Commensurate and Incommensurate Phases of a Spin-Peierls System

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by
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J. Srivatsava
Abstract

The interest in the study of spin-Peierls phenomenon has increased with the discovery of copper germanium oxide (\(CuGeO_3\)) as an example of spin-Peierls systems. The availability of this inorganic compound as large, high quality single crystals, allow experimental measurements which aid in understanding the spin-Peierls phenomenon. This report details the numerical and analytical work done on the various magnetic phases that occur in a quasi one-dimensional spin-Peierls system (like that of copper germanium oxide). Taking the system to be finite, the bond displacements, single particle energies, energy eigenfunctions, spin densities and phonon frequencies are calculated numerically for all possible magnetizations, which includes both the commensurate and incommensurate phases, at zero temperature. Solitons of fractional spin are found to be present in the system for appropriate magnetizations. The uniform to dimerized phase transition occurring in this system is also modelled numerically. The single particle and ground-state energies are later obtained theoretically for the uniform and dimerized phases. In addition, the lattice spin displacements are analytically modelled for a particular magnetization of the system.
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Chapter 1

Introduction

1.1 Spin-Peierls systems

An interest in the theoretical study of quantum spin systems exhibiting the spin-Peierls transition has grown ever since the discovery of the first inorganic spin-Peierls compound, copper germanium oxide ($CuGeO_3$). A spin-Peierls transition is a structural transition associated with quantum spin systems where spin phonon coupling leads to distortions of the lattice. This magneto-elastic phenomenon gives rise to a variety of phases in the system as a function of field $H$ and temperature $T$ [1]. This report is aimed at analyzing these various phases of the spin-Peierls system and the associated physical quantities.

In this chapter, the spin-Peierls systems are introduced by first discussing the structure of the spin-Peierls compound $CuGeO_3$. Its phase diagram is studied later and the section is concluded by writing the model Hamiltonian for this spin-Peierls system.

1.2 Structure of $CuGeO_3$

The crystal structure of $CuGeO_3$ is shown in Fig. (1.1). The crystal is constructed of $CuO_2$ ribbons connected via $GeO_4$ tetrahedra. The $Cu^{2+}$ ions in $3d^9$ configuration form antiferromagnetic spin $1/2$ chain in $c$ direction. There are two different types of $O^{2-}$ shown in the figure in black ($O2$) and grey ($O1$). The $Ge^{4+}$ ions connect adjacent $CuO_2$ ribbons. The lattice parameters of the
orthorhombic unit cell are $a = 4.81\,\text{Å}$, $b = 8.43\,\text{Å}$ and $c = 2.95\,\text{Å}$ [1]. The Cu-O2-Cu (with a bonding angle $\eta \sim 99^\circ$) is responsible for the super exchange
intrachain couplings. The lattice distortions that occur in the dimerized phase obtained by the neutron diffraction measurements are shown in Fig. (1.2). The arrows indicate the direction of atomic displacements.

1.3 (H,T) Phase diagram of \( CuGeO_3 \)

![Figure 1.3: (H,T) phase diagram of the spin-Peierls compound \( CuGeO_3 \)](image)

The (H,T) phase diagram of a spin-Peierls compound \( CuGeO_3 \) which closely resembles the theoretical predictions is shown in Fig. (1.3). The diagram consists of three phases: the uniform \( U \) phase, the dimerized \( D \) phase and the incommensurate \( I \) phase. At high temperatures, the system is in the uniform phase. In this phase, the magnetic chains have uniform spacing \( l \) and one exchange coupling \( J \) between the neighbouring spins. As the temperature is decreased, a second order structural transition is observed at \( T_{sp} \sim 14k \) in the case of \( CuGeO_3 \). In zero or low fields, this transition occurs and it corresponds to a dimerization of lattice. In that dimerized phase, two lattice parameters \( l_1 \) and \( l_2 \) and two exchange couplings \( J_1 \) and \( J_2 \) are needed to define the magnetic chains. Increasing the magnetic field from the \( D \) phase yields a new transition occurring at specific value of the field \( H_c, \sim 12.5T \) at zero temperature in \( CuGeO_3 \). This field induced transition corresponds to a new deformation of
the lattice. Above $H_c$, the lattice becomes incommensurate i.e., the period of modulation of spin density is generally not a rational multiple of the lattice constant $l$ as against the uniform and dimerized phases. Eventually, as the applied magnetic field becomes very large, all the spins get polarized and we get a ferromagnetic state.

### 1.4 Modeling the spin-Peierls compound $CuGeO_3$

The Hamiltonian $H_{sp}$ used to model the spin-Peierls system is given by

$$H_{sp} = J \sum_{n=1}^{N} [1 - \lambda(u_{n+1} - u_n)] \left[ S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z \right] - h \sum_{n=1}^{N} S_n^z + \frac{k}{2} \sum_{n=1}^{N} (u_{n+1} - u_n)^2 + \sum_{n=1}^{N} \frac{P_n^2}{2M}$$

(1.1)

where $N$ is the number of sites, $h$ is the strength of the magnetic field, $\vec{S}_n$ represents the $n^{th}$ spin, $u_n$ is the displacement of lattice point $n$, $P_n$ represents the momentum of lattice point $n$, $M$ is the mass of each lattice point and $\lambda$ is the positive constant which is a measure of the coupling that exists between the lattice points and spins. In the above equation, periodic boundary conditions are assumed i.e., $\vec{S}_{N+1} \equiv \vec{S}_1$.

