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Condensed Matter Theory - Lecture Notes
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Theory & Notes

1. XX-MODEL

Consider the XX-Heisenberg model, with its Hamiltonian given in terms of the traditional $\frac{1}{2}$-spin operators ie.

$$\mathbf{H} = J\sum_{i=1}^{L}(\mathbf{S}_j^x\mathbf{S}_{j+1}^x + \mathbf{S}_j^y\mathbf{S}_{j+1}^y) - \lambda\sum_{j=1}^{L}\mathbf{S}_j^z, \tag{1}$$

which describes interacting spins in a one-dimensional chain, with periodic boundary conditions. (1)'s first terms represents nearest neighbour interactions in the x and $y-$directions interactions, with J being either positive or negative and quantifying the strength and type of interactions, while the second term represents a magnetic field of strength λ, applied in the z-direction of the spins.

In order to solve this problem, it is necessary to rewrite (1) and apply a Jordan-Wigner transformation, mapping the spin problem into a fermionic problem. But first, it is convenient to write the spin-operators in terms of the raising and lowering $\mathfrak{su}(2)$-operators, ie.

$$\mathbf{S}_j^{\pm} = \mathbf{S}_j^x \pm i\mathbf{S}_j^y \;\Rightarrow\; \begin{array}{c} \mathbf{S}_j^x = \frac{1}{2}(\mathbf{S}_j^+ + \mathbf{S}_j^-), \\ \mathbf{S}_j^y = \frac{1}{2i}(\mathbf{S}_j^+ - \mathbf{S}_j^-). \end{array}$$

Then, the XX-Hamiltonian can be re-written as

$$\mathbf{H} = \frac{J}{2}\sum_{i=1}^{L}(\mathbf{S}_j^+\mathbf{S}_{j+1}^- + \mathbf{S}_j^-\mathbf{S}_{j+1}^+) - \lambda\sum_{j=1}^{L}\mathbf{S}_j^z \tag{2}$$

where the interacting terms in the first summation, flip neighboring spins if said spins are anti-aligned[1]. In addition, the XX-Hamiltonian has a total magnetization symmetry, since the Hamiltonian given by (2) conmutes with the magnetization operator.

Now, we use a Jordan-Wigner transformation whereby the spin operators are mapped to fermionic operators, as follows

[1]In effect, consider for example, a two-spin problem. Then, the interaction term is given by

$$\mathbf{S}_1^+\mathbf{S}_2^- + \mathbf{S}_1^-\mathbf{S}_2^+,$$

and consider an anti-aligned state $|\downarrow\uparrow\rangle$. Then, the action of the previous two-spin operator over this state yields

$$(\mathbf{S}_1^+\mathbf{S}_2^- + \mathbf{S}_1^-\mathbf{S}_2^+)\,|\downarrow\uparrow\rangle = |\uparrow\downarrow\rangle + 0,$$

since $\mathbf{S}_1^-\mathbf{S}_2^+$ destroys the state. Similarly, $(\mathbf{S}_1^+\mathbf{S}_2^- + \mathbf{S}_1^-\mathbf{S}_2^+)\,|\uparrow\downarrow\rangle = |\downarrow\uparrow\rangle$. However, note that, should both spins be either up or down, the state remain invariant under the action of the two-spin operator.

$$(\mathbf{S}_1^+\mathbf{S}_2^- + \mathbf{S}_1^-\mathbf{S}_2^+)\,|\downarrow\downarrow\rangle = |\downarrow\downarrow\rangle \text{ and } (\mathbf{S}_1^+\mathbf{S}_2^- + \mathbf{S}_1^-\mathbf{S}_2^+)\,|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle \tag{3}$$

$$\mathbf{S}_j^z = f_j^\dagger f_j - \tfrac{1}{2}$$

(4) $$\mathbf{S}_j^- = \exp\Big(i\pi \textstyle\sum_{\ell=1}^{L-1} f_\ell^\dagger f_\ell\Big)$$

$$\mathbf{S}_j^+ = \exp\Big(-i\pi \textstyle\sum_{\ell=1}^{L-1} f_\ell^\dagger f_\ell\Big)$$

