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Superconducting phase stiffness and coherence length from a finite momentum pairing constraint

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Even Einstein [...] had attempted to construct a theory of superconductivity. Fortunately, I was unaware of these many unsuccessful attempts. So when John invited me to join him (he, somehow, neglected to mention these previous efforts), I decided to take the plunge.

<div style="text-align: right">

Leon Cooper
"Remembrance of Superconductivity Past", BCS: 50 Years [1].

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Kurzzusammenfassung

Abstract

CONTENTS

I Introduction

II SUPERCONDUCTIVITY

III Quantum Geometry, normal state something?

III.1 EG-X model

The tight-binding Hamiltonian for the model reads

$$
\begin{aligned}
H_0 = &- t_X \sum_{\langle ij \rangle, \sigma} d_{i,\sigma}^\dagger d_{j,\sigma} - t_{Gr} \sum_{\langle ij \rangle, \sigma} \left(c_{i,\sigma}^{(A),\dagger} c_{j,\sigma}^{(B)} + c_{j,\sigma'}^{(B),\dagger} c_{i,\sigma}^{(A)} \right) \\
&+ V \sum_{i,\sigma} d_{i,\sigma}^\dagger c_{i,\sigma}^{(A)} + \text{h.c.}
\end{aligned}
\tag{III.1}
$$

with:

- d operators on the X atom
- $c^{(\epsilon)}$ operators on the Graphene site ($\epsilon = A, B$)
- t_X next-nearest hopping for the X atoms
- t_{Gr} next-nearest hopping on the Graphene
- V hopping between X and Graphene B sites

This describes the

In material terms, this can be thought of as a sheet of graphene on top of another material, providing the additional X atoms, but in this thesis the model will be taken as a toy model, providing certain favorable aspects.

III.2 Lattice Structure of Graphene

This section reviews the lattice structure of graphene and by extension also of the flat-band model, following the review [2].
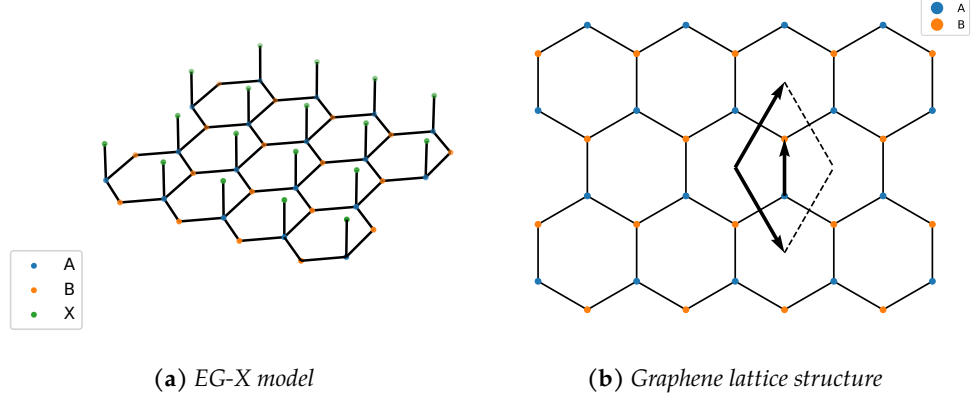
(a) *EG-X model*   (b) *Graphene lattice structure*

Figure III.1: *EG-X model and Hexagonal lattice structure*

Monolayer graphene forms a hexagonal lattice as seen in fig. III.1b. This is formed by two triangular sub lattices, so the unit cell of the hexagonal lattice has two atoms. The primitive vectors of the hexagonal lattice are

$$\mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad \mathbf{a}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix}, \tag{III.2}$$

Te with lattice constant $a \approx 2.46\,\text{Å}$ for graphene. The distance between nearest neighbor is

$$a = \sqrt{3}a_0 . \tag{III.3}$$

The primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$ fulfill

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \text{ and}$$
$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0 , \tag{III.4}$$

so

$$\mathbf{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad \mathbf{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} . \tag{III.5}$$

Graphic for primitive BZ

Explain primitive BZ

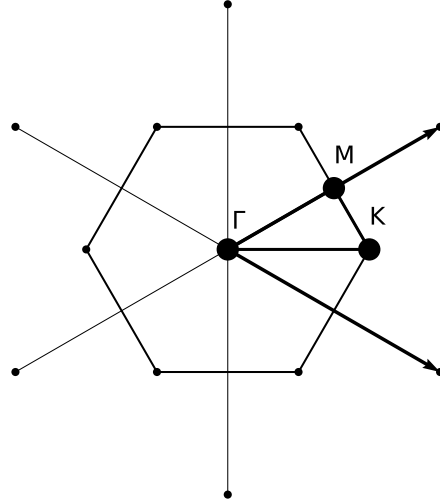Explain: what symmetries does EG-X break? How does that influence BZ?

Figure III.2: *Graphene Brillouin Zone*

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ M = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \ K = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \tag{III.6}$$

III.3 Band structure

aka why is the model interesting?

The detailed derivation can be found in appendix A.

$$H_0 = \sum_{\mathbf{k},\sigma} \begin{pmatrix} c_{k,\sigma}^{A,\dagger} & c_{k,\sigma}^{B,\dagger} & d_{k,\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{k,\sigma}^{A} \\ c_{k,\sigma}^{B} \\ d_{k,\sigma} \end{pmatrix} \tag{III.7}$$

III.4 Quantum Metric normal state?

