

Book proposal

**Problems in quantum condensed matter**

From our experience as both teachers and students, the best way to learn subject matter is through problem-solving. When we look for collections of condensed matter physics problems available to the advanced undergraduate or beginning graduate student, however, the only book one readily finds is Mihály and Martin's "Solid State Physics: Problems and Solutions" [1]. Textbooks often have problems in the end of chapters, but these are mostly problems that demonstrate and practice the preceding analytical technique introduced.

We propose a book of quantum condensed matter physics problems that will fill this gap and provide students with a tool for practicing and sharpening their understanding of the varied and complex topics of our field. This book will concentrate on modern condensed matter theory. It will cater to advanced undergraduates, any level of graduate students, and engineering professionals. The only prerequisites for efficacious use of the book would be having taken electromagnetism, quantum mechanics, and introductory solid-state (Ashcroft and Mermin level) classes. The problems will range in difficulty from simple problems meant to acquaint the student with the physical (or experimental) system, all the way to open-ended problems reflecting contemporary research. Intermediate problems will require some knowledge of various techniques, and detailed solutions will allow students to learn the techniques necessary. Emphasis will be put on the understanding of both the experimental details and the analytical techniques. Needless to say that the most advanced problems will be addressed to theorists, but at least half of the problems will be intended to both theory- and experiment-oriented readers.

We expect that each chapter will consist of a brief introduction, list of general references and reviews, collection of about ten problems, and solutions with appropriate specific references.

**1 Table of contents**

A tentative table of contents follows. In each topic we give a list of likely themes for the problems, as well as the specific experimental aspects we intend to cover. Needless to say, since condensed matter is an integrated subject, many problems will pertain to more than just the subject matter of the chapter their grouped under.

1. A review of the theory of metals; second quantization; tight-binding Hamiltonians; Landau theory of Fermi liquids. Experimental topics: transport and magneto-resistance measurements.
2. Introduction to mesoscopic physics. Transport; Coulomb blockade; weak localization; shot-noise.
3. Quantum phase transitions. Dynamical scaling; transverse-field Ising model; Kosterlitz-Thouless transition in 1D quantum systems.
4. Luttinger liquid and Bosonization. Sine-Gordon model, Kane-Fisher impurity tunneling, Landauer-Büttiker formalism. Experimental topics: transport measurements; nanotubes.
5. Superconductivity. This chapter will encompass several extended sub-topics:
  - (a) Low-temperature superconductivity; BCS wave-function.
  - (b) High-temperature superconductivity; Cuprates phase-diagram phenomenology; Hubbard model.
  - (c) Superconductor-metal-insulator transitions. Disorder effects in metals; phase-fluctuations; Chakravarty-Schmid transition of Josephson junctions.
  - (d) Experimental topics: tunneling, ARPES, STM, surface-acoustic waves.



Figure 1: The AKLT state is constructed by considering each spin-1 site as consisting of two spin-1/2 parts that are symmetrized. In each site, one part forms a singlet (solid line) to its right, and the other part forms a singlet to its left. Parameterizing the spin-1/2 parts using Schwinger Bosons enforces their symmetrization.

6. Quantum magnetism. Origin and models; signatures of ground states; spin-wave theory. Experimental topics: susceptibility measurements, neutron scattering.
7. Quantum Hall effect. Phenomenology; composite bosons and fermions; edge-channels; zero-resistance states. Experimental topics: transverse transport, semi-conductor heterostructures.
8. Low-temperature atomic physics. Bose-Einstein condensation; Gross-Pitaevskii equation; Feshbach resonances; Superfluid-insulator transitions. Experimental topics: time-of-flight measurements; noise measurements.
9. Heavy-Fermion materials. Phenomenology; slave-boson methods; DMFT.

## 2 Sample problems

### 2.1 The AKLT state of a 1-D spin-1 Heisenberg model

#### Problem

Consider the spin-1 Heisenberg chain,

$$\mathcal{H} = \sum_i J \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1}. \quad (1)$$

This Hamiltonian has very special properties: unlike its half-integer spin counterparts, it has a single ground state which has an excitation gap. It describes very well the compound  $Ni(C_2H_8N_2)_2NO_2ClO_4$ , or NENP [2].

A state close to the ground state of the spin-1 Heisenberg model is the AKLT state, named after Affleck, Kennedy, Lieb, and Tasaki [3]. In terms of Schwinger-Boson operators (Schwinger bosons will be described in the background material, currently in footnote[4]), it is given by:

$$|AKLT\rangle = \frac{1}{N} \left[ \prod_i \left( \hat{a}_i^\dagger \hat{b}_{i+1}^\dagger - \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger \right) \right] |0\rangle. \quad (2)$$

This state literally considers each spin-1 site as consisting of two spin-1/2 parts, where one of the parts forms a singlet to the right, and the other to the left (see Fig. 1). This maximizes antiferromagnetic correlations without breaking any symmetry of the system, which is forbidden by the Mermin-Wagner theorem [5].

1. Show that the state  $|AKLT\rangle$  is (a) an eigenstate and (b) the ground state of the AKLT Hamiltonian:

$$\mathcal{H}_{AKLT} = \sum_i J \left[ \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} + \frac{1}{3} \left( \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \right)^2 \right] \quad (3)$$

Hint: what is the projection operator for two spins to the  $s_{total} = 2$  subspace?

