Eidgenössische Technische Hochschule Zürich
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Computational Quantum Physics
Solution 7

FS 16
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Problem 7.1 Tight-Binding Model on a Square Lattice

Here we consider the problem of a tight-binding model with nearest-neighbour hoppings on a square lattice, i.e.

$$H = \sum_{\langle i,j \rangle,\sigma} \left(t_{i,j}\, \hat{c}^{\dagger}_{i,\sigma}\, \hat{c}_{j,\sigma} + h.c. \right) \tag{1}$$

We start off by Fourier-transforming the creation and annihilation operators using

$$\begin{aligned} \hat{c}_{j,\sigma} &= \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}\in B.Z.} e^{i\mathbf{k}\cdot\mathbf{r}_j}\, \hat{c}_{\mathbf{k},\sigma} \\ \hat{c}^{\dagger}_{j,\sigma} &= \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}\in B.Z.} e^{-i\mathbf{k}\cdot\mathbf{r}_j}\, \hat{c}^{\dagger}_{\mathbf{k},\sigma} \end{aligned}$$

Substituting in eq. (1) gives

$$H = \sum_{\langle i,j \rangle,\sigma} \frac{t_{i,j}}{N} \sum_{\mathbf{k},\mathbf{k}'} e^{-i(\mathbf{k}\cdot\mathbf{r}_i - \mathbf{k}'\cdot\mathbf{r}_j)}\, \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k}',\sigma} + h.c.$$

Assuming the hoppings to be $t_{i,j} = -t$ and using the fact that only nearest-neighbour hoppings are non-vanishing we rearrange the summations over sites to give

$$H = -\frac{t}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}'} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} \left\{ e^{i\mathbf{k}'\cdot\mathbf{a}_1} + e^{i\mathbf{k}'\cdot\mathbf{a}_2} \right\} \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k}',\sigma} + h.c.$$

Using the identity $\sum_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} = \delta_{\mathbf{k}',\mathbf{k}} N$, we may simplify then to

$$H = -t \sum_{\mathbf{k},\sigma} \left\{ e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2} \right\} \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} + h.c.$$

Finally, grouping everything together with the terms in h.c. we may write

$$H = -2t \sum_{\mathbf{k},\sigma} \left\{ \cos(\mathbf{k}\cdot\mathbf{a}_1) + \cos(\mathbf{k}\cdot\mathbf{a}_2) \right\} \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma}$$

which allows us to identify the energy dispersion relation for the model

$$\epsilon(\mathbf{k}) = -2t \left\{ \cos(\mathbf{k}\cdot\mathbf{a}_1) + \cos(\mathbf{k}\cdot\mathbf{a}_2) \right\}, \tag{2}$$

with $\mathbf{a}_1 = a(1,0)$ and $\mathbf{a}_2 = a(0,1)$ as basis vectors for the square lattice and a the lattice constant. See fig. 1 for a plot of the dispersion relation in eq. (2).

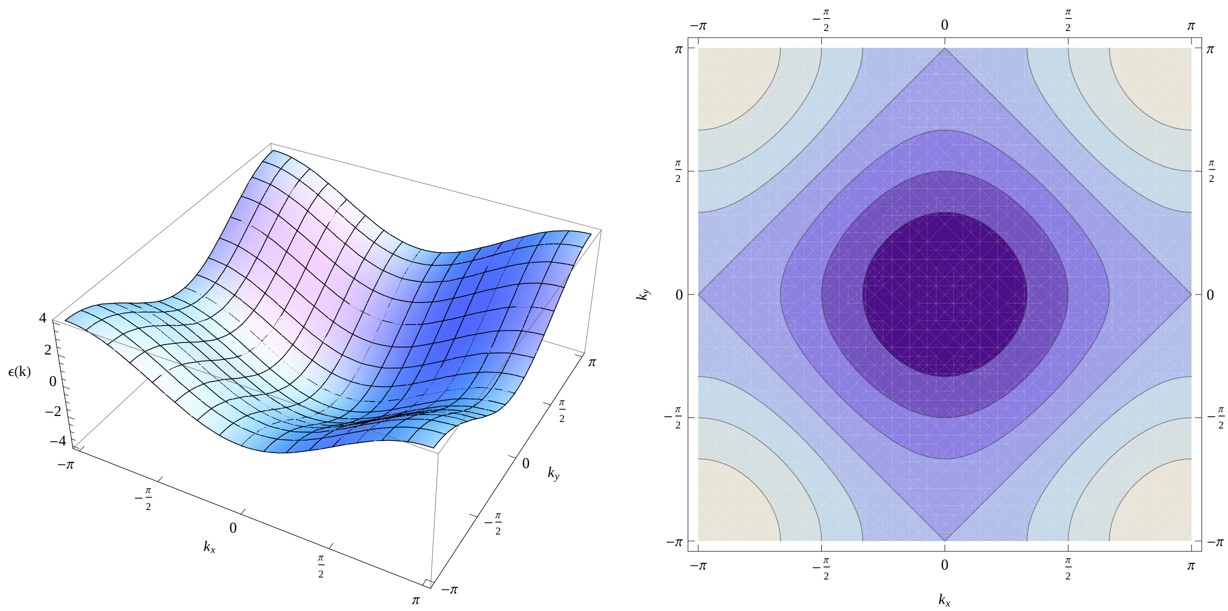

Figure 1: Dispersion relation for the square lattice tight-binding model over the first Brillouin zone.