The first term in the Hamiltonian gives an antiferromagnetic interaction between the nearest neighbour Heisenberg spins along the $c$ direction of the lattice with their exchange coupling $J$ modified to take into account the spin-phonon interactions to the first order in bond displacements. Thus $J$ is replaced by $J [1 - \lambda(u_{n+1} - u_n)]$. The interactions between the spins in the other two lattice directions and between the spins other than the nearest neighbour in $c$ direction of the lattice are neglected. Considering the distance of separation between the spins, this is a good approximation and the system can be analyzed as a quasi one-dimensional (1D) system. The second term is the Zeeman term giving the effect of magnetic field on the system with net magnetization $\sum_{n=1}^{N} S_n^z$. The third term is the harmonic energy of the lattice and the final term represents the kinetic energy of the lattice.

This Hamiltonian is simplified later to calculate the ground state energies and other physical quantities of interest discussed in the next chapter.
Chapter 2

Numerical Results

2.1 Simplification of the Hamiltonian

The full Hamiltonian for the general spin-Peierls system is shown in the previous chapter, Eq. (1.1). It is difficult to work with this Hamiltonian to calculate quantities of interest like single-particle energies and wave functions at zero temperature, spin densities etc. Hence the full Hamiltonian is simplified using the physical arguments discussed below so that the quantities calculated from the simplified Hamiltonian reproduce the physics of the full Hamiltonian to a very good approximation.

2.1.1 Approximations involved and their justification:

- *Soft phonon limit:* The time scales involved in the motion of lattice are known to be much larger than the time scales involved in the motion of spins arising due to the interactions between the spins and phonons. Hence the lattice points are initially taken to be at fixed positions while calculating the unperturbed single-particle energies at zero temperature and zero field. At the end, the lattice movements are however taken into account using the perturbation theory and the perturbed single-particle energies due to motion of lattice points are calculated to second order in bond displacements.

- *XY spins:* The generalised Heisenberg spins in the model are replaced by the XY spins, i.e., the spin-spin interactions in the $\hat{z}$ direction are
Chapter 2. Numerical Results

neglected. This is done to simplify the calculations. When the spins are transformed into Jordan-Wigner fermions, the interactions in the \( \hat{z} \) direction involves four spinless fermion operators \([4]\). It is known from numerical analysis that reducing the Heisenberg spins to XY spins does not qualitatively affect the phase diagram of a quasi 1D spin-Peierls system.

The simplified Hamiltonian, \( H_s \), thus obtained using the above approximations is given by

\[
H_s = -J \sum_{n=1}^{N} \left[ 1 + \delta_{n+\frac{1}{2}} \right] \left[ S_n^x S_{n+1}^x + S_n^y S_{n+1}^y \right] - \hbar \sum_{n=1}^{N} S_n^z + \frac{c}{2} \sum_{n=1}^{N} \delta_{n+\frac{1}{2}}^2 (2.1)
\]

where \( \delta_{n+\frac{1}{2}} = -\lambda (u_{n+1} - u_n) \) is the bond displacement and \( \lambda \) is the positive constant which is a measure of the coupling that exists between the lattice points and spins.

It is to be noted that in addition to the mentioned approximations, a unitary transformation of the form shown in Eqs. \((2.2)\) is performed on the Hamiltonian given in Eq.\((1.1)\) to reverse the sign of the first term.

\[
\begin{align*}
S_n^x &\rightarrow (-1)^n S_n^x \\
S_n^y &\rightarrow (-1)^n S_n^y \\
S_n^z &\rightarrow S_n^z
\end{align*}
\]

**2.1.2 Jordan-Wigner transformation**

Jordan-Wigner transformation transforms a spin Hamiltonian into a spinless fermion Hamiltonian \([2, 6, 10]\). Here, two spinless fermion operators, the creation and annihilation operators, are defined as shown below

\[
\begin{align*}
C_n &= \prod_{j=1}^{n-1} (-\sigma_j^z) S_n^- \\
C_n^+ &= \prod_{j=1}^{n-1} S_n^+ (-\sigma_j^z)
\end{align*}
\]
where

\[
\begin{align*}
S_n^- &= S_n^x - iS_n^y \\
S_n^+ &= S_n^x + iS_n^y
\end{align*}
\]

and \(\sigma\)'s are the Pauli matrices. Using the properties of Pauli matrices, it follows from the relations (2.3) between spin operators and fermion operators that the total magnetization, \(m\), of the system is

\[
m = \sum_{n=1}^{N} S_n^z = N_F - \frac{N}{2}
\]

(2.4)

where \(N_F = \sum_{n=1}^{N} C_n^+ C_n\) is the number of Jordan-Wigner fermions.

