

HOMEWORK FOR THE COURSE «QUANTUM MANY-BODY PHYSICS»

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1 Bosons

1.a Hamiltonian diagonalization

i. $h = h^\dagger = S^\dagger D S$ with $D = \text{diag}(\varepsilon_1, \varepsilon_2, \dots)$ and S orthogonal

ii. $\hat{H} = \mathbf{a}^\dagger h \mathbf{a} = (\mathbf{S}\mathbf{a})^\dagger D(S\mathbf{a}) = \tilde{\mathbf{a}}^\dagger D \tilde{\mathbf{a}}$ with $\tilde{a}_i = S_{ij} a_j$, $\tilde{a}_i^\dagger = S_{ij}^\dagger a_j^\dagger$

We can check the canonicity of a transformation by direct substitution. Taking into account the known commutation relations and orthogonality of S

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = 0, \quad s_{ik} S_{kj}^\dagger = \delta_{ij},$$

we could check

$$[\tilde{a}_i, \tilde{a}_j^\dagger] = [S_{ki} a_i, a_j^\dagger S_{jp}^\dagger] = S_{ki} (\delta_{ij} + a_j^\dagger a_i) S_{jp}^\dagger - a_j^\dagger S_{jp}^\dagger S_{ki} a_i = S_{ki} \delta_{ij} S_{jp}^\dagger + (S_{ki} S_{jp}^\dagger - S_{jp}^\dagger S_{ki}) a_j^\dagger a_i = \delta_{kp}.$$

Similarly $[\tilde{a}_i, \tilde{a}_j]$ will be reduced to 0.

iii. Since $\varepsilon_k > 0$ ground state will be reduced to the absence of excitations, namely $|0\rangle$.

1.b Heisenberg representation

i. Let's start with calculating the commutator in diagonal case

$$[a_q, a_k^\dagger a_k] = (\delta_{qk} + a_k^\dagger a_q) a_k - a_k^\dagger a_k a_q = a_q, \quad (1)$$

which means the equation of motion can be obtained in the form

$$i\partial_t a(t) = [a_q(t), \hat{H}] = \varepsilon_q a_q(t), \quad \Rightarrow \quad a_q(t) = e^{-i\varepsilon_q t} a_q(0).$$

In the off-diagonal case

$$a_q(t) = S_{qk}^\dagger \tilde{a}_k(t) = \sum_k S_{qk}^\dagger e^{-i\varepsilon_k t} \tilde{a}_k(0). \quad (2)$$

ii. Notice, that

$$[\hat{H}, a_q] = -\varepsilon_q a_q, \quad [\hat{H}, [\hat{H}, a_q]] = (-\varepsilon_q)^2 a_q, \quad \dots \quad \Rightarrow \quad [\hat{H}, a_q]_m = (-\varepsilon_q)^m a_q$$

Using the Baker-Campbell-Hausdorff formula

$$a_q(t) = e^{i\hat{H}t} a_q(0) e^{-i\hat{H}t} = a_q + (-i\varepsilon_q t) a_q + \dots + \frac{(-i\varepsilon_q t)^m}{m!} a_q + \dots = e^{-i\varepsilon_q t} a_q(0),$$

which is in accordance with the previous result.

iii. $a_q^\dagger(t) = a_q(t)^\dagger = e^{i\varepsilon_q t} a_q^\dagger(0)$

iv. Expression (1) will not change for fermions, so evolution will occur according to the same law.