2. Although  $|AKLT\rangle$  is not an eigenstate of the Heisenberg Hamiltonian, Eq. (1), we can use it to estimate the ground-state energy of the model. For this purpose, calculate the expectation value

$$\langle AKLT | \mathcal{H} | AKLT \rangle. \quad (4)$$

This energy should be compared to the energy of a spin-1/2 singlet per bond. How different are these energies?

### Solution

1. The AKLT state is unique in the following way: if we concentrate on each pair of neighboring states, and ignore completely the rest of the chain, we see that at most the two sites have total spin 1. This is since the basic element in the AKLT wave function is the Schwinger boson singlet operator:

$$\left(\hat{a}_i^\dagger \hat{b}_{i+1}^\dagger - \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger\right). \quad (5)$$

Therefore the AKLT wave function must be an exact ground state of operators projecting neighboring spins on the  $S_{total} = 2$  subspace. We will now show that the AKLT Hamiltonian consists of a sum of such operators.

To construct such a projection operator, we write an operator which will vanish for the  $S_{total} = 1$  and  $S_{total} = 0$  states:

$$P = \frac{1}{6 \cdot 4} (S_{total}^2 - 2) (S_{total}^2) \quad (6)$$

where the normalization is obtained by putting  $S_{total} = 2$  and  $S_{total}^2 = 3$ . This operator is either 0, or 1 in the case of  $S_{total} = 2$ .

By assigning  $S_{total} = S_i + S_{i+1}$  we find:

$$\begin{aligned} P_i &= \frac{1}{6 \cdot 4} (S_i^2 + S_{i+1}^2 + 2S_i \cdot S_{i+1} - 2) (S_i^2 + S_{i+1}^2 + 2S_i \cdot S_{i+1}) \\ &= \frac{1}{2} \left( \frac{2}{3} + S_i \cdot S_{i+1} + \frac{1}{3} (S_i \cdot S_{i+1})^2 \right). \end{aligned} \quad (7)$$

But this looks exactly like one term in the AKLT Hamiltonian. In fact:

$$H_{AKLT} = \sum_i (2P_i - 2/3) \quad (8)$$

Since for each  $P_i$  we have  $P_i |AKLT\rangle = 0$ , and  $\langle P_i \rangle \geq 0$ ,  $|AKLT\rangle$  is a ground state of  $H_{AKLT}$ , with:

$$H_{AKLT} |AKLT\rangle = -\frac{2}{3} L |AKLT\rangle. \quad (9)$$

It turns out that this state is also unique; for proof see Ref. [3].

2. Our goal is to calculate  $\langle AKLT | \mathcal{H} | AKLT \rangle$ . Let us first calculate the normalization  $N$  of the AKLT state:

$$N^2 \langle AKLT | AKLT \rangle = \langle 0 | \prod_i \left( \hat{a}_i \hat{b}_{i+1} - \hat{b}_i \hat{a}_{i+1} \right) \prod_i \left( \hat{a}_i^\dagger \hat{b}_{i+1}^\dagger - \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger \right) | 0 \rangle. \quad (10)$$

This complicated product is simplified in a similar fashion to that of one-dimensional partition functions, using transfer matrices. First, we note that when we expand the product on the left, each term must be matched with its hermitian conjugate in the product to the right, in order to produce a non-zero contribution to this expectation value. Let us make the following definition:

$$f_i^1 = \hat{a}_i \hat{b}_{i+1} \quad f_i^2 = \hat{b}_i \hat{a}_{i+1} \quad (11)$$

With this definition we can write:

$$N^2 \langle AKLT | AKLT \rangle = \sum_{\{\tau_i=1,2\}} \tau \langle 0 | \prod_i f_i^{\tau_i} \prod_i (f_i^{\tau_i})^\dagger | 0 \rangle \quad (12)$$

The Schwinger-Boson (SB) vacuum can be written as a product of the SB vacuum for each site:

$$|0\rangle = \prod_i |0_i\rangle. \quad (13)$$

hence Eq. (12) consists of products of the expectation value of f-operators with respect to the vacuum each individual site. For site  $i$  this product is roughly:

$$\langle 0_i | f_{i-1}^{\tau_{i-1}} f_i^{\tau_i} f_{i-1}^{\tau_{i-1} \dagger} f_i^{\tau_i \dagger} | 0_i \rangle \quad (14)$$

Since  $\tau_i$  and  $\tau_{i-1}$  can each be 1 or 2, let us organize this product in a  $2 \times 2$  matrix. For:

$$T_{\tau_{i-1}, \tau_i} = \begin{pmatrix} T_{1,1} & T_{1,2} \\ T_{2,1} & T_{2,2} \end{pmatrix} \quad (15)$$

we have:

$$T = \begin{pmatrix} \langle 0_i | b_i a_i b_i^\dagger a_i^\dagger | 0_i \rangle & \langle 0_i | b_i b_i b_i^\dagger b_i^\dagger | 0_i \rangle \\ \langle 0_i | a_i a_i a_i^\dagger a_i^\dagger | 0_i \rangle & \langle 0_i | a_i b_i a_i^\dagger b_i^\dagger | 0_i \rangle \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \quad (16)$$

Now, it is easy to see that:

$$N^2 \langle AKLT | AKLT \rangle = N^2 = \sum_{\{\tau_i=1,2\}} \prod_{i=0}^{L-1} T_{\tau_i, \tau_{i+1}} \quad (17)$$

with  $\tau_0 = \tau_L$ . But this is just the trace:

$$= Tr(T^L). \quad (18)$$

The trace of a power of a matrix is most easily obtained using its diagonal form.  $T$  is readily diagonalized by the eigenvectors:

$$(1, 1), (1, -1) \quad (19)$$

with eigenvalues:

$$3 \quad -1 \quad (20)$$

respectively. Hence:

$$N^2 = 3^L + (-1)^L. \quad (21)$$

Moving next to the evaluation of  $\langle AKLT | \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} | AKLT \rangle$ , we begin by noting that since the AKLT state is rotationally invariant, we should have:

$$\langle AKLT | \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} | AKLT \rangle = 3 \langle AKLT | \hat{S}_i^z \cdot \hat{S}_{i+1}^z | AKLT \rangle, \quad (22)$$

which simplifies things dramatically.

