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Condensed Matter Theory - Lecture Notes
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Theory & Notes

1. Numerical solution to Fermionic models

Consider a Hamiltonian describing a fermionic system, given by

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

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[1]. Said Hamiltonian has open boundaries conditions since there is no hopping term across the boundary. Note that we can rewrite (1) as

$$\mathbf{H} = \sum_{i,j=1}^{L}\mathcal{M}_{ij}f_i^\dagger f_j \text{ with } \begin{matrix}\mathcal{M}\in \mathrm{GL}(L,\mathbb{R}),\\ \mathcal{M}_{ij} = \begin{cases}\lambda_i & \text{if } i=j\\ J & \text{if } j=i+1 \text{ or } i=j+1\\ 0 & \text{otherwise}\end{cases},\end{matrix} \tag{2}$$

which is a positive-defined tri-diagonal matrix. Let $\mathbf{f} = (f_1\ f_2\ \cdots f_L)^{\mathrm{T}}$ be a vector of the L fermionic operators. Then, (1) can be rewritten as

$$\mathbf{H} = \mathbf{f}^\dagger\mathcal{M}\mathbf{f}. \tag{3}$$

Since $\mathcal{M}$ is symmetric, then it can be diagonalized $\mathcal{M} = A\mathcal{D}A^{\mathrm{T}}$, 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 (1) to be rewritten as

$$\mathbf{H} = \mathbf{f}^\dagger A\mathcal{D}A^{\mathrm{T}}\mathbf{f} = \mathbf{d}^\dagger\mathcal{D}\mathbf{d} \tag{4}$$

where $\mathbf{d} = A^{\mathrm{T}}\mathbf{f}$. Since the A-matrix is orthogonal, the new d_k-operators are fermionic operators as well, satisfying (1)'s anti-commutation rules. Then, the new fermionic operators are

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

Then, we can expand (4) in terms of the lattices, as follows

$$\mathbf{H} = \sum_{k=1}^{L}\epsilon_k d_k^\dagger d_k, \tag{5}$$

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

[1] 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.

$$\frac{d}{dt}d_k = i[\mathbf{H}, d_k], \tag{6}$$

and using that $d_k^2 = 0$, it turns out that (6)'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

$$\mathcal{N}_{jk} = \langle d_j^\dagger d_k\rangle = \begin{cases} 0 \text{ or } 1 \text{ if } j = k \\ 0 \text{ if } j \neq k \end{cases}, \tag{7}$$

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,

$$\mathcal{N}_{jk} = \langle d_j^\dagger d_k\rangle_{\text{th}} = \frac{1}{1 + e^{\beta\epsilon_k + \mu}}\delta_{jk}. \tag{8}$$

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 (9), we can evolve any number operator or two-body correlation operator, ie.

$$\langle f_j^\dagger f_k\rangle = \sum_{k,l=1}^{n} A_{jk}A_{jl}\langle d_k^\dagger d_l\rangle. \tag{9}$$

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

$$\langle f_j^\dagger(t) f_k(t)\rangle = \sum_{k,l=1}^{L} e^{i(\epsilon_k - \epsilon_l)t}A_{jk}A_{jl}\langle d_k^\dagger d_l\rangle, \tag{10}$$

which can then be numerically solved.