1.c Correlation function

Let's consider the correlation function

$$f_{qk}(t) = \langle 0 | a_q(t) a_k^\dagger(0) | 0 \rangle.$$

Using (2), we get

$$f_{qk}(t) = S_{qp}^\dagger S_{kj} e^{-i\varepsilon_p t} \delta_{pj} = \sum_j S_{qj}^\dagger S_{kj} e^{-i\varepsilon_j t},$$

and with $h_{qk} = \delta_{qk} \varepsilon_k$

$$f_{qk}(t) = \delta_{qk} e^{-i\varepsilon_q t}.$$

2 Fermions

We work in the grand canonical ensemble and assume periodic boundary conditions:

$$\hat{H} = -J \sum_l (c_l^\dagger c_{l+1} + \text{h.c.}) - \mu \sum_j c_j^\dagger c_j.$$

(a) Let's do a discrete Fourier transform

$$|j\rangle = \frac{1}{\sqrt{L}} \sum_{n=0}^{N-1} e^{-i\frac{2\pi}{L}nj} |n\rangle,$$

which corresponds to impulses $k = \frac{2\pi}{La}n$. Using the orthonormality of the chosen system of functions, we obtain

$$\hat{H} = \sum_{n=0}^{L-1} (\varepsilon_n - \mu) c_n^\dagger c_n, \quad \varepsilon_n = -2J \cos\left(\frac{2\pi}{L}n\right) = -2J \cos(ka).$$

(b) In the thermodynamic limit $L \rightarrow \infty$ the Hamiltonian can be rewritten as

$$\hat{H} = \int_0^{2\pi} \frac{dk}{2\pi} (\varepsilon_k - \mu) c_k^\dagger c_k, \quad \varepsilon_k = -2J \cos(ka).$$

So we could introduce DOS (density of states)

$$g(\varepsilon) = \int \frac{dk}{2\pi} \delta(\varepsilon - \varepsilon_k) \propto \int \frac{d\varepsilon_k}{\sqrt{(2J)^2 - \varepsilon_k^2}} \delta(\varepsilon - \varepsilon_k) = \frac{1}{\sqrt{4J^2 - \varepsilon^2}},$$

with characteristic behavior $g(\varepsilon \rightarrow \pm 2J) \rightarrow \infty$.