Under the Jordan-Wigner map, nearest-neighbours spin flipping is translated into to nearest-neighbours fermionic hopping, ie. $\mathbf{S}_j^+\mathbf{S}_{j+1}^- = f_j^\dagger f_{j+1}$ and $\mathbf{S}_j^-\mathbf{S}_{j+1}^+ = f_{j+1}^\dagger f_j$. However, due to the boundary conditions' periodicity, the XX-Hamiltonian cannot be rewritten as a fermionic model yet since (it will contain an additional boundary term), for example, the fermionic counterparts to the $\mathbf{S}_L^+\mathbf{S}_1^-$ interaction are highly non-local operators and are not desirable. Indeed, under the Jordan-Wigner mapping

$$\mathbf{S}_L^+\mathbf{S}_1^- = f_L^\dagger \exp\Big(-i\pi \sum_{\ell=1}^{L-1} f_\ell^\dagger f_\ell\Big) f_1,$$

which is not problematic, since it accounts for all L-lattice sites. Let

(5) $$\begin{aligned}\mathbf{S}_L^+\mathbf{S}_1^- &= \mathcal{Q} f_L^\dagger f_1,\\ \mathbf{S}_L^-\mathbf{S}_1^+ &= \mathcal{Q} f_1^\dagger f_L,\end{aligned}$$

then (2) can be rewritten as

(6) $$\mathbf{H} = \frac{J}{2}\sum_{i=1}^{L-1}\Big(f_j^\dagger f_{j+1} + f_{j+1}^\dagger f_j\Big) - \lambda\sum_{j=1}^{L}\Big(f_j^\dagger f_j - \frac{1}{2}\Big) + \frac{J}{2}\mathcal{Q}(f_L^\dagger f_1 + f_1^\dagger f_L),$$

where the first term accounts for fermionic nearest-neighbour hopping, the second term accounts for the magnetic field, and the third term being the non-local boundary term. Note that this fermionic Hamiltonian hasn't got any type of boundary conditions, since the L-lattice site is disconnected in any way whatsoever from the first lattice site. Then, the standard procedure is to add and subtract terms from the Hamiltonian, so that the nearest-neighbour hopping term in (6) can also have periodic boundary conditions, thus yielding

(7) $$\mathbf{H} = \frac{J}{2}\sum_{i=1}^{L}\Big(f_j^\dagger f_{j+1} + f_{j+1}^\dagger f_j\Big) - \lambda\sum_{j=1}^{L}\Big(f_j^\dagger f_j - \frac{1}{2}\Big) + \frac{J}{2}(\mathcal{Q}-1)(f_L^\dagger f_1 + f_1^\dagger f_L),$$

where now the fermionic hopping term has the standard boundary conditions. The third term, since it does not involve any type of summation over lattice sites, only contributes at $\mathcal{O}\Big(\frac{1}{L}\Big)$-order to any microscopic quantity. In the thermodynamic limit, this non-local term can be dropped, thus yielding an $\mathcal{O}(L)$-Hamiltonian given by

(8) $$\mathbf{H} = \frac{J}{2}\sum_{i=1}^{L}\Big(f_j^\dagger f_{j+1} + f_{j+1}^\dagger f_j - \lambda f_j^\dagger f_j\Big) + \frac{\lambda L}{2},$$

which is now fully cyclic and where its operators obey fermionic algebras. This Hamiltonian can then be diagonalized via a discrete Fourier transform on the fermionic operators

(9) $$f_j = \frac{1}{\sqrt{L}}\sum_{\substack{k=2\pi m/L\\ m\in\mathbb{Z}_{[1,L]}}} e^{ijk} d_k, \qquad f_j^\dagger = \frac{1}{\sqrt{L}}\sum_{\substack{k=2\pi m/L\\ m\in\mathbb{Z}_{[1,L]}}} e^{-ijk} d_k^\dagger,$$

with the inverse transformation given by

$$d_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ikj} f_j \qquad d_k^\dagger = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikj} f_j^\dagger. \tag{10}$$

Note that the d_k-operators follow the standard fermionic anticonmutation algebra. Note as well, that the f_j-vacuum state, defined such that $f_j |0\rangle_f = 0,\ \forall j$, is the same as the d_k-vacuum state, defined such that $d_j |0\rangle_d = 0,\ \forall k$, ie. $|0\rangle_f = |0\rangle_d$. Another important relationship is the Fourier transform's consistency condition, ie.