Using the Jordan-Wigner transformation on the simplified spin Hamiltonian (2.1), a spinless fermion Hamiltonian is obtained as shown in Eq. (2.5)

\[
\begin{align*}
\tilde{H} &= -\frac{J}{2} \sum_{n=1}^{N-1} \left(1 + \delta_{n+\frac{1}{2}}\right) \left[C_n^+ C_{n+1} + C_{n+1}^+ C_n\right] + (-1)^{N_F+1} (C_N^+ C_1 + C_1^+ C_N) \\
&\quad - \hbar \sum_{n=1}^{N} \left[C_n^+ C_n - \frac{1}{2}\right] + \frac{c}{2} \sum_{n=1}^{N} \delta_{n+\frac{1}{2}}^2
\end{align*}
\]

(2.5)

### 2.2 Single particle energies

The Hamiltonian used to calculate the single-particle energies at zero temperatures for all phases (for all possible magnetizations) is given by

\[
\begin{align*}
H &= -\frac{J}{2} \sum_{n=1}^{N-1} \left[1 + \delta_{n+\frac{1}{2}}\right] \left[C_n^+ C_{n+1} + C_{n+1}^+ C_n\right] + (-1)^{N_F} \left[C_N^+ C_1 + C_1^+ C_N\right] \\
&\quad - \hbar \sum_{n=1}^{N} \left[C_n^+ C_n - \frac{1}{2}\right] + \frac{c}{2} \sum_{n=1}^{N} \delta_{n+\frac{1}{2}}^2
\end{align*}
\]

(2.6)

It can be seen that the boundary term of this Hamiltonian has a relative minus sign compared to the Hamiltonian shown in the Eq. (2.5). This
appears to break the translation invariance. However, Eq. (2.6) can be made translation invariant by transforming all the fermion operators as

\[
\begin{align*}
C_n & \rightarrow e^{i\pi/N} C_n \\
C_n^+ & \rightarrow e^{-i\pi/N} C_n^+
\end{align*}
\]

which distributes the minus sign at the boundary over all the sites equally. As \( N \rightarrow \infty \), such a transformation produces a vanishingly small change in the single-particle energies.

The system size \( N \) is chosen to be 100 spins. The constant \( c \) in the final term in the Hamiltonian (2.6) showing the harmonic energy of the lattice is set equal to unity. The lattice constant \( l \) is also fixed to be unity so that all lengths which are multiples of the lattice constant are now just integers. In order to obtain the single-particle energies for any particular magnetization or any particular filling of Jordan-Wigner fermions, \( N_F \), of the ground-state, it is necessary to obtain the set of bond displacements, \( \delta_{n+\frac{1}{2}} \)'s which minimize the Hamiltonian given in Eq. (2.6). The procedure followed to achieve this is

- Set all \( \delta_{n+\frac{1}{2}} \)'s to zero initially.
- Increment or decrement each \( \delta_{n+\frac{1}{2}} \) separately in steps of 0.0005 and change each of the remaining spins by 0.0005/99 with the reverse sign, so that for each such change the sum of all displacements continues to remain zero as required for a periodic lattice.
- Calculate the new ground-state energy for each such change and iterate in a loop running over all the lattice sites, so as to minimize the Hamiltonian.

Then the eigenvalues of the Hamiltonian with these bond displacements, \( \delta_{n+\frac{1}{2}} \)'s give the single-particle energies for the particular filling at zero temperature. The eigenfunctions similarly give the single-particle wave functions. The bond displacements and single-particle energies are obtained for all possible magnetizations, few interesting ones of which are shown in the following sections.
2.2.1 For zero magnetization (for \( N_F = 50 \))

The bond displacements for the case of zero magnetization, i.e., for \( N_F = 50 \), obtained by minimizing the Hamiltonian in Eq. (2.6) using the above procedure are shown in the lower part of Fig. (2.1). It can be seen that the value of the displacement of the bond alternates in sign between any two consecutive lattice spins with its magnitude remaining constant. This corresponds to dimerization of the lattice. The magnitude of each of the bond displacements, \( \delta \), is 0.0642.

![Graph showing bond displacements and expectation values of \( S_n^z \) for zero magnetization.](image)

Figure 2.1: The bond displacements and expectation values of \( S_n^z \) for zero magnetization.

The single-particle energy spectrum obtained by diagonalizing this Hamiltonian with these bond displacements is shown in Fig. (2.2). It is observed that

- There are an equal number of positive and negative energy levels.
- For every positive energy level there is a corresponding negative energy level which is equal in magnitude but opposite in sign.
Figure 2.2: The single-particle energy spectrum of the zero magnetization.

- Each level is doubly degenerate. Exceptions to this fact are the maximum level (1), the minimum level (-1), the largest negative level (-0.0642) and the smallest positive level (0.0642) which are non-degenerate.

- There is a gap between the largest negative level and smallest positive level which is twice of $\delta$. It is to be noted that all the quoted energies are in units of $J$.