(c) The population of the state can be written as

$$\bar{n}_k = \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1},$$

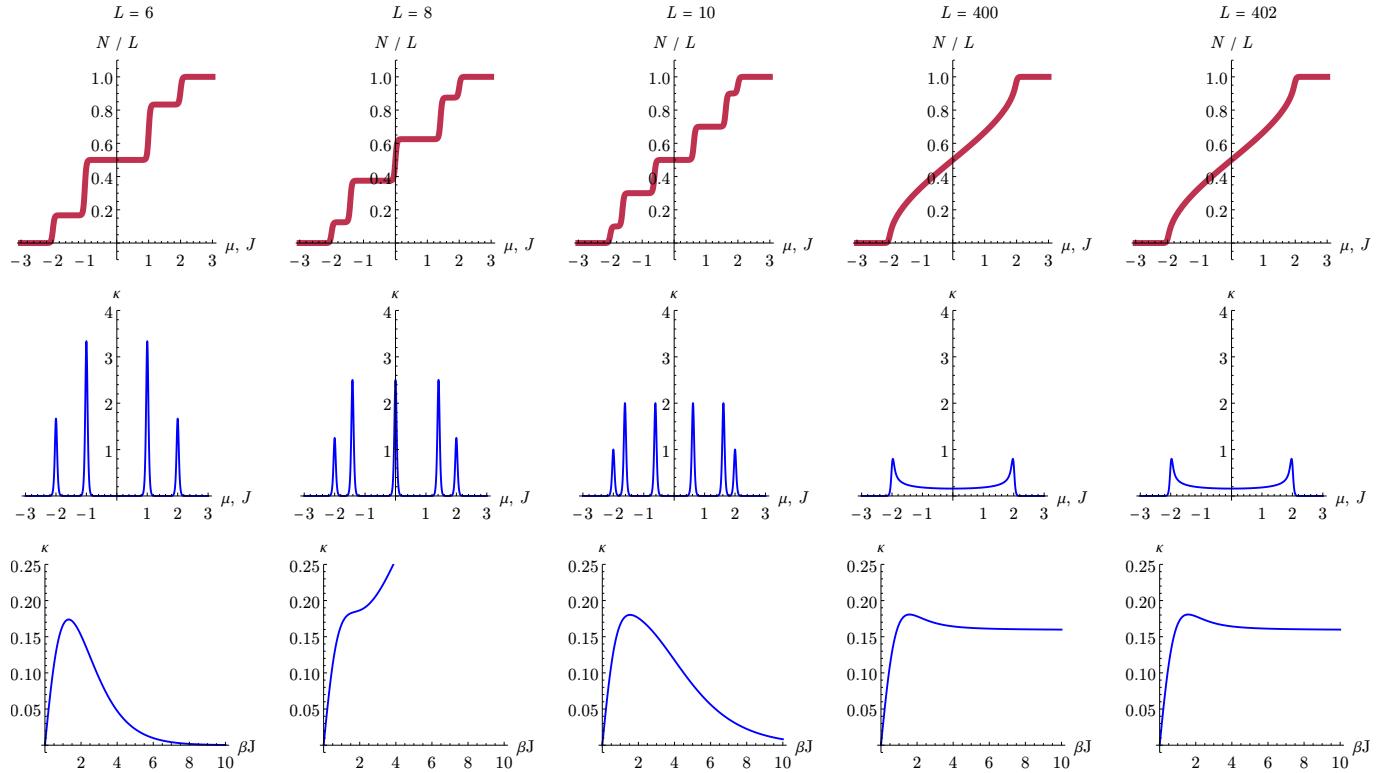
Substituting the energy value, we find

$$\frac{1}{L} \langle N(\mu) \rangle = \frac{1}{L} \sum_k \frac{1}{\exp(-2\beta J \cos(ka) - \beta\mu)},$$

And, rewriting through the density of states

$$\frac{1}{L} \langle N(\mu) \rangle = \int_{-2J}^{2J} \frac{g(\varepsilon) d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1}.$$

(d) For $\beta J = 40$ let's plot $\langle \hat{N} \rangle(\mu)$ and $\kappa = \partial_\mu \langle \hat{N} \rangle$. For a small L , characteristic steps are noticeable, corresponding to the population of a new state.



2.1 Second Quantization

We could consider

$$|\alpha_1, \dots, \alpha_N\rangle = \frac{1}{\sqrt{N!}} \sum_P \zeta^{\sigma(P)} |\alpha_{P(1)}\rangle \otimes \dots \otimes |\alpha_{P(N)}\rangle,$$

where $\zeta = \pm 1$ for bosons and fermions respectively. We define creation operator via

$$a_\beta^\dagger |\alpha_1, \dots, \alpha_N\rangle \stackrel{\text{def}}{=} |\beta, \alpha_1, \dots, \alpha_N\rangle.$$

1. Adjoint a_β could be expressed as

$$\begin{aligned} a_\beta^\dagger &= \sum_{\{\theta\}} |\beta, \theta_1, \dots, \theta_M\rangle \langle \theta_1, \dots, \theta_M|, \\ a_\beta &= \sum_{\{\theta\}} |\theta_1, \dots, \theta_M\rangle \langle \beta, \theta_1, \dots, \theta_M|. \end{aligned}$$

Than it could be shown that

$$a_\beta |\alpha_1, \dots, \alpha_N\rangle = \sum_k C_k |\alpha_1, \dots, \cancel{\alpha_k}, \dots, \alpha_N\rangle,$$

with

$$C_k = \langle \beta, \alpha_1, \dots, \cancel{\alpha_k}, \dots, \alpha_N | \alpha_1, \dots, \alpha_N \rangle = \frac{1}{\sqrt{N!}} \sum_P \langle \alpha_{P(1)} | \otimes \dots \otimes \langle \beta |_{P(k)} \otimes \dots \otimes \langle \alpha_{P(N)} | \alpha_1, \dots, \alpha_N \rangle,$$