Looking Eq. (17) above, the insertion of  $\hat{S}_i^z \cdot \hat{S}_{i+1}^z$  to the AKLT product modifies the transfer matrix  $T_{\tau_i, \tau_{i+1}}$  in locations  $i$  and  $i+1$ . At  $i$  we have:

$$T_{\tau_i, \tau_{i+1}} \rightarrow S_{\tau_i, \tau_{i+1}} = \begin{pmatrix} \langle 0_i | b_i a_i \hat{S}_i^z b_i^\dagger a_i^\dagger | 0_i \rangle & \langle 0_i | b_i b_i \hat{S}_i^z b_i^\dagger b_i^\dagger | 0_i \rangle \\ \langle 0_i | a_i a_i \hat{S}_i^z a_i^\dagger a_i^\dagger | 0_i \rangle & \langle 0_i | a_i b_i \hat{S}_i^z a_i^\dagger b_i^\dagger | 0_i \rangle \end{pmatrix} = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \quad (23)$$

And, therefore:

$$\begin{aligned} \langle AKLT | \hat{S}_i^z \cdot \hat{S}_{i+1}^z | AKLT \rangle &= \frac{1}{3^L} \sum_{\{\tau_i=1,2\}} \prod_{j=0}^{i-2} T_{\tau_j, \tau_{j+1}} S_{\tau_{i-1}, \tau_i} S_{\tau_i, \tau_{i+1}} \prod_{j=i+1}^{L-1} T_{\tau_j, \tau_{j+1}} \\ &= \frac{1}{3^L} Tr(T^{L-2} S^2) \end{aligned} \quad (24)$$

Now, we know that the trace on the RHS (24) is dominated by the eigenvalue  $\lambda = 3$  of the matrix  $T$ , which corresponds to the eigenvector  $(1, 1)/\sqrt{2}$ . Therefore, neglecting the contribution of the other eigenvalue of  $T$  due to the large length of the chain, we can write:

$$\langle AKLT | \hat{S}_i^z \cdot \hat{S}_{i+1}^z | AKLT \rangle = \frac{1}{3^L} \frac{1}{2} (1, 1) T^{L-2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \frac{1}{2} (1, 1) S^2 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = -\frac{4}{9} \quad (25)$$

Thus, we have:

$$\langle AKLT | J \sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} | AKLT \rangle = -\frac{4}{3} JL. \quad (26)$$

Note that a spin-1/2 singlet with a Heisenberg Hamiltonian would have the energy  $-3/4J$  per bond, hence the AKLT state exceeds this energy by almost a factor of 2. On the other hand, a singlet between two spin-1 sites has energy  $-2J$  per bond, which is nearly twice the energy per bond of the AKLT state.

## 2.2 The Haldane gap

### Problem

In 1983, Duncan Haldane discovered that a spin-1 Heisenberg chain,

$$\mathcal{H} = \sum_i J \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1}, \quad (27)$$

has an excitation gap [6]. He had done so by developing a mapping of the Heisenberg Hamiltonian to a non-linear sigma model. Using the AKLT state of the previous problem, however, it is possible to demonstrate and evaluate the gap in a much simpler way.

1. For the purpose of finding the Haldane gap, we are going to use the single-mode approximation. Assuming that we know the ground state of  $\mathcal{H}$  to be  $|GS\rangle$ , we can guess that there will be a band of excited states with wave number  $k$  is given by  $\hat{A}_k |GS\rangle = \sum_n e^{ikn} \hat{A}_n |GS\rangle$ , with  $\hat{A}_n$  a local operator on site  $n$ . Show that the expectation value of the excitation energy of  $\hat{A}_k |GS\rangle$  is given by:

$$\langle \Delta_k \rangle = \frac{1}{2} \langle GS | \left[ \hat{A}_k^\dagger, \left[ \mathcal{H}, \hat{A}_k \right] \right] | GS \rangle \quad (28)$$

Assume that the following condition applies:  $\hat{A}_k |GS\rangle$  and  $\hat{A}_k^\dagger |GS\rangle$  have the same expectation of the excitation energy, and the same normalization - a consequence of time reversal.

2. Given that the lowest excited states of the Haldane spin-1 chain have total spin  $S_{total} = 1$  (as opposed to the ground state which is a full singlet, with  $S_{total} = 0$ ), construct approximations to these states using the AKLT state of the previous problem. How many such excitation branches are there?
3. By finding the appropriate operator  $\hat{A}_n$ , the states of (2) and the identity of (1), evaluate the Haldane gap. Here too, use the AKLT state as an approximation for the ground state.