The ground-state energy of this system is obtained by summing the lowest fifty levels i.e., all the states lying below the gap (negative energy states). This is the state of the system at zero temperature and its energy is -31.8634.

The upper half of Fig. (2.1) gives the variation of spin density with the site index. It can be seen that this remains constant at half throughout the chain as expected. Also the bond displacements, single-particle energies and spin densities remain independent of an applied magnetic field for small values of the field because the net magnetization in this case is zero.
2.2.2 For magnetization=1 (for $N_F=51$)

Figure 2.3: The bond displacements and expectation values of $S^z_n$ for magnetization=1.

The bond displacements for the case of 51 fermions i.e., one away from dimerization, obtained by minimizing the Hamiltonian in Eq. (2.6) for the case of zero magnetic field using the same procedure, are shown in the lower part of Fig. (2.3). It can be seen that the displacements of the bonds oscillate around the value zero and have an envelope whose periodicity is 50, their maximum magnitude being 0.058. The pattern obtained is similar to that of beats in sound waves.

The single-particle energy spectrum obtained in this case is shown in Fig. (2.4). The features of the spectrum that get modified compared to $N_F = 50$ are

- There is an increase in the number of non-degenerate levels by four. The doubly degenerate levels lying next to the non-degenerate levels of the last case become non-degenerate.
Figure 2.4: The single-particle energy spectrum for magnetization=1.

- The size of the energy gap existing between the greatest negative level and smallest positive level falls from 0.0128 to 0.02.

The ground-state energy of this system is now obtained by summing the lowest fifty one levels and its value is -31.8219.

The upper half of the Fig. (2.3) gives the variation of spin density with the site index. The pattern obtained is seen to be similar to that of bond displacements except that the spin density maximum occurs at the site where the bond displacement is minimum and the oscillations within each envelope remain always above the value half. Also, the area under each of these envelopes, say from \( n = 35 \) to \( n = 85 \), is half and the sum of the areas under the two envelopes is equal to unity. This implies the extra (51st) fermion distributes itself into these two envelopes with equal probability. Thus, the solitons with half integral spin are seen in the system.
2.2.3 For magnetization=49 (for $N_F=99$)

![Graph showing bond displacements and expectation values of $S_n^z$ for magnetization=49.](image)

Figure 2.5: The bond displacements and expectation values of $S_n^z$ for magnetization=49.

The bond displacements for the magnetization of the system being 49 or fermion filling being just one less than the maximum allowed, for the case of zero magnetic field are shown in the lower part of Fig. (2.5). It can be seen that the system has a single peak ($\sim 0.18$) in bond displacements localized over a small region chosen randomly by the system by spontaneously breaking the translation symmetry.

The upper half of Fig. (2.3) gives the variation of spin density with the site index. It can be seen that there is a dip in the spin density over the region where there is a peak in bond displacements, showing that there is a localization of the missing ($100^{th}$) fermion over a small region.
2.2.4 For \( N = 102 \), magnetization=18 (for \( N_F = 69 \))

The bond displacements for a system size of 102 spins, \( N_F \) being one away from trimerization i.e, 69, obtained by minimizing the Hamiltonian in Eq. (2.6) for the case of zero magnetic field are shown in the lower part of Fig. (2.6). The bond displacements of the lattice spins are seen to oscillate around the value zero, their maximum magnitude being 0.022 and have an envelope whose periodicity is 34. The pattern is similar to \( N_F = 51 \) case. Also, the single-particle energy spectrum is seen to be gapless in this case.

The upper half of Fig. (2.3) gives the variation of spin density with the site index. The pattern obtained is similar to that of bond displacements except that the spin density maximum occurs at the site where the bond displacement is minimum and oscillations within each envelope remain always above the value 0.667. Also, the area under each of these envelopes, say from \( n = 24 \) to \( n = 57 \), is 0.333 and sum of the areas under all three envelopes is unity. This
means that the extra (69th) fermion distributes itself into the three envelopes with equal probability. Thus, solitons with fractional (1/3) spin are seen here in the system.

### 2.3 Variation of ground-state magnetization with magnetic field

![Graph showing the variation of ground-state energy with magnetization](image.png)

Figure 2.7: The variation of ground-state energy with magnetization $m$ for zero magnetic field $h$.

The single-particle energy spectrum, the ground-state energies and the spin densities at zero temperatures are calculated for each of the magnetizations (0 to 50) possible in the system. Fig. (2.7) shows the variation of ground-state energy $E_0$ with magnetization $m$, with the magnetic field term set to zero in the Hamiltonian (2.6).

The variation of ground-state magnetization of the spin-Peierls system with magnetic field at zero temperature is now studied numerically, by
Figure 2.8: The variation of ground-state magnetization $m$ with magnetic field $h$.

varying the magnetic field $h$ from -1.1 to 1.1 in steps of 0.001 in the Zeeman term, $h \sum_{n=1}^{N} [C_{n}^{+}C_{n} - \frac{1}{2}]$, of the Hamiltonian (2.6). The ground-state energies for each of the possible magnetizations are calculated and the magnetization which minimizes the ground-state energy is identified for each value of the magnetic field. The plot in Fig. (2.8) shows the variation of ground-state magnetization $m$ with magnetic field $h$. It is seen that the saturation magnetic field of this system is 1.035 and above this, the system exists only in the ferromagnetic state.