IV Conclusion and Outlook

A EG-X Hamiltonian in Reciprocal Space

In the following chapter, the model Hamiltonian

$$H_0 = -t_X \sum_{\langle ij \rangle, \sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_{Gr} \sum_{\langle ij \rangle, \sigma} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma} + V \sum_{i,\sigma} d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma} + \text{h.c.} \qquad (A.1)$$

will be treated to obtain the band structure. The first step is to write out the sums over nearest neighbors $\langle i, j \rangle$ explicitly, writing $\delta_X, \delta_\epsilon$ ($\epsilon = A, B$) for the vectors to the nearest neighbors of the X atoms and Graphene A, B sites. Doing the calculation for example of the X atoms:

$$-t_X \sum_{\langle ij \rangle, \sigma} (d^\dagger_{i,\sigma} d_{j,\sigma} + d^\dagger_{j,\sigma} d_{i,\sigma}) = -\frac{t_X}{2} \sum_{i,\sigma} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} - \frac{t_X}{2} \sum_{j,\sigma} \sum_{\delta_X} d^\dagger_{j,\sigma} d_{j+\delta_X,\sigma}$$
$$(A.2)$$

$$= -t_X \sum_{i,\sigma} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} \qquad (A.3)$$

The factor $1/2$ in eq. (A.2) is to account for double counting when going to the sum over all lattice sites i. By relabeling $j \rightarrow i$ in the second sum, the two sum are the same and eq. (A.3) is obtained. Using now the discrete Fourier transform

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}, \quad c^\dagger_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_i} c^\dagger_{\mathbf{k}} \qquad (A.4)$$

with the completeness relation

$$\sum_i e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'} , \qquad (A.5)$$

eq. (A.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma} = -t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\delta_X} \left(e^{-i\mathbf{k}\mathbf{r}_i} d_{\mathbf{k},\sigma}^\dagger \right) \left(e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma} \right) \quad \text{(A.6)}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\delta_X,\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k}',\sigma} e^{i\mathbf{k}'\delta_X} \sum_i e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \quad \text{(A.7)}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k}',\sigma} \sum_{\delta_X} e^{i\mathbf{k}'\delta_X} \left(N \delta_{\mathbf{k},\mathbf{k}'} \right) \quad \text{(A.8)}$$

$$= -t_X \sum_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} . \quad \text{(A.9)}$$

This part is now diagonal in $\mathbf{k}$ space. The nearest neighbours vectors δ_X for the X atoms are the vectors $\delta_{AA,i}$ from section III.2. With that, the sum over δ_X can be explicitly calculated:

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad \text{(A.10)}$$

$$= -t_X \left[\exp\left(ia \left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) \right) + e^{iak_x} + e^{ia(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right. \quad \text{(A.11)}$$

$$\left. + e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right] \quad \text{(A.12)}$$

$$= -t_X \left(2\cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos\left(\frac{a}{2}k_x\right) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos\left(\frac{a}{2}k_x\right) \right) \quad \text{(A.13)}$$

$$= -2t_X \left(\cos(ak_x) + 2\cos\left(\frac{a}{2}k_x\right) \cos\left(\sqrt{3}\frac{a}{2}k_y\right) \right) . \quad \text{(A.14)}$$

The same can be done for the hopping between Graphene sites, for example :

$$-t_{\text{Gr}} \sum_{\langle ij \rangle, \sigma\sigma'} c_{i,\sigma}^{(A),\dagger} c_{j,\sigma'}^{(B)} = -t_{\text{Gr}} \sum_{i,\sigma\sigma'} \sum_{\delta_{AB}} c_{i,\sigma}^{(A),\dagger} c_{i+\delta_{AB},\sigma'}^{(B)} \quad \text{(A.15)}$$

$$= -t_{\text{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c_{\mathbf{k},\sigma}^{(A)\dagger} c_{\mathbf{k},\sigma'}^{(B)} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad \text{(A.16)}$$

We note

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left(\sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \quad \text{(A.17)}$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{A.18}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{i\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{i\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{A.19}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{-i\frac{a}{2\sqrt{3}}k_y} \left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x} \right) \right) \tag{A.20}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + 2e^{-i\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) \tag{A.21}$$

All together, we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c_{k,\sigma}^{A,\dagger} & c_{k,\sigma}^{B,\dagger} & d_{k,\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{k,\sigma}^{A} \\ c_{k,\sigma}^{B} \\ d_{k,\sigma} \end{pmatrix} \tag{A.22}$$

Bibliography

[1] L. N. Cooper and D. Feldman. *BCS: 50 Years*. WORLD SCIENTIFIC, Nov. 2010. ISBN: 978-981-4304-64-1. DOI: 10.1142/7728 (cit. on p. iii).

[2] G. Yang et al. "Structure of Graphene and Its Disorders: A Review". In: *Science and Technology of Advanced Materials* 19.1 (Aug. 29, 2018), pp. 613–648. ISSN: 1468-6996. DOI: 10.1080/14686996.2018.1494493 (cit. on p. 5).

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ACKNOWLEDGEMENT