### Answer

1. We begin by assuming that the excited states is approximated by:

$$|A\rangle = \frac{1}{\sqrt{\langle GS | \hat{A}^\dagger \hat{A} | GS \rangle}} \hat{A} |GS\rangle. \quad (29)$$

The excitation energy with respect to the Hamiltonian  $\mathcal{H}$  is then:

$$\langle \Delta \rangle = \langle A | \mathcal{H} | A \rangle - \langle GS | \mathcal{H} | GS \rangle. \quad (30)$$

Since  $|GS\rangle$  is assumed to be the ground state of  $\mathcal{H}$ ,  $\mathcal{H} |GS\rangle = E_0 |GS\rangle$  we can write:

$$\Delta = \frac{\langle GS | \left( \hat{A}^\dagger \mathcal{H} \hat{A} - \mathcal{H} \hat{A}^\dagger \hat{A} \right) | GS \rangle}{\langle GS | \hat{A}^\dagger \hat{A} | GS \rangle} = \frac{\langle GS | \left( \hat{A} \mathcal{H} \hat{A}^\dagger - \mathcal{H} \hat{A} \hat{A}^\dagger \right) | GS \rangle}{\langle GS | \hat{A} \hat{A}^\dagger | GS \rangle}. \quad (31)$$

In the second equality we used the fact that the normalization of  $\hat{A} |GS\rangle$  and  $\hat{A}^\dagger |GS\rangle$ , as well as their energy expectation values are the same. Adding the two expressions for  $\Delta$ , and dividing by two, we arrive at:

$$\Delta = \frac{1}{2} \frac{\langle GS | \left[ \hat{A}^\dagger, \left[ \mathcal{H}, \hat{A} \right] \right] | GS \rangle}{\langle GS | \hat{A}^\dagger \hat{A} | GS \rangle} \quad (32)$$

2. The next step is to guess what the excited states look like. An excited state would presumably have a structure of a quasi-particle, delocalized at the equivalent of a  $k$  momentum state. Starting with the  $|AKLT\rangle$  state, it seems plausible that the role of the quasiparticle would be played by a triplet replacing the singlet operator  $(\hat{a}_i^\dagger \hat{b}_{i+1}^\dagger - \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger)$ . This would indeed yield a spin-1 state. The triplet operator can be one of three:  $(\hat{a}_i^\dagger \hat{b}_{i+1}^\dagger + \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger)$ ,  $\hat{a}_i^\dagger \hat{a}_{i+1}^\dagger$ ,  $\hat{b}_i^\dagger \hat{b}_{i+1}^\dagger$ . Thus we find three branches, or bands of excitations:

$$\begin{aligned} |k, +\rangle &= \frac{1}{N_{k+}} \sum_n e^{ikn} (\hat{a}_n^\dagger \hat{a}_{n+1}^\dagger) \prod_{m \neq n} (\hat{a}_m^\dagger \hat{b}_{m+1}^\dagger - \hat{b}_m^\dagger \hat{a}_{m+1}^\dagger) |0\rangle, \\ |k, 0\rangle &= \frac{1}{N_{k0}} \sum_n e^{ikn} (\hat{a}_n^\dagger \hat{b}_{n+1}^\dagger + \hat{b}_n^\dagger \hat{a}_{n+1}^\dagger) \prod_{m \neq n} (\hat{a}_m^\dagger \hat{b}_{m+1}^\dagger - \hat{b}_m^\dagger \hat{a}_{m+1}^\dagger) |0\rangle, \\ |k, -\rangle &= \frac{1}{N_{k-}} \sum_n e^{ikn} (\hat{b}_n^\dagger \hat{b}_{n+1}^\dagger) \prod_{m \neq n} (\hat{a}_m^\dagger \hat{b}_{m+1}^\dagger - \hat{b}_m^\dagger \hat{a}_{m+1}^\dagger) |0\rangle. \end{aligned} \quad (33)$$

Due to rotational symmetry, these three states will give rise to states with the same energy. They represent the  $m_z = 1, 0, -1$  states of the triplet of excitations.

3. Because the three states in Eq. (33) are degenerate, it suffices us to consider one of them. It is most convenient to take the  $m_z = 0$  triplet state, since it can be produced using the application of  $\hat{S}_i^z$ . Also, since we are after the lowest energy state, we need to choose  $k = 0$  or  $\pi$ .

Let us define the states  $|j\rangle$  with a localized  $m_z = 0$  triplet:

$$|j\rangle = \frac{1}{N} (\hat{a}_j^\dagger \hat{b}_{j+1}^\dagger + \hat{b}_j^\dagger \hat{a}_{j+1}^\dagger) \prod_{i \neq j} (\hat{a}_i^\dagger \hat{b}_{i+1}^\dagger - \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger) |0\rangle, \quad (34)$$

$N$  is the same normalization as for the AKLT state. Our guess for the lowest excited state is thus:

$$|A\rangle = \sum_j (-1)^j |j\rangle, \quad (35)$$

corresponding to the state  $|\pi, 0\rangle$  in Eq. (33). In principle, we need to check whether the  $(-1)^j$  staggering term gives a lower energy than just having a constant ( $|0, 0\rangle$ ). As it turns out, it does. We leave it to the reader to verify that the energy for a non-staggered triplet state is higher.