2.4 Dimerized to uniform phase transition

The dimerized to uniform structural phase transition in the spin-Peierls system shown in figure (1.3) is obtained numerically, for the case of zero magnetic field ($h=0$) and zero magnetization ($m=0$, $N_{F}=50$), as discussed below.

By taking the bond displacements to be of the form $\delta_{n} = \delta(-1)^{n}$,
which is true for dimerized phase, the value of $\delta$ that minimizes the free energy is obtained for each non-zero temperature, by following the same procedure mentioned in section (2.2), except that free energy is minimized instead of the ground-state energy. The free energy $U$ at any temperature $T$, using the Fermi-Dirac statistics, is given by

$$U = -\frac{1}{k_BT} \sum_{n=1}^{n=N} \log [1 + \exp \left( \frac{E(n) - h}{k_BT} \right)] \quad (2.8)$$

where $E(n)$ are the single-particle energies at temperature $T$, and $k_B$ is the Boltzmann constant.

The step sizes chosen in varying the temperature and the magnitude of the bond displacement while minimizing the free energy are both equal to 0.0001. Fig. (2.9) shows the second order phase transition, the critical parameter being the magnitude of the bond displacement, $\delta$, plotted as a function of...
temperature, $T$. The critical temperature as obtained from the graph is 0.036. It is to be noted that though the system is 1D in the Hamiltonian (2.6) it still has a phase transition. This is because our calculation is equivalent to a mean-field theory which allows a non-zero displacement $\delta$. In a real CuGeO$_3$ system the interchain couplings justify this mean-field treatment and led to a finite temperature phase transition.

### 2.5 Calculation of the phonon frequencies

#### 2.5.1 Analytical method

In Section (2.2), single-particle energies were calculated assuming static lattice displacements. In this section, we will calculate the phonon frequencies using perturbation theory.

The simplified spin-Peierls Hamiltonian is given by the Eq. (2.6).

The $i^{th}$ bond displacement, $\delta_{i+\frac{1}{2}}$, is given by

$$\delta_{i+\frac{1}{2}} = -\lambda (u_{i+1} - u_i)$$

Now the first order change in the ground-state energy (at zero temperature) $E_0$ due to the displacement of $i^{th}$ bond proportional to $\frac{\partial E_0}{\partial \delta_{i+\frac{1}{2}}}$. This is zero since $E_0$ is calculated by minimizing $H$ in Eq. (2.6) with respect to all the bond displacements. Hence to realize the contribution of bond displacements to a change in the ground-state energy, we have to find the derivative of second order with respect to the bond displacements.

Defining the elements of the dynamical matrix $D$ to be

$$D_{i+\frac{1}{2}, j+\frac{1}{2}} = \frac{\partial^2 E_0}{\partial \delta_{i+\frac{1}{2}} \partial \delta_{j+\frac{1}{2}}}$$

where all the derivatives are evaluated at those values of $\delta$'s which are obtained by minimizing the Hamiltonian (2.6) [6]. Using this definition for $D$ we get the lattice Hamiltonian to be
Chapter 2. Numerical Results

\[ H_{ph} = \frac{1}{2} M \sum_i \ddot{u}_i^2 + \frac{1}{2} \sum_{i,j} D_{i+\frac{1}{2},j+\frac{1}{2}} \left[ \lambda(u_{i+1} - u_i) + \delta_{i+\frac{1}{2}}^{(0)} \right] \left[ \lambda(u_{j+1} - u_j) + \delta_{j+\frac{1}{2}}^{(0)} \right] \]  \hspace{1em} (2.9)

where \( u_i \) is the displacement of the ion at the lattice point \( i \), \( M \) its mass, \( \delta_{i+\frac{1}{2}}^{(0)} \) is the equilibrium value of \( \delta_{i+\frac{1}{2}} \) which minimizes the Hamiltonian and \( \lambda \) is the positive constant which is a measure of the coupling that exists between the lattice points and spins.

Now we define a transformation on displacements of lattice points as shown below,

\[ \tilde{u}_i = u_i - c_i \]  \hspace{1em} (2.10)

we see that with periodic boundary conditions, and with the choice \( c_1 = 0 \) we have

\[ \lambda(c_{i+1} - c_i) + \delta_{i+\frac{1}{2}}^{(0)} = 0 \]

since \( \sum_i \delta_{i+\frac{1}{2}} = 0 \).