$$\sum_{j=1}^{L} e^{i(k-q)j} = L\delta_{kq}.$$

Under the Fourier transform, (8)'s terms are mapped as follows

$$\begin{aligned}
\sum_{j=1}^{L} f_j^\dagger f_{j+1} &= \sum_{j=1}^{L} \frac{1}{L} \sum_{k,\,q} e^{-ikj} e^{iq(j+1)} d_k^\dagger d_q = \sum_{j=1}^{L} \frac{1}{L} \sum_{k,\,q} e^{i(q-k)j} e^{iq} d_k^\dagger d_q \\
&= \sum_{k,\,q} \frac{1}{L} e^{iq} \delta_{qk} d_k^\dagger d_q = \sum_k e^{ik} d_k^\dagger d_k \\
\sum_{j=1}^{L} f_{j+1}^\dagger f_j &= \sum_{j=1}^{L} \frac{1}{L} \sum_{k,\,q} e^{-ik(j+1)} e^{iqj} d_k^\dagger d_q = \sum_{j=1}^{L} \frac{1}{L} \sum_{k,\,q} e^{i(q-k)j} e^{-ik} d_k^\dagger d_q \\
&= \sum_{k,\,q} \frac{1}{L} e^{-ik} \delta_{qk} d_k^\dagger d_q = \sum_k e^{-ik} d_k^\dagger d_k \\
\sum_{j=1}^{L} f_j^\dagger f_j &= \sum_{j=1}^{L} \frac{1}{L} \sum_{k,\,q} e^{-ikj} e^{iqj} d_k^\dagger d_q = \sum_{j=1}^{L} \frac{1}{L} \sum_{k,\,q} e^{i(q-k)j} d_k^\dagger d_q \\
&= \sum_{k,\,q} \frac{1}{L} \delta_{qk} d_k^\dagger d_q = \sum_k d_k^\dagger d_k
\end{aligned}$$

Therefore, using these identities, the new Hamiltonian is given by

$$\mathbf{H} = \frac{J}{2} \sum_k \left(e^{ik} d_k^\dagger d_k + e^{-ik} d_k^\dagger d_k - \lambda d_k^\dagger d_k \right) + \frac{\lambda L}{2} \tag{11}$$

$$= \sum_k \left(J \cos k - \lambda \right) d_k^\dagger d_k + \frac{\lambda L}{2}, \tag{12}$$

which can be rewritten as

(13)

$$\boxed{\mathbf{H} = \sum_k \epsilon_k d_k^\dagger d_k + \frac{\lambda L}{2} \quad \begin{array}{c} \text{with the eigenvalues being given by } \epsilon_k = J\ cosk - \lambda + \frac{\lambda L}{2} \\ \text{and the eigenvectors being given by } |E_n\rangle = \prod_n (d_k^\dagger)^n, \text{ with eigenvalue } E_n = \sum_n \epsilon_n \end{array}},$$

thus the problem has been solved.

As for its thermal properties, since this is a fermionic model, the fermions will obey the Fermi-Dirac distribution, ie.

$$\mathcal{N}_{jk} = \langle d_j^\dagger d_k \rangle_{\text{th}} = \frac{1}{1 + e^{\beta\epsilon_k + \mu}} \delta_{jk}. \tag{14}$$

2. NUMERICAL SOLUTION TO FERMIONIC MODELS

Consider a Hamiltonian describing a fermionic system, given by

$$\mathbf{H} = J\sum_{j=1}^{L-1}(f_j^\dagger f_{j+1} + f_{j+1}^\dagger f_j) + \sum_{j=1}\lambda_j f_j^\dagger f_j, \quad \text{with the usual conmutation rules} \quad \begin{array}{c}\{f_j, f_k\} = \{f_j^\dagger, f_k^\dagger\} = 0 \\ \{f_j, f_k^\dagger\} = \delta_{jk}\end{array} \tag{15}$$

where L indicates the number of lattice sites, J is the hopping strength, which could be either positive or negative, and where λ_j is the on-site potential strength[2]. Said Hamiltonian has open boundaries conditions since there is no hopping term across the boundary. Note that we can rewrite (15) as

$$\mathbf{H} = \sum_{i,j=1}^{L}\mathcal{M}_{ij}f_i^\dagger f_j \text{ with } \begin{array}{c}\mathcal{M}\in \mathrm{GL}(L,\mathbb{R}), \\ \mathcal{M}_{ij} = \begin{cases}\lambda_i & \text{if } i=j \\ J & \text{if } j=i+1 \text{ or } i=j+1 \\ 0 & \text{otherwise}\end{cases}\end{array}, \tag{16}$$

which is a positive-defined tri-diagonal matrix. Let $\mathbf{f} = (f_1\ f_2\ \cdots\ f_L)^{\mathbf{T}}$ be a vector of the L fermionic operators. Then, (15) can be rewritten as

$$\mathbf{H} = \mathbf{f}^\dagger\mathcal{M}\mathbf{f}. \tag{17}$$

Since $\mathcal{M}$ is symmetric, then it can be diagonalized $\mathcal{M} = A\mathcal{D}A^{\mathbf{T}}$, where $A\in\mathbb{R}^{L\times L}$ is a real orthogonal matrix and with $\mathcal{D}_{ij}\in\mathbb{R}^{L\times L} \mid \mathcal{D}_{ij} = \epsilon_i\delta_{ij}$. In this context, the A-matrix acts on the fermionic operator as a Bogoliubov transformation, allowing for (15) to be rewritten as