The next step is to construct this state, and find the appropriate  $\hat{A}$ . We first note the following commutator:

$$[\hat{S}_i^z, \hat{a}_j^\dagger \hat{b}_{j+1}^\dagger - \hat{b}_j^\dagger \hat{a}_{j+1}^\dagger] = \frac{1}{2} (\delta_{i,j} - \delta_{i,j+1}) (\hat{a}_j^\dagger \hat{b}_{j+1}^\dagger + \hat{b}_j^\dagger \hat{a}_{j+1}^\dagger) \quad (36)$$

Thus:

$$\sum_j (-1)^j |j\rangle = \sum_j (-1)^j \hat{S}_j^z |AKLT\rangle \quad (37)$$

And we have:

$$\hat{A} = \sum_j (-1)^j \hat{S}_j^z \quad (38)$$

which is also Hermitian.

Note that using the spin operators we can construct all three branches of triplet excitations:

$$\begin{aligned} |k, \pm\rangle &\propto \sum_n e^{ikn} S_n^\pm |AKLT\rangle, \\ |k, 0\rangle &\propto \sum_n e^{ikn} S_n^z |AKLT\rangle. \end{aligned} \quad (39)$$

In antiferromagnetic spin systems it is often the case that the operator used for the single-mode approximation are indeed the spin operators. Since the full spin operator is a vector, it produces a spin-1 state out of singlets, fulfilling the expectation out of the lowest excited states over a singlet

ground state. Note that formula (39) fails at  $k = 0$ , since the  $|AKLT\rangle$  state is an exact singlet state. In this case the appropriate state requires  $e^{ikn} \rightarrow n$  - an interesting fact to show.

Now we need to evaluate the commutator  $[\hat{A}, [\mathcal{H}, \hat{A}]]$ . We have:

$$\begin{aligned} [\mathcal{H}, \hat{A}] &= \left[ \sum_i \frac{1}{2} (\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+), \sum_j (-1)^j \hat{S}_j^z \right] \\ &= \frac{1}{4} \sum_i (-1)^i (\hat{S}_{i-1}^+ [\hat{S}_i^-, \hat{S}_i^z] + \hat{S}_{i-1}^- [\hat{S}_i^+, \hat{S}_i^z] \\ &\quad + [\hat{S}_i^+, \hat{S}_i^z] \hat{S}_{i+1}^- + [\hat{S}_i^-, \hat{S}_i^z] \hat{S}_{i+1}^+) \end{aligned} \quad (40)$$

where another  $1/2$  was added to offset the double counting from the  $\hat{S}_i^z$  sum. Using  $[\hat{S}_i^-, \hat{S}_i^z] = \hat{S}_i^-$ , and  $[\hat{S}_i^+, \hat{S}_i^z] = -\hat{S}_i^+$ , we get:

$$= \frac{1}{2} \sum_i (-1)^i (-\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+) \quad (41)$$

And repeating the same steps give:

$$[\hat{A}, [\mathcal{H}, \hat{A}]] = -\frac{1}{2} \sum_i (\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+) \quad (42)$$

By using rotational symmetry again we find:

$$\langle AKLT | [\hat{A}, [\mathcal{H}, \hat{A}]] | AKLT \rangle = - \sum_i 2 \langle AKLT | \hat{S}_i^z \cdot \hat{S}_{i+1}^z | AKLT \rangle = \frac{8}{9} L. \quad (43)$$

The remaining part is the evaluation of the denominator,  $\langle AKLT | \hat{A} \hat{A} | AKLT \rangle$ . For this purpose we need to know the z-z correlation function in the AKLT state. Following the methods of problem 2.1, we have:

$$\langle AKLT | \hat{S}_i^z \cdot \hat{S}_j^z | AKLT \rangle = \frac{1}{3^L} \frac{1}{2} (1, 1) T^{L-1-(j-i)} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \frac{1}{2} (1, 1) S \cdot T^{j-i-1} \cdot S \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (44)$$

The matrix  $S$  switches the dominating eigenvector of  $T$ ,  $(1, 1)$ , into the sub-dominant eigenvector:

$$S \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = -2 \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (45)$$

which has eigenvalue under  $T$ ,  $\lambda = -1$ . Note that also:

$$(1, 1) S = 2(1, -1) \quad (46)$$

without the extra minus sign. Hence:

$$\frac{1}{2} (1, 1) S \cdot T^{j-i-1} \cdot S \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 4 \cdot (-1)^{j-i} \quad (47)$$

and thus:

$$\langle AKLT | \hat{S}_i^z \cdot \hat{S}_j^z | AKLT \rangle = \frac{4}{3^{j-i+1}} \cdot (-1)^{j-i}. \quad (48)$$

In order to calculate the denominator of Eq. (32) we also need:

$$\langle AKLT | (\hat{S}_i^z)^2 | AKLT \rangle = \frac{1}{3} \langle AKLT | (\hat{S}_i)^2 | AKLT \rangle = \frac{2}{3} \quad (49)$$

Now:

$$\begin{aligned} \langle AKLT | \hat{A}\hat{A} | AKLT \rangle &= \sum_i \sum_j (-1)^{j-i} \langle AKLT | \hat{S}_i^z \cdot \hat{S}_j^z | AKLT \rangle \\ &= L \left( \frac{2}{3} + 2 \sum_{j>i} \frac{4}{3^{j-i+1}} \right) = L \left( \frac{2}{3} + 2 \cdot \frac{4}{9} \frac{1}{1-\frac{1}{3}} \right) = 2L \end{aligned} \quad (50)$$

Finally, we can evaluate the gap:

$$\Delta \approx \frac{J}{2} \frac{8}{9} \cdot \frac{1}{2} = J \frac{2}{9} = 0.22J. \quad (51)$$

This should be compared to the numerical result: [7]

$$\Delta = 0.325J. \quad (52)$$

## 2.3 Graphene: Tight-binding model on a honeycomb lattice

### problem:

Solving the tight-binding model on the honeycomb lattice is the starting point for understanding the electronic structure of *graphene* - a single sheet of graphite. Ever since the success in producing single-layer Graphene sheets, the system has become a central topic of investigation in Condensed Matter Physics and nanotechnology.

