high temperature: <u>thermal fluctuations</u> wash out sharp jumps in $\rho(\mu)$

at $T=0$, $t\neq 0$: <u>quantum fluctuations</u> 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.

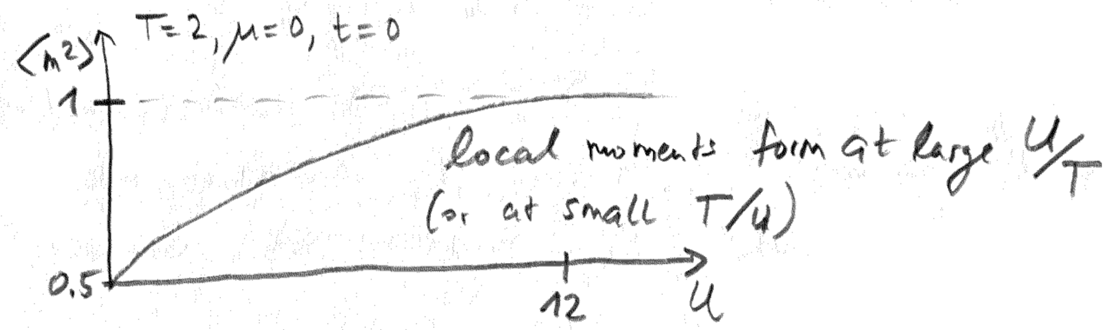
<u>Local spin moment:</u>

$$\langle \hat{m}^2 \rangle = \langle (\hat{n}_\uparrow - \hat{n}_\downarrow)^2 \rangle = \underbrace{\langle \hat{n}_\uparrow + \hat{n}_\downarrow \rangle}_{\equiv \rho \text{ density}} - 2 \underbrace{\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle}_{\equiv D \text{ double occupancy}} = \rho - 2D$$

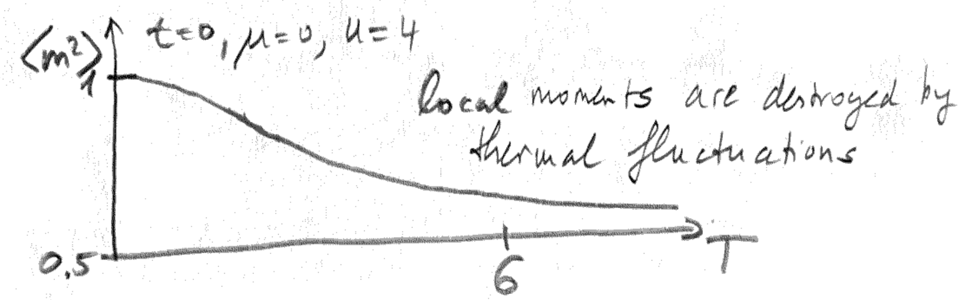
$\Rightarrow$ local moment is zero for $|0\rangle$ and $|\uparrow\downarrow\rangle$ but takes maximal value $(=1)$ for either $|\uparrow\rangle$ or $|\downarrow\rangle$.

Quiz: $\boxed{\text{(A) Plot } \langle m^2 \rangle \text{ as a function of } U \in [0,12] \text{ for } T=2, \mu=0 \quad \text{(B) Plot } \langle m^2 \rangle \text{ as a function of } T \in [0,6] \text{ for } U=4, \mu=0}$

Answer: (A)



(B)



1.6 Noninteracting limit

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

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) - \mu \sum_{j\sigma} \hat{n}_{j\sigma}$$

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

(i) real space:

$[\hat{H}, \hat{N}_\uparrow] = 0$, $[\hat{H}, \hat{N}_\downarrow] = 0$ (task: show this!)

where $\hat{N}_\sigma \equiv \sum_j \hat{n}_{j\sigma}$.

How to see this? Use a bond $i-j$

$\Rightarrow [c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}, \hat{n}_{i\sigma'} + \hat{n}_{j\sigma'}] = 0$ can be shown

using $[AB, C] = A\{B, C\} - \{A, C\} B$.