where we could «move» $\langle \beta |$ to the start, by $P(k) - 1$ transpositions, and due to $N!$ equal permutations we could neglect $\frac{1}{N!}$ coming to

$$C_k = \zeta^{k-1} \langle \beta | \alpha_k \rangle.$$

2. We also could find, that a_β and a_β^\dagger fulfills the (anti)-commutation relations

$$\begin{aligned} a_\beta^\dagger a_\alpha |\theta_1, \dots, \theta_N\rangle &= a_\beta^\dagger \sum_{k=1}^N \zeta^{k-1} \langle \alpha | \theta_k \rangle |\theta_1, \dots, \cancel{\theta_k}, \dots, \theta_N\rangle = \sum_{k=1}^N \zeta^{k-1} \langle \alpha | \theta_k \rangle |\beta, \theta_1, \dots, \cancel{\theta_k}, \dots, \theta_N\rangle, \\ a_\alpha a_\beta^\dagger |\theta_1, \dots, \theta_N\rangle &= a_\alpha |\beta, \theta_1, \dots, \theta_N\rangle = \sum_{k=1}^N \zeta^k \langle \alpha | \theta_k \rangle |\beta, \theta_1, \dots, \cancel{\theta_k}, \dots, \theta_N\rangle + \langle \alpha | \beta \rangle |\theta_1, \dots, \theta_N\rangle, \end{aligned}$$

so for bosons $\zeta = 1$ we have

$$[a_\alpha, a_\beta^\dagger] \stackrel{\text{def}}{=} a_\alpha a_\beta^\dagger - a_\beta^\dagger a_\alpha = \langle \alpha | \beta \rangle = \delta_{\alpha, \beta},$$

and in the same way for fermions $\zeta = -1$ and

$$\{a_\alpha, a_\beta^\dagger\} \stackrel{\text{def}}{=} a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = \langle \alpha | \beta \rangle = \delta_{\alpha, \beta}.$$

3. For density operator

$$\hat{\rho}(x) = \sum_{j=1}^N \delta(x - \hat{x}_j),$$

we could find second quantized form

$$\hat{\rho}(x) = \sum_{\alpha \beta} \langle \alpha | \delta(x - \hat{x}) | \beta \rangle \hat{a}_\alpha^\dagger \hat{a}_\beta = \sum_{\alpha \beta} \int \langle \alpha | x' \rangle \langle x' | \beta \rangle \delta(x - x') dx' \hat{a}_\alpha^\dagger \hat{a}_\beta = \sum_{\alpha \beta} \langle \alpha | x \rangle \langle x | \beta \rangle \hat{a}_\alpha^\dagger \hat{a}_\beta,$$

what could be reduced to the $\hat{a}_x^\dagger \hat{a}_x$ form if $|\alpha\rangle$ and $|\beta\rangle$ corresponds to the coordinates.

2.2 Mapping between Quantum and Classical Systems

We could rewrite classical 1D Ising chain partitin function as

$$\mathcal{Z}_c = T_{s_1, s_2} \dots T_{s_{N-1}, s_N} T_{s_N, s_1} = \text{tr}(T^N),$$

with transfer matrix

$$T = T^a T^b = \begin{pmatrix} e^{h_c + K_c} & e^{h_c - K_c} \\ e^{-h_c - K_c} & e^{K_c - h_c} \end{pmatrix}, \quad T^a = \begin{pmatrix} e^{h_c} & 0 \\ 0 & e^{-h_c} \end{pmatrix}, \quad T^b = \begin{pmatrix} e^{K_c} & e^{-K_c} \\ e^{-K_c} & e^{K_c} \end{pmatrix}.$$