The tight-binding Hamiltonian is defined, in the second-quantized notation, as

$$\hat{\mathcal{H}}_{\text{TB}} = \mu \sum_{\mathbf{i}} c_{\mathbf{i}}^{\dagger} c_{\mathbf{i}} - t \sum_{\langle i,j \rangle} \left( c_{\mathbf{i}}^{\dagger} c_{\mathbf{j}} + c_{\mathbf{j}}^{\dagger} c_{\mathbf{i}} \right) \quad (53)$$

where the summation in the second term is performed over all pairs of nearest neighbor sites  $i, j$ . The spin indices are omitted for clarity; the Hamiltonian is spin-independent. This is a single-particle Hamiltonian, so it can be conveniently written in the basis of Wannier states  $|\mathbf{R}\rangle$ :

$$\hat{\mathcal{H}}_{\text{TB}} = \mu \sum_{\mathbf{R}} |\mathbf{R}\rangle \langle \mathbf{R}| - t \sum_{\mathbf{R}} \sum_{\boldsymbol{\delta}} |\mathbf{R}\rangle \langle \mathbf{R} + \boldsymbol{\delta}| \quad (54)$$

where  $\boldsymbol{\delta}$ 's are the vectors connecting each site to one of its neighbors. (Wannier states are the orthonormal states which are localized in the vicinity of a given site:  $|\mathbf{R}_i\rangle \equiv c_i^{\dagger}|0\rangle$ .) For the purpose of this problem, we concentrate on the case of a two-dimensional honeycomb lattice.

1. The primitive cell of a honeycomb lattice contains two sites (e.g., a pair of sites connected by a vertical bond, as depicted in Fig. 2). These two sites belong to two different sublattices, e.g., the bottom site only connects to top sites in the same and other primitive cells of the honeycomb lattice.

Introduce two sets of Wannier functions,  $\langle \mathbf{r} | \mathbf{R}_A \rangle$  and  $\langle \mathbf{r} | \mathbf{R}_B \rangle$  describing the electrons localized around the sites of each sublattice. Rewrite Equation (54) in terms of  $|\mathbf{R}_A\rangle$ 's and  $|\mathbf{R}_B\rangle$ 's. This should allow you to specify the sets of  $\boldsymbol{\delta}$ 's for each sublattice.

2. Diagonalize this Hamiltonian and find the energy eigenvalues. How many bands are there?
3. What is the Brillouin zone for this lattice? Plot the energy spectrum as a function of  $\mathbf{k}$  along two directions of high symmetry.

### Solution:

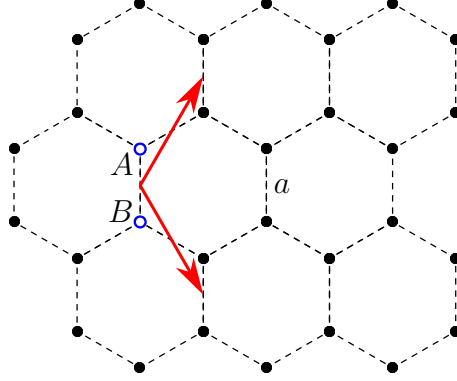


Figure 2: The honeycomb lattice with the two sites,  $A$  and  $B$  forming the basis. Two primitive vectors  $\mathbf{d}_{1,2}$  are also shown.

1. Let us start by simply re-labeling the states:

$$|\mathbf{R}_A\rangle \equiv |\mathbf{R} + \mathbf{v}_A\rangle \equiv |\mathbf{R}, A\rangle \quad (55)$$

and

$$|\mathbf{R}_B\rangle \equiv |\mathbf{R} + \mathbf{v}_B\rangle \equiv |\mathbf{R}, B\rangle \quad (56)$$

where we choose  $\mathbf{R}$  to point to the middle of the vertical edge connecting the two atoms of one basis. In this case,  $\mathbf{v}_A = -\mathbf{v}_B = a(1/2, 0)$ . In fact, the particular choice of which point in the basis is specified by  $\mathbf{R}$ , and what are the corresponding  $\mathbf{v}_{1,2}$  is immaterial; as you will see,  $\mathbf{v}_{1,2}$  do not enter any the following. What is important, is to keep track of the two sublattices because the sets of vectors  $\delta$  connecting each atom to its neighbors is different for these sublattices.