$$\mathbf{H} = \mathbf{f}^\dagger A\mathcal{D}A^{\mathbf{T}}\mathbf{f} = \mathbf{d}^\dagger\mathcal{D}\mathbf{d} \tag{18}$$

where $\mathbf{d} = A^{\mathbf{T}}\mathbf{f}$. Since the A-matrix is orthogonal, the new d_k-operators are fermionic operators as well, satisfying (15)'s anti-commutation rules. Then, the new fermionic operators are

$$\begin{array}{c} d_k = \sum_{j=1}^{L}A_{jk}f_j \\ \\ f_j = \sum_{k=1}^{L}A_{jk}d_k\end{array} \quad \text{since } A^{\mathbf{T}}A = \sum_{j,k=1}^{L}A_{jk}A_{kj} = \mathbb{1}_L.$$

Then, we can expand (18) in terms of the lattices, as follows

$$\mathbf{H} = \sum_{k=1}^{L}\epsilon_k d_k^\dagger d_k, \tag{19}$$

which is a sum of number operators with potentials. The eigenstates can then be constructed from the the theory's vacuum state, by applying the $d_k^\dagger$-fermionic operators. In the Heisenberg-picture, the d_k-operators can be evolved via the Heisenberg equation of motion

$$\frac{d}{dt}d_k = i[\mathbf{H}, d_k], \tag{20}$$

and using that $d_k^2 = 0$, it turns out that (20)'s solution is simply $d_k(t) = e^{-i\epsilon_k t}d_k$. The system's correlation can be easily found by analyzing the following matrix. Let $\mathcal{N}_{jk} = \langle d_j^\dagger d_k\rangle$, where the expectation value is taken via calculating the operator's trace along the Fock space, which takes the following values

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[2]The λ_j-term frequently appears in many condensed matter models, with different numerical values and interpretations, eg.

- In the XX model, $\lambda_j = \lambda\ \forall j$.
- While for the Anderson model $\lambda_j \in \mathcal{U}_{\mathbb{R}_{[-W,W]}}$, a uniform random variable, with W being the disorder strength.
- In the Aubry-André model, $\lambda_j = \lambda\cos(2\pi\sigma j)$, with $\sigma\in\mathbb{I}$ and λ quantifying the disorder strength.

$$\mathcal{N}_{jk} = \langle d_j^\dagger d_k \rangle = \begin{cases} 0 \text{ or } 1 \text{ if } j = k \\ 0 \text{ if } j \neq k \end{cases}, \tag{21}$$

ie. different lattice-sites are not correlated and there can only be a single fermion at most per lattice site, in accordance with Pauli's principle. A ground state, for example, would choose to turn on all fermions in the eigenmode d-space such that $\epsilon_k < 0$. If instead, the expectation value is taken with thermal states, the Fermi-Dirac distribution is returned,

$$\mathcal{N}_{jk} = \langle d_j^\dagger d_k \rangle_{\text{th}} = \frac{1}{1 + e^{\beta\epsilon_k + \mu}} \delta_{jk}. \tag{22}$$

Another interesting quality is a system with an initial configuration where the system's initial state, in real space, is known. In this setting, $\mathcal{N}_{jk}$ is known for all lattices. Consider for example the Anderson model, where the system's initial state is given by a single tensor product of n-fermionic states in real space, with $n < L$. Then, for all lattice sites, we have that $\mathcal{N}_{jj}$ is either zero or one. The $\mathcal{N}_{jk}$-matrix entries can then be evaluated as

$$\langle d_j^\dagger d_k \rangle = \sum_{i,j=1}^{n<L} A_{ik} A_{jl} \langle f_i^\dagger f_j \rangle = \sum_{j=1} A_{jk} A_{jl} \langle f_j^\dagger f_j \rangle,$$

which can then be numerically computed to obtain the LHS expectation value. In general, this $\mathcal{N}_{jk}$-matrix will not be diagonal, which is reasonable since the system's real configuration is not an eigenstate. In principle and in practice, by inverting (23), we can evolve any number operator or two-body correlation operator, ie.

$$\langle f_j^\dagger f_k \rangle = \sum_{k,l=1}^{n} A_{jk} A_{jl} \langle d_k^\dagger d_l \rangle. \tag{23}$$

This quantities' time evolution can then be found out to be

$$\langle f_j^\dagger(t) f_k(t) \rangle = \sum_{k,l=1}^{L} e^{i(\epsilon_k - \epsilon_l)t} A_{jk} A_{jl} \langle d_k^\dagger d_l \rangle, \tag{24}$$

which can then be numerically solved.