Writing the lattice Hamiltonian (2.9) in terms of \( \tilde{u}_i \)'s, thus simplifies it to the form

\[ H_{ph} = \frac{1}{2} M \sum_i \ddot{\tilde{u}}_i^2 + \frac{\lambda^2}{2} \sum_{i,j} \tilde{D}_{i,j}(\tilde{u}_{i+1} - \tilde{u}_i)(\tilde{u}_{j+1} - \tilde{u}_j) \]  \hspace{1em} (2.12)

Simplifying it further by defining

\[ \tilde{D}_{i,j} = D_{i-\frac{1}{2},j-\frac{1}{2}} + D_{i+\frac{1}{2},j+\frac{1}{2}} - D_{i-\frac{1}{2},j+\frac{1}{2}} - D_{i+\frac{1}{2},j-\frac{1}{2}} \]  \hspace{1em} (2.11)

we get the lattice Hamiltonian \( H_{ph} \) (2.9) to be

\[ H_{ph} = \frac{1}{2} M \sum_i \ddot{\tilde{u}}_i^2 + \frac{\lambda^2}{2} \sum_{i,j} \tilde{D}_{i,j}\tilde{u}_i\tilde{u}_j \]  \hspace{1em} (2.12)
Now the frequency, $\omega_i$, of the $i^{th}$ phonon, (proportional to its energy) is given by

$$\omega_i = \lambda \sqrt{\frac{\mu_i}{M}} \quad (2.13)$$

where $\mu_i$ is the $i^{th}$ eigenvalue of the transformed dynamical matrix, $\tilde{D}$, and $M$ is the mass of each lattice point [6].

![Figure 2.10: Square root of eigenvalues of the transformed dynamical matrix for the system in dimerized phase.](image)

The transformed dynamical matrix for the dimerized phase is evaluated assuming bond displacements of the form $\delta_i = \delta(-1)^i$ and the root of the eigenvalues of the corresponding Hamiltonian are plotted in an increasing order as shown in Fig. (2.10). This curve gives the phonon dispersion for the dimerized phase accurate upto a constant factor given by Eq. (2.13) [8]. While evaluating the elements of the transformed dynamical matrix, various symmetries like inversion symmetry about the bonds, translational symmetry of lattice
points, etc., are used to generate all the elements from just the first few rows or columns.

2.5.2 Numerical method

The eigenfunctions of the Hamiltonian, $H$ for the case of dimerized phase (zero magnetization) are used to evaluate the transformed dynamical matrix using the second order perturbation theory as shown below

$$ D(m,n) = \sum_{j,k} \left[ \frac{<n+1|H|n><n|H|n+1> + <m+1|H|m><m|H|m+1>}{E(j) - E(k)} \right] $$

(2.14)

where $N$ is the system size, $j$ represents an occupied single-particle state and takes the values from 1 to 50, $k$ represents an unoccupied single-particle state and ranges from 51 to 100, $E(j)$ and $E(k)$ denote the single-particle energies, $m$ and $n$ denote the site numbers with $|m>$ representing a state in which the $m^{th}$ site is occupied. While most of the matrix elements of $D$ obtained using the above equation are found to agree very well with those determined by the analytical method described in the previous section, a few off-diagonal elements are seen to differ slightly.
Chapter 3

Analytical Methods

3.1 Uniform phase

The Hamiltonian for the system in uniform phase is given by

\[
H = -\frac{J}{2} \sum_{n=1}^{N-1} [C_n^+ C_{n+1} + C_{n+1}^+ C_n] + (-1)^{N_F} [C_N^+ C_1 + C_1^+ C_N] \\
+ \frac{c}{2} \sum_{n=1}^{N} \delta_{n+\frac{1}{2}}^2.
\]  (3.1)

This is obtained by setting each \( \delta_{n+\frac{1}{2}} \) and also the total magnetization, \( m \), to zero in (2.6). The single-particle energy spectrum of this Hamiltonian is obtained by taking the discrete Fourier transform for this equation [9, 10]. This is given by \( e_k = -J \cos(k) \), where \( k \) is the Fourier momentum and is shown in the left half of Fig. (3.1). In the plot, the value of exchange integral \( J \) is chosen to be unity. Also the lattice constant \( l \) of uniform phase is set to unity all throughout this report. Imposing periodic boundary conditions on the system, \( k \) assumes the form \( k = 2\pi n/N \) where \( N \) is the system size and \( n \) takes values from 0 to \( N - 1 \).

The ground-state energy of the system per site at zero temperature, \( E_k \) is now obtained by summing the lower half of the energy spectrum and dividing it by the system size \( N \), and is found to be \(-J/\pi\).
3.2 Dimerized phase

In dimerized phase, the bond displacements are of the form $\delta_{n+\frac{1}{2}} = (-1)^n \delta$. The total magnetization of the system remains zero. The Hamiltonian of the system is shown in (3.2).

$$H = -\frac{J}{2} \sum_{n=1}^{N-1} [1 + (-1)^n \delta] \left[ C_n^+ C_{n+1} + C_{n+1}^+ C_n \right] + (-1)^N \left[ C_N^+ C_1 + C_1^+ C_N \right] + \frac{c}{2} \sum_{n=1}^{N} \delta^2. \quad (3.2)$$