With this labeling of the states, the Hamiltonian becomes

$$\begin{aligned} \hat{\mathcal{H}}_{\text{TB}} = & \mu \sum_{\mathbf{R}} \{ |\mathbf{R}, A\rangle \langle \mathbf{R}, A| + |\mathbf{R}, B\rangle \langle \mathbf{R}, B| \} \\ & - t \sum_{\mathbf{R}} \{ |\mathbf{R}, B\rangle \langle \mathbf{R}, A| + |\mathbf{R} + \mathbf{d}_1, B\rangle \langle \mathbf{R}, A| + |\mathbf{R} - \mathbf{d}_2, B\rangle \langle \mathbf{R}, A| \\ & + |\mathbf{R}, A\rangle \langle \mathbf{R}, B| + |\mathbf{R}, A\rangle \langle \mathbf{R} + \mathbf{d}_1, B| + |\mathbf{R}, A\rangle \langle \mathbf{R} - \mathbf{d}_2, B| \} \quad (57) \end{aligned}$$

Here the vectors  $\mathbf{d}_{1,2} = a\sqrt{3}(1/2, \pm\sqrt{3}/2) = d_0(1/2, \pm\sqrt{3}/2)$  are the primitive vectors of the underlying triangular (also sometimes referred to as hexagonal – not to be confused with honeycomb!) Bravais lattice with the lattice constant  $d_0 = a\sqrt{3}$ . The second line of Eq. (57) describes “hops” from a given A-site to all three of its surrounding B-sites, one within the same basis and two in the neighboring ones. The third line describes “hops” in the opposite direction. Convince yourself that all possible “hops” are included in this Hamiltonian. Written this way, the Hamiltonian is explicitly Hermitian, as of course it should be.

2. The next step is to perform the Fourier transform. Write

$$|\mathbf{R}, A\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} |\mathbf{k}, A\rangle \quad (58)$$

which can be inverted as  $|\mathbf{k}, A\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \exp(i\mathbf{k}\cdot\mathbf{R}) |\mathbf{R}, A\rangle$ , with the identical expressions for  $|\mathbf{k}, B\rangle$  and  $|\mathbf{R}, B\rangle$ .

Now, the Hamiltonian becomes

$$\begin{aligned} \hat{\mathcal{H}}_{\text{TB}} = \mu \sum_{\mathbf{k}} \{ & |\mathbf{k}, A\rangle \langle \mathbf{k}, A| + |\mathbf{k}, B\rangle \langle \mathbf{k}, B| \} \\ & - t \sum_{\mathbf{k}} \{ |\mathbf{k}, B\rangle \langle \mathbf{k}, A| (1 + e^{i\mathbf{k} \cdot \mathbf{d}_1} + e^{-i\mathbf{k} \cdot \mathbf{d}_2}) + |\mathbf{k}, A\rangle \langle \mathbf{k}, B| (1 + e^{-i\mathbf{k} \cdot \mathbf{d}_1} + e^{i\mathbf{k} \cdot \mathbf{d}_2}) \}. \end{aligned} \quad (59)$$

In this form, the Hamiltonian is *almost* diagonal – its terms do not mix states with different wave vectors  $\mathbf{k}$ . However, it still mixes  $|\mathbf{k}, A\rangle$  and  $|\mathbf{k}, B\rangle$  – in other words, we just block-diagonalized the Hamiltonian. The remaining task is to diagonalize these blocks, which in matrix notation (i.e., in  $|\mathbf{k}, A\rangle, |\mathbf{k}, B\rangle$  basis) look like this:

$$\hat{\mathcal{H}}_{\mathbf{k}} = \begin{pmatrix} \mu & -t(1 + e^{-i\mathbf{k} \cdot \mathbf{d}_1} + e^{i\mathbf{k} \cdot \mathbf{d}_2}) \\ -t(1 + e^{i\mathbf{k} \cdot \mathbf{d}_1} + e^{-i\mathbf{k} \cdot \mathbf{d}_2}) & \mu \end{pmatrix}. \quad (60)$$

The eigenvalue equation is

$$\begin{aligned} (\mu - \mathcal{E}_{\mathbf{k}})^2 &= t^2 (1 + e^{-i\mathbf{k} \cdot \mathbf{d}_1} + e^{i\mathbf{k} \cdot \mathbf{d}_2}) (1 + e^{i\mathbf{k} \cdot \mathbf{d}_1} + e^{-i\mathbf{k} \cdot \mathbf{d}_2}) \\ &= t^2 [3 + 2 \cos \mathbf{k} \cdot \mathbf{d}_1 + 2 \cos \mathbf{k} \cdot \mathbf{d}_2 + 2 \cos \mathbf{k} \cdot (\mathbf{d}_1 + \mathbf{d}_2)] \end{aligned} \quad (61)$$

or

$$\begin{aligned} \mathcal{E}_{\mathbf{k}} &= \mu \pm t \sqrt{3 + 2 \cos \mathbf{k} \cdot \mathbf{d}_1 + 2 \cos \mathbf{k} \cdot \mathbf{d}_2 + 2 \cos \mathbf{k} \cdot (\mathbf{d}_1 + \mathbf{d}_2)} \\ &= \mu \pm t \sqrt{3 + 4 \cos \left( \frac{1}{2} k_x d_0 \right) \cos \left( \frac{\sqrt{3}}{2} k_y d_0 \right) + 2 \cos k_y d_0} \end{aligned} \quad (62)$$

This is the desired dispersion relation. Clearly it has *two* bands, corresponding to the choice of sign in the last expression.

3. The reciprocal lattice is another triangular lattice, rotated by  $\pi/6$ , with the primitive vectors

$$\begin{aligned} \mathbf{b}_1 &= \frac{2\pi}{d_0} \left( 1, \frac{1}{\sqrt{3}} \right) = \frac{2\pi}{3a} (\sqrt{3}, 1) \\ \mathbf{b}_2 &= \frac{2\pi}{d_0} \left( -1, \frac{1}{\sqrt{3}} \right) = \frac{2\pi}{3a} (-\sqrt{3}, 1) \end{aligned}$$

The first Brillouin zone is a hexagon with two most symmetric directions being that pointing from its center to one of its corners (e.g., along the  $k_x$  axis) and the other one being that pointing to the middle of one of its sides (e.g., along the  $k_y$  axis) – see Figure 3 below.