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

Upshot: sectors of total $N_\uparrow, N_\downarrow$ can be considered separately. (This is even true for $U \neq 0$).

Example: $N_\uparrow = 1$, $N_\downarrow = 0$

Basis in this sector of Hilbert space:

$$\underbrace{\{ |10000\ldots\rangle, |01000\ldots\rangle, |00100\ldots\rangle, \ldots \}}_{\text{dimension} = L \text{ for } L\text{-site model (e.g. 1D chain)}}$$

$\Rightarrow$ It is enough to know on which of the L sites the single electron with $\uparrow$-spin is.

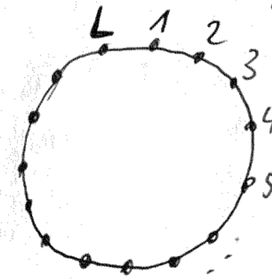
$$\hat{H}\,|01000\ldots\rangle = -\mu\,|01000\ldots\rangle - t\,|10000\ldots\rangle$$
$$- t\,|00100\ldots\rangle$$

$\Rightarrow$ in this basis we have

$$\hat{H} = \begin{bmatrix} -\mu & -t & & & & & -t \\ -t & -\mu & -t & & & & \\ & -t & -\mu & -t & & & \\ & & -t & -\mu & & & \\ & & & & \ddots & & \\ & & & & & -\mu & -t \\ -t & & & & & -t & -\mu \end{bmatrix}$$

periodic boundary conditions

= a closed ring



$\Rightarrow$ hopping $-t$ between 1 and L

$\Rightarrow$ $L \times L$ tridiagonal matrix with a on diagonal and b on upper/lower diagonal has eigenvalues

$$\boxed{\begin{aligned} \lambda_n &= a + 2b\cos(k_n) \\ k_n &= \frac{2\pi n}{L} \qquad n = 1, \ldots, L \end{aligned}}$$

How to see this? Ansatz $v_\ell = e^{ik\ell}$ into eigenvalue equation:

$$a v_\ell + b v_{\ell-1} + b v_{\ell+1} \stackrel{!}{=} \lambda v_\ell$$

+ periodicity condition $v_0 = v_L$, $v_1 = v_{L+1}$ etc. } automatically fulfilled by ansatz provided that $k_n = \frac{2\pi n}{L}$

enforces discrete values of k_n.

$$a e^{ik\ell} + b\left(e^{-ik} + e^{ik}\right)e^{ik\ell} = \lambda e^{ik\ell}$$

$$\Rightarrow \lambda = a + b\left(e^{ik} + e^{-ik}\right) = a + 2b\cos(k)$$

and k_n have to fulfill $1 \stackrel{!}{=} e^{ik_n L}$

$\Leftrightarrow k_n L = n \cdot 2\pi$, $n \in \mathbb{Z}$

choice of $n = 1, \ldots, L$ corresponds to one possible choice of Brillouin zone.

$\Rightarrow$ 1D chain has eigenvalues $\varepsilon(k) = -2t\cos(k) - \mu$

and eigenvectors $\underbrace{(\vec{V}_k)_\ell}_{\substack{\ell\text{-th spatial component of eigenvector} \\ \text{with index } \ell}} = e^{ik\ell}$

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 $U \neq 0$!

(ii) momentum space: More direct way to solve $U=0$ HH:

Canonical transformation of operators.

$$c^+_{k\sigma} = \frac{1}{\sqrt{L}} \sum_\ell e^{ik\ell} c^+_{\ell\sigma}$$

orthogonality:
$$\frac{1}{L}\sum_\ell e^{i(k_n - k_m)\ell} = \delta_{n,m}$$
$$\frac{1}{L}\sum_n e^{ik_n(\ell - j)} = \delta_{\ell,j}$$

Quiz: $\boxed{\begin{array}{l} \text{(A) Prove that the inverse Fourier transform is given by} \\ \qquad c^+_{\ell\sigma} = \frac{1}{\sqrt{L}}\sum_k e^{-ik\ell} c^+_{k\sigma} \\ \text{(B) Prove that } \{c_{k\sigma}, c^+_{p\sigma'}\} = \delta_{kp}\delta_{\sigma\sigma'}. \end{array}}$