The Hamiltonian can be solved using the translation symmetry by redefining the size of unit cell in the dimerized phase to be twice that of the uniform phase and then applying the continuous Fourier transform as shown below. In equation (3.2), $A_k, B_k$ represents the annihilation operators for fermions.
with momentum \( k \) associated with first and second of the pair of lattice points present in the unit cell respectively and their Hermitian conjugates represent the respective creation operators.

\[
H = \int_{-\pi}^{\pi} \frac{dk}{4\pi} \left[ A_k^+ B_k^+ \right] \begin{bmatrix}
0 & -\frac{J+\delta}{2} & \frac{J-\delta}{2} e^{ik}\\
-\frac{J+\delta}{2} & \frac{J-\delta}{2} e^{-ik} & 0
\end{bmatrix} \begin{bmatrix}
A_k \\ B_k
\end{bmatrix} \tag{3.3}
\]

The single-particle energy spectrum \( e_k \), of this Hamiltonian is given by

\[
e_k = \pm \sqrt{\frac{J^2 + \delta^2}{2}} \sqrt{1 + \frac{J^2 - \delta^2}{J^2 + \delta^2} \cos k} \tag{3.4}
\]

where \( k \) goes from \(-\pi\) to \( \pi \) as shown in right half of Fig. (3.1). In the plot, exchange integral \( J \) is set to unity. The ground-state energy of the system in this dimerized phase at zero temperature is calculated in the following section.

### 3.2.1 Ground-state energy

The total energy of the ground-state is obtained by summing all the negative energy states. From last section, it can be seen that the crystal momentum \( k \) takes values from \(-\pi\) to \( \pi \). Hence, the Ground-state energy per site, \( E_d \) is given by

\[
E_d = -\frac{J b}{4\pi \sqrt{2}} \int_{-\pi}^{\pi} dk \sqrt{1 + a \cos k}
\]

where

\[
a = 1 - \frac{2\delta^2}{J^2} \\
b = 1 + \frac{\delta^2}{2J^2} \tag{3.5}
\]

This is an elliptical integral of the second kind. Using the series approximation for this integral and truncating the series to the quadratic power of \((\delta/J)\),

\[
E_d = -\frac{J}{\pi} \sqrt{1 - \frac{\delta^2}{J^2}} \epsilon(1 - \frac{J}{\delta})
\]
\[ \approx -\frac{J}{\pi} \left[ 1 - \frac{\delta^2}{J^2} \left( \frac{1}{2} - a_1 + 2b_1 \log\left( \frac{J}{\delta} \right) \right) \right] \]
\[ \approx -\frac{J}{\pi} \left[ 1 + \frac{\delta^2}{J^2} 2b_1 \log\left( \frac{J}{\delta} \right) \right] \]

where \( \epsilon(1 - \frac{J}{\delta}) = 1 + a_1 \left( \frac{\delta^2}{J^2} \right) - 2b_1 \left( \frac{\delta^2}{J^2} \right) \log\left( \frac{J}{\delta} \right) \)

and \( a_1 \approx 0.46301, \ b_1 \approx 0.24527 \) \( (3.6) \)

Thus, the ground-state energy of the system in dimerized phase is lower compared to that of uniform phase for sufficiently smaller values of \( \delta/J \) and hence dimerization occurs.

### 3.3 Modeling the bond displacements for the case of magnetization=49 \( (N_F = 99) \)

The Hamiltonian for the spin-Peierls system at zero temperature is shown in \( (2.4) \). In the continuum limit, the eigenfunctions of this are of the form \( \psi_n = e^{in(\pi+k)} \) where the lattice spacing is chosen to be unity and the magnetic field, \( h \), is taken to be zero. Substituting this in the above Hamiltonian, we get

\[ E_0 = \frac{1}{2} (1 + \delta_{n+\frac{1}{2}}) (e^{i(k+\pi)} + e^{-i(k+\pi)}) \]
\[ = -\left( 1 + \delta_{n+\frac{1}{2}} \right) \cos k \]
\[ \approx -1 + v(x) + \frac{k^2}{2} \] \( (3.7) \)

where \( E_0 \) is the energy eigenvalue corresponding to \( \psi_n \) and \( v(x) = -\delta_{n+\frac{1}{2}} \). It is to be noted that in the following discussion the lattice label \( n \) is replaced by the continuum label \( x \) whenever convenient.

Using this form of \( \delta_{n+\frac{1}{2}} \) in the Hamiltonian \( (2.7) \) we get

\[ H = -1 - \frac{1}{2} \partial^2 + v(x) + \frac{c}{2} \int dx \ v^2(x) \] \( (3.8) \)
subject to the constraint \( \int dv(x) = 0 \).