Allowing  $\mathbf{k} = k_x \hat{\mathbf{e}}_x$  and  $\mathbf{k} = k_y \hat{\mathbf{e}}_y$ , we obtain

$$\mathcal{E}_{k_x} = \mu \pm t \sqrt{3 + 4 \cos \frac{k_x d_0}{2} + 2 \cos k_x d_0} \quad (63)$$

$$\mathcal{E}_{k_y} = \mu \pm t \sqrt{5 + 4 \cos \frac{\sqrt{3}}{2} k_y d_0}. \quad (64)$$

While in the  $k_y$ -direction, the gap between the bands,  $2t \sqrt{5 + 4 \cos \frac{\sqrt{3}}{2} k_y d_0}$  always remains positive, in the  $k_x$ -direction it vanishes at the corner of the Brillouin zone, i.e. at  $k_x = 4\pi/3d_0$ . Since the Brillouin zone is a hexagon, it has six corners, but they can be broken into two set of three so that within each set the corners are identifiable with each other: they are related to one another by the reciprocal lattice vectors  $\mathbf{b}_{1,2}$ . Therefore, there are two distinct points in the first Brillouin zone where the band gap vanishes linearly – these are known as *Dirac* points and are the main feature of the electronic spectrum in graphene.

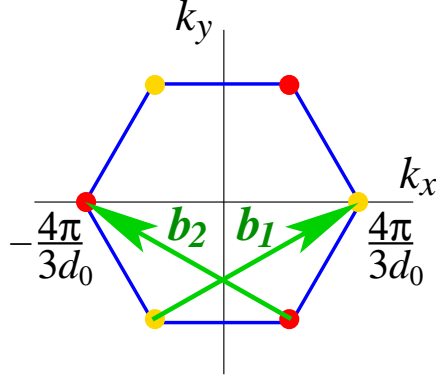


Figure 3: The first Brillouin zone for graphene.  $\mathbf{b}_1$  and  $\mathbf{b}_2$  are two primitive vectors (whose choice is not unique for the reciprocal triangular lattice). The corners of the Brillouin zone that are related by the reciprocal lattice translations (and therefore identifiable with each other) are color-coded red and yellow.

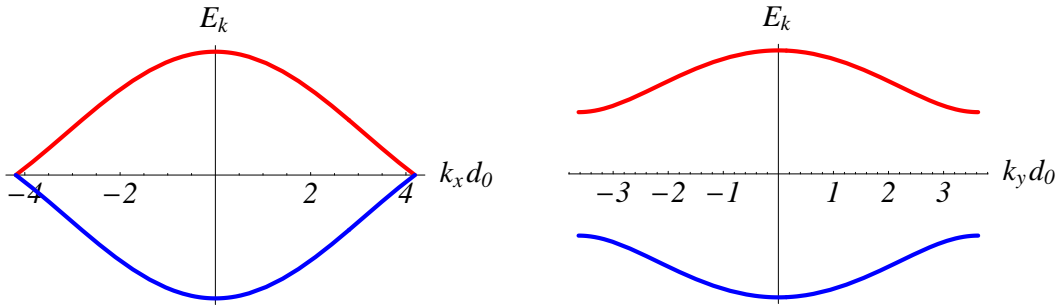


Figure 4: The energy spectrum for  $\mathbf{k}$  in  $x$  and  $y$  directions in the first Brillouin zone of graphene.

## References

- [1] László Mihály and Michael C. Martin. *Solid State Physics : Problems and Solutions*. John Wiley, New York, 1996.
- [2] Partha P. Mitra, Bertrand I. Halperin, and Ian Affleck. Temperature dependence of the electron-spin-resonance spectrum of the chain-end  $s=1/2$  modes in an  $s=1$  antiferromagnetic chain. *Phys. Rev. B*, 45(10):5299–5306, Mar 1992.
- [3] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki. Rigorous results on valence-bond ground states in antiferromagnets. *Phys. Rev. Lett.*, 59:799, 1987.
- [4] The Schwinger-Boson parametrization of spins uses two flavors of Bosons with annihilation operators,  $\hat{a}$  and  $\hat{b}$ , with usual commutation relations:  $[\hat{a}, \hat{a}^\dagger] = [\hat{b}, \hat{b}^\dagger] = 1$ . The  $\hat{a}$  Bosons represent a spin-1/2 part pointing up, and  $\hat{b}$  Bosons a spin-1/2 part pointing down. The spin operators become:  $\hat{S}_{total} = \frac{1}{2}(\hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b})$ ,  $\hat{S}^z = \frac{1}{2}(\hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b})$  and  $\hat{S}^+ = \hat{a}^\dagger \hat{b}$ ,  $\hat{S}^- = \hat{b}^\dagger \hat{a}$ .
- [5] N. D. Mermin and H. Wagner. Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic heisenberg models. *Phys. Rev. Lett.*, 17(22):1133–1136, Nov 1966.
- [6] F. D. M. Haldane. Nonlinear field theory of large-spin heisenberg antiferromagnets: Semiclassically quantized solitons of the one-dimensional easy-axis nel state. *Phys. Rev. Lett.*, 50:1153, 1983.
- [7] A. Auerbach. *Interacting electrons and quantum magnetism*. Springer Verlag, New York, 1994.