Total number operator: $\hat{N} = \sum_{j\sigma} \hat{n}_{j\sigma} = \sum_{k\sigma} \hat{n}_{k\sigma}$

$\hat{n}_{k\sigma} \equiv c^+_{k\sigma} c_{k\sigma}$ = occupation operator in momentum space

Quiz: $\boxed{\text{Derive the } U=0 \text{ HH in momentum space.}}$

Answer: $\hat{H} = \sum_{k\sigma} (\epsilon_k - \mu)\, c^+_{k\sigma} c_{k\sigma} = \sum_{k\sigma} (\epsilon_k - \mu)\, \hat{n}_{k\sigma}$

$\epsilon_k = -t \sum_\ell e^{i\vec{k}\cdot\vec{a}_\ell}$, $\vec{a}_\ell$ = nearest-neighbor connections

1D chain: $\vec{a}_\ell = \pm\hat{x}$, $\epsilon_k = -2t\cos k$ (lattice constant $\equiv 1$)

Useful quantity: density of states (DOS)

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

Thermodynamic limit on hypercubic lattice, $L \to \infty$:

$$\frac{1}{L}\sum_k \xrightarrow[L\to\infty]{} \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \quad , \; d = \text{spatial dimension}$$

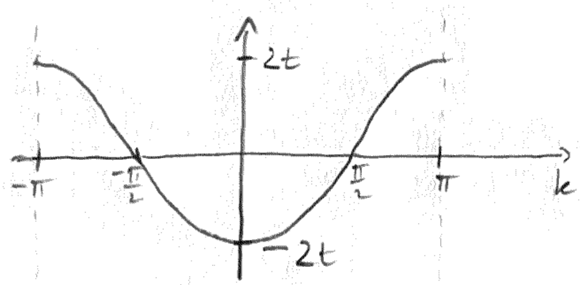
Quiz: $\boxed{\text{Compute and plot } N(E) \text{ for 1D chain } \epsilon_k = -2t\cos k.}$

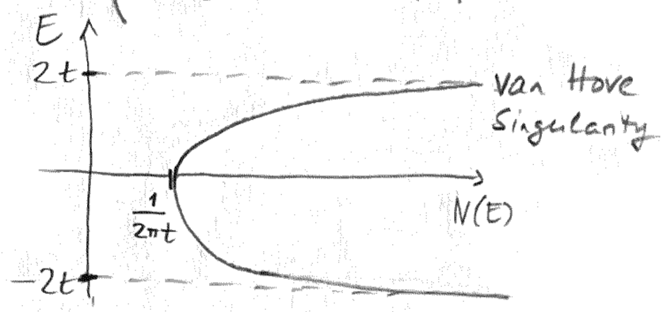
Answer: $x = -2t \cos k$, $dx = 2t \sin k \, dk = 2t\sqrt{1-\cos^2 k}\, dk$

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

$$N(E) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \; \delta(E + 2t\cos k) \underset{\substack{\uparrow \\ \text{Symmetry} \\ k \to -k}}{=} \frac{1}{\pi}\int_0^{\pi} dk \; \delta(E + 2t\cos k) =$$

$$= \frac{1}{\pi}\int_{-2t}^{2t} \frac{dx}{\sqrt{4t^2 - x^2}} \, \delta(E - x) = \begin{cases} \dfrac{1}{\pi\sqrt{4t^2 - E^2}} & |E| \le 2t \\ 0 & |E| > 2t \end{cases}$$





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

Partition function $Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] = \prod_k \prod_{n_k \in \{0,1\}} e^{-\beta(\epsilon_k - \mu)} = \prod_k \left(1 + e^{-\beta(\epsilon_k - \mu)}\right)$

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

$\langle \hat{n}_k \rangle$

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

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

entropy $S = \beta(E - F) \underset{\uparrow}{=} \beta E - \ln Z$

$F = -\ln Z/\beta$, $E = F - TS$