The minimum energy solution of this Hamiltonian, (3.8), is obtained using a trial function \( \psi(x) = 1/\cosh(\alpha x) \) where \( \alpha > 0 \). Consequently, it reduces to

\[
\frac{\tilde{e}_0}{\cosh(\alpha x)} = \frac{-1}{\cosh(\alpha x)} - \frac{1}{2} \left( \frac{\alpha^2}{\cosh(\alpha x)} - \frac{2\alpha^2}{\cosh^3(\alpha x)} \right) + \frac{v(x)}{\cosh(\alpha x)} + \left( \frac{c}{2} \int dy \ v^2(y) \right) \frac{1}{\cosh(\alpha x)} \]

(3.9)

Hence we choose \( v(x) = -\alpha^2/\cosh^2(\alpha x) \). Then matching the coefficient of \( \psi(x) = 1/\cosh(\alpha x) \) on the two sides gives the equation

\[
\tilde{e}_0 = -1 - \frac{\alpha^2}{2} + \frac{c\alpha^3}{2} \int_{-\infty}^{\infty} dt \frac{1}{\cosh^4 t} \]

\Rightarrow \tilde{e}_0 = -1 - \frac{\alpha^2}{2} + \frac{2c\alpha^3}{3} \]

(3.10)

The minimum energy of \( \tilde{e}_0 \) is attained when \( \alpha = \frac{1}{2c} \) and it is equal to \( -1 - \frac{1}{24c^2} \) and the corresponding \( v(x) = -\delta_{n+\frac{1}{2}} = -1/4c^2 \cosh^2(\frac{x}{2c}) \). For \( c = 1 \), this value is equal to -1.125. From section (2.2.3), numerically this value is found to be -1.091. This discrepancy in the value of \( v(x) \) arises because the continuum approximation is valid only for \( c >> 1 \). Also it can be noted that

\[
\sum_n \delta_{n+\frac{1}{2}} = \int_{-\infty}^{\infty} \frac{dx}{4c^2 \cosh^2(\frac{x}{2c})} = \frac{1}{c} \]

(3.11)

So in a finite system with \( N \) sites where \( N >> c \), we introduce a Lagrangian multiplier in Eq. (3.8 to enforce the constraint \( dx f v(x) = 0 \). We then find \( \delta_{n+\frac{1}{2}} = -\frac{1}{Nc} \) for \( n >> c \) instead of \( \delta_{n+\frac{1}{2}} = 0 \). Then

\[
\tilde{e}_0 = -1 - \frac{1}{24c^2} + \frac{1}{2Nc^2} \]

(3.12)
It can be verified that this solution for $\psi(x)$ is indeed the minimum energy solution since the first order change in Hamiltonian (3.1) is zero. The analytical function of $\delta_{n+\frac{1}{2}}$ obtained here agrees perfectly well with the lower curve in Fig. (2.5) for the values $c = 1, N = 100$. 
Chapter 4

Scope for future work

4.1 Finite temperature calculations

All the ground-state energies and eigenfunctions for the magnetizations discussed in section (2.2) are calculated at zero temperature. An attempt is made to extend these calculations using the same algorithm to non-zero temperatures using Fermi statistics as shown below. The free-energy $U$ at temperature $T$ is now given by

$$U = -\frac{1}{k_B T} \sum_{n=1}^{N} \log [1 + \exp\left( \frac{E(n) - \hbar}{k_B T} \right)]$$

(4.1)

where $E(n)$ are the single particle energies at temperature $T$ obtained after minimizing the Hamiltonian (2.6) and $k_B$ is the Boltzmann constant [8]. However, it is noticed that convergence in finding the set of lattice displacements which minimize the free-energy could not be achieved. Also, the same problem was encountered while calculating the single particle energies and eigenfunctions for low-lying excited states at zero temperature. A Solution is yet to be found to overcome this problem. This is required to obtain the complete phase diagram and compare it with Fig. (1.3).
4.2 Calculation of change in eigenfunctions due to dynamical phonons

In section (2.2), a procedure has been detailed to evaluate all the eigenfunctions assuming the lattice points to be static. The phonon frequencies are then calculated in section (2.5) to leading order in lattice displacements by using perturbation theory. The corrections to the unperturbed eigenfunctions due to these phonons can thereafter be obtained self-consistently. Work to accomplish this is in progress. This will give a more accurate picture of the soliton profile in the presence of dynamical phonons. For instance, the soliton profiles shown in Figs. (2.3) and (2.6) which do not take phonons into account now get modified.

4.3 Modeling the lattice spin displacements for all possible magnetizations

The lattice spin displacements for all possible magnetizations can be modelled by adopting a procedure similar to the one discussed in section (3.3). A trial function for the lattice displacements is used to minimize the Hamiltonian for that particular magnetization. The necessary constraints required to be satisfied are incorporated in this equation using Lagrangian multipliers. By comparing the analytical shapes of the bond displacements with those observed numerically, one can find the value of the lattice-spin coupling parameter $\lambda$.

4.4 Inclusion of the $S^n_z S^z_{n+1}$ term in the Hamiltonian

As detailed in section (2.2.1), for all calculations in this report the generalised Heisenberg spins in the full Hamiltonian (1.1) are replaced by the XY spins. This is done to simplify the calculations without qualitatively affecting the phase diagram. However, a more realistic picture requires the inclusion of the spin-spin interactions in the $z$ direction which on Jordan-Wignerization become four fermion interactions [4, 5]. Techniques like the density matrix renormalisation group and bosonization can be employed to study the Hamiltonian of such a system [3].
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