high temperature: thermal fluctuations wash out sharp jumps in $S/m$ 

at $T=0$, $t\neq 0$: quantum fluctuations due to hopping can play a
similar role destroying the Mott plateau —
this is much more complicated to evaluate
than the finite-$T$ single-site limit though.

Local spin moment:
\[
\langle m^2 \rangle = \langle \hat{n}_\uparrow \hat{n}_\uparrow - \hat{n}_\uparrow \hat{n}_\downarrow \rangle - 2\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle = s - 2D
\]
\[\equiv \text{density} \equiv D \text{ double occupancy}\]

\[\Rightarrow \text{ local moment is zero for } 10 \text{ and } 11 \text{ but takes}
\text{ maximal value } (= 1) \text{ for either } 10 \text{ or } 11 \).

**Quiz:**

A) Plot $\langle m^2 \rangle$ as a function of $U \in [0, 12]$ for $T=2, \mu=0$

B) Plot $\langle m^2 \rangle$ as a function of $T \in [0, 6]$ for $U=4, \mu=0$

**Answer:**

A)

\[\langle m^2 \rangle \text{ vs } U \text{ at } T=2, \mu=0, t=0\]

Local moments form at large $U$ (or at small $T/4$)

B)

\[\langle m^2 \rangle \text{ vs } T \text{ at } t=0, \mu=0, U=4\]

Local moments are destroyed by thermal fluctuations
1.6 Noninteracting limit

After studying the atomic limit \((U \neq 0, t \neq 0)\), we now study the "opposite" limit \((U = 0, t \neq 0)\), in which the kinetic energy dominates and we recover the band picture.

\[
\hat{H} = -t \sum_{\langle \sigma \sigma' \rangle} (\hat{c}_{\sigma}^+ \hat{c}_{\sigma' + h.c.}) - \mu \sum_{\sigma} \hat{n}_{\sigma}
\]

Two points of view: (i) real space, (ii) momentum space.

(i) real space:

\[
[\hat{H}, \hat{N}_{\sigma}] = 0, \quad [\hat{H}, \hat{N}_0] = 0 \quad \text{(task: show this!)}
\]

Where \(\hat{N}_{\sigma} = \sum_{\sigma} \hat{n}_{\sigma}.\)

How to see this? Use a bond \(i-j\):

\[
\Rightarrow [\hat{c}_{\sigma}^+ \hat{c}_{\sigma} + \hat{c}_{\sigma}^+ \hat{c}_{\sigma}, \hat{n}_{\sigma} + \hat{n}_{\sigma}] = 0 \quad \text{can be shown}
\]

using \([A,B,C] = A \langle B,C \rangle - \langle A,C \rangle B,\)

Another way to understand it: \(\hat{c}_{\sigma}^+ \hat{c}_{\sigma}\) has as many annihilation as creation operators for spin \(\sigma\) \(\Rightarrow\) does not change the particle number for either spin (does not flip a spin).

Upshot: sectors of total \(N_{\sigma}, N_0\) can be considered separately.

(This is even true for \(U \neq 0\).

Example: \(N_0 = 1, N_\sigma = 0\)

Basis in this sector of Hilbert space:

\[
\{ |10000... >, |01000... >, |00100... >, ... \}
\]

Dimension = \(L\) for \(L\)-site model (e.g. 1D chain)

\(\Rightarrow\) it is enough to know on which of the \(L\) sites the single electron with \(\uparrow\)-spin is.
\[ \hat{A} |101000...\rangle = -\mu |101000...\rangle - t |10000...\rangle - t |00100...\rangle \]

⇒ in this basis we have

\[ \hat{A} = \begin{bmatrix} -\mu & -t & 0 & \cdots & 0 \\ -t & -\mu & -t & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ -t & 0 & \cdots & -\mu & -t \\ 0 & -t & \cdots & -t & -\mu \end{bmatrix} \]

periodic boundary conditions

⇒ hopping \(-t\) between 1 and L

⇒ \( L \times L \) tridiagonal matrix with \( a \) on diagonal and \( b \) on upper/lower diagonal has eigenvalues

\[ \begin{align*}
\lambda_n &= a + 2b \cos(\frac{2\pi n}{L}) \\
\kappa_n &= \frac{2\pi n}{L} \\
n &= 1, \ldots, L
\end{align*} \]

How to see this? Ansatz \( V_\epsilon = e^{i\kappa x} \) into eigenvalue equation:

\[ \alpha V_\epsilon + bV_{\epsilon-1} + bV_{\epsilon+1} = \lambda V_\epsilon \]

+ periodicity condition \( V_0 = V_L \)

\( V_1 = V_{L+1} \)

e.g., automatically fulfilled by ansatz provided that \( \kappa_n = \frac{2\pi n}{L} \)

enforces discrete values of \( \kappa_n \).

\[ a e^{i\kappa} + b (e^{-i\kappa} + e^{i\kappa}) e^{i\kappa} = \lambda e^{i\kappa} \]

⇒ \( \lambda = a + b (e^{i\kappa} + e^{-i\kappa}) = a + 2b \cos(\kappa) \)

and \( \kappa_n \) have to fulfill \( 1 \equiv e^{i\kappa_n L} \)

⇒ \( \kappa_n L = n \cdot 2\pi, n \in \mathbb{Z} \)

choice of \( n = 1, \ldots, L \) corresponds to one possible choice of Brillouin zone.
A 1D chain has eigenvalues \( \varepsilon(k) = -2t \cos(k) - \mu \)
and eigenvectors \( \frac{1}{\sqrt{L}} e^{i k \ell} \)
where \( \ell \) is the spatial component of eigenvector with index \( \ell \).

