldsymbol{R'}-\boldsymbol{R}+\boldsymbol{\tau}_{j'}-\boldsymbol{\tau}_j)} =$$

$$\frac{A_{\mathrm{uc}}}{(2\pi)^2\sqrt{N_l N_{l'}}} \int d\boldsymbol{q}\, t(\boldsymbol{q}, z) \sum_{\boldsymbol{R},\boldsymbol{R'}} e^{i(\boldsymbol{k}-\boldsymbol{q})\cdot(\boldsymbol{R}+\boldsymbol{\tau}_j)} e^{-i(\boldsymbol{k'}-\boldsymbol{q})\cdot(\boldsymbol{R'}+\boldsymbol{\tau}_{j'})},$$

and, by summing over lattice vectors in both layers,

$$\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{R}} = N \sum_{\boldsymbol{G}} \delta_{\boldsymbol{k}-\boldsymbol{q},\boldsymbol{G}}, \tag{4}$$

we get

$$\langle \boldsymbol{k'}, j', l'|\boldsymbol{\delta\hat{H}}|\boldsymbol{k}, j, l\rangle = \frac{A_{\mathrm{uc}}\sqrt{N_l N_{l'}}}{(2\pi)^2} \int d\boldsymbol{q} \sum_{\boldsymbol{G},\boldsymbol{G'}} t(\boldsymbol{q}, z) \delta_{\boldsymbol{k}-\boldsymbol{q},\boldsymbol{G}} \delta_{\boldsymbol{q}-\boldsymbol{k'},\boldsymbol{G'}} e^{i\boldsymbol{G}\cdot\boldsymbol{\tau}_j} e^{i\boldsymbol{G'}\cdot\boldsymbol{\tau}_{j'}}.$$

We now turn the integration into a sum over $\boldsymbol{q}$,

$$\int d\boldsymbol{q} \rightarrow \frac{(2\pi)^2}{\sqrt{S_l S_{l'}}} \sum_{\boldsymbol{q}}, \tag{5}$$

where S_l is the area of the layer l. This allows us to use one of the Kronecker deltas to remove the sum over $\boldsymbol{q}$ and, because $S_l = N_l A_{\mathrm{uc}}$ (we assume both layers are identical), we obtain

$$\langle \boldsymbol{k'}, j', l'|\boldsymbol{\delta\hat{H}}|\boldsymbol{k}, j, l\rangle = \sum_{\boldsymbol{G},\boldsymbol{G'}} t(\boldsymbol{k'} + \boldsymbol{G'}, z) e^{i\boldsymbol{G}\cdot\boldsymbol{\tau}_j} e^{i\boldsymbol{G'}\cdot\boldsymbol{\tau}_{j'}}\, \delta_{\boldsymbol{k}-\boldsymbol{G},\boldsymbol{k'}+\boldsymbol{G'}}, \tag{6}$$

a form equivalent to the main result of Ref. [1]. An important point is that for a general twist angle, only at most one set of $\boldsymbol{G}$ and $\boldsymbol{G'}$ connects the given initial and final wave vectors $\boldsymbol{k}$ and $\boldsymbol{k'}$. This means that once we have determined the sets of $\boldsymbol{k}$ and $\boldsymbol{k'}$ that are coupled by the moiré and that we include in our basis set, a matrix element of the interlayer coupling block is either zero or corresponds to one of the terms of the sum in Eq. (6).

References

[1] M. Koshino, New J. Phys. **17**, 015014 (2015).