For \( U = 0 \) one can simply build eigenstates for arbitrary particle number as product states (obeying Pauli principle) of single-particle eigenstates. This does not work any more when \( U \neq 0 \)!

For \( U = 0 \) \textbf{momentum space: more direct way to solve } U=0 \textbf{ HH:}

**Canonical transformation of operators.**

\[
\begin{align*}
    c_k^+ &= \frac{1}{\sqrt{L}} \sum_{\ell} e^{i k \ell} c_{\ell}^+ \\
    \text{orthogonality: } \frac{1}{L} \sum_{\ell} e^{-i k \ell_m} \ell_n &= \delta_{n,m} \\
    \frac{1}{L} \sum_{n} e^{i k \ell_n (k-j)} &= \delta_{k,j}
\end{align*}
\]

**Quiz:**

A) Prove that the inverse Fourier transform is given by

\[
    c_{\ell_0}^+ = \frac{1}{\sqrt{L}} \sum_{k} e^{-i k \ell_0} c_k^+
\]

B) Prove that \( \{ c_{k_0}, c_{-k_0}^+ \} = \delta_{k_0} \delta_{-k_0} \).

**Total number operator**

\( \hat{N} = \sum_{\ell_0} \hat{N}_{\ell_0} = \sum_{k_0} \hat{N}_{k_0} \)

\( \hat{N}_{k_0} = c_{k_0}^+ c_{k_0} = \text{occupation operator in momentum space} \)

**Derive the } U=0 \textbf{ HH in momentum space.**

**Answer:**

\[
\begin{align*}
    \hat{A} &= \sum_{k_0} (\varepsilon_{k_0} - \mu) c_{k_0}^+ c_{k_0} = \sum_{k_0} (\varepsilon_{k_0} - \mu) \hat{N}_{k_0} \\
    \varepsilon_{k_0} &= -t \sum_{\ell} e^{i k \ell} \hat{a}_{\ell_0}^2 \\
    \hat{a}_{\ell} &= \text{nearest-neighbor connections} \\
    \text{1D chain: } \hat{a}_{\ell} = \pm \hat{x} \\
    \varepsilon_{k} &= -2t \cos k \text{ (lattice constant } \ell \text{) }
\end{align*}
\]
Useful quantity: density of states (DOS)

\[ N(E) = \frac{1}{L} \sum_k \delta(E - \epsilon_k) \]

Thermodynamic limit on hypercubic lattice, \( L \to \infty \):

\[ \frac{1}{L} \sum_k \xrightarrow{L \to \infty} \int_0^\pi \frac{dk}{(2\pi)^d}, \quad d = \text{spatial dimension} \]

Quit: Compute and plot \( N(E) \) for 1D chain \( \epsilon_k = -2t \cos k \).

Answer: \( x = -2t \cos k \), \( dx = 2t \sin k \, dk = 2t \sqrt{1 - \cos^2 k} \, dk \)

\[ k \in [0, \pi] \Rightarrow x \in [-2t, 2t] \]

\[ N(E) = \frac{1}{2\pi} \int_0^\pi \delta(E + 2t \cos k) = \frac{1}{\pi} \int_0^\pi \delta(E + 2t \cos k) = \]

\[ = \frac{1}{\pi} \int_{-2t}^{2t} \frac{dx}{\sqrt{4t^2 - x^2}} \delta(E - x) = \begin{cases} \frac{1}{\pi \sqrt{4t^2 - E^2}} & |E| \leq 2t \\ 0 & |E| > 2t \end{cases} \]

Knowledge of \( \epsilon_k \Rightarrow \) knowledge of all statistical properties (analogous to free Fermi gas).

Partition function \( Z = \text{Tr} \left[ e^{-\beta \hat{H}} \right] = \prod \prod \left( 1 + e^{-\beta (\epsilon_k - \mu)} \right) = \prod \left( 1 + e^{-\beta (\epsilon_k - \mu)} \right) \)

density \( g = Z^{-1} \text{Tr} \left[ \sum_k \hat{n}_k e^{-\beta \hat{H}} \right] = \sum_k \left( 1 + e^{\beta (\epsilon_k - \mu)} \right)^{-1} \equiv \sum_k f(\epsilon_k) = \sum_k f_k \)

\( f(\epsilon_k) \equiv \left( 1 + e^{\beta (\epsilon_k - \mu)} \right)^{-1} \) Fermi function

Internal energy \( E = Z^{-1} \text{Tr} \left[ \hat{H} e^{-\beta \hat{H}} \right] = \sum_k \epsilon_k \left( 1 + e^{\beta (\epsilon_k - \mu)} \right)^{-1} = \sum_k \epsilon_k f_k \)

Entropy \( S = \beta (E - F) = \beta E - \ln Z \)

\( F = -\ln Z / \beta, \quad E = F - TS \)