There are different ways to define T , because important just eigenvalues

$$\lambda_{1,2} = \frac{1}{2} e^{-h_c - K_c} \left(e^{2(h_c + K_c)} + e^{2K_c} \pm \sqrt{e^{4K_c} (e^{2h_c} - 1)^2 + 4e^{2h_c}} \right).$$

For a quantum system the partitin function

$$\mathcal{Z}_q = \text{tr } e^{-\beta H},$$

and we want to achieve

$$\mathcal{Z}_q = \mathcal{Z}_c = \text{tr} \left(e^{-\frac{\beta}{N} H_1} e^{-\frac{\beta}{N} H_2} \right)^N, \quad e^{-\frac{\beta}{N} H_1} = T^a, \quad e^{-\frac{\beta}{N} H_2} = T^b.$$

Using formulas to the Pauli matrix exponents, we could find

$$H_1 = \frac{N}{-\beta} \alpha_3 \sigma_z, \quad H_2 = \frac{N}{-\beta} (\alpha_0 \mathbb{1} - \alpha_1 \sigma_x),$$

with $\alpha_0 = \ln \sinh(2K_c) + \ln 2$, $\alpha_1 = \ln \tanh K_c$ and $\alpha_3 = h_c$. I think it is possible to find other H_1 and H_2 , my choice was ruled by separating K_c and h_c dependences.

3.1 The Transverse Field Ising Model

Consider the Hamiltonian of the Transverse Field Ising Model (TFIM)

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^x \hat{\sigma}_j^x - h \sum_j \hat{\sigma}_j^z$$

where $J, h > 0$ with PBC $\hat{\sigma}_L^x \hat{\sigma}_{L+1}^x = \hat{\sigma}_L^x \hat{\sigma}_1^x$.

1. We could try to map spins to bosonic operators

$$\begin{cases} \hat{\sigma}_j^x = \hat{b}_j + \hat{b}_j^\dagger \\ \hat{\sigma}_j^y = i(\hat{b}_j^\dagger - \hat{b}_j) \\ \hat{\sigma}_j^z = 1 - 2\hat{b}_j^\dagger \hat{b}_j \end{cases} \Leftrightarrow \begin{cases} \hat{b}_j = \hat{\sigma}_j^+ = \frac{1}{2}\hat{\sigma}_j^x + \frac{i}{2}\hat{\sigma}_j^y \\ \hat{b}_j^\dagger = \hat{\sigma}_j^- = \frac{1}{2}\hat{\sigma}_j^x - \frac{i}{2}\hat{\sigma}_j^y \end{cases}$$

- (a) Bosons as define above are «hard-core bosons». We know that

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 0 \text{ with } i \neq j, \quad [\hat{\sigma}^a, \hat{\sigma}^b] = 2i\varepsilon_{abc}\hat{\sigma}^c, \quad \{\hat{\sigma}^a, \hat{\sigma}^b\} = 2\delta_{ab}.$$

So bosons commute at different sites, but

$$\{\hat{b}_j, \hat{b}_j^\dagger\} = \frac{1}{2}\hat{\sigma}_j^x \hat{\sigma}_j^x + \frac{1}{2}\hat{\sigma}_j^y \hat{\sigma}_j^y = 1, \quad \hat{b}_j^\dagger \hat{b}_j^\dagger = \frac{1}{4}\hat{\sigma}_j^x \hat{\sigma}_j^x - \frac{1}{4}\hat{\sigma}_j^y \hat{\sigma}_j^y + \frac{1}{4}\{\hat{\sigma}_j^x, \hat{\sigma}_j^y\} = 0,$$

thus at most one boson is allowed on each site.

- (b) In 1D it's useful to modify bosons to spinless fermions by *Jordan Wigner transformation*

$$\hat{b}_j = \hat{K}_j \hat{c}_j = \hat{c}_j \hat{K}_j, \quad \hat{K}_j = \prod_{i=1}^{j-1} (1 - 2\hat{n}_i) = \pm 1,$$

where non-local string operator \hat{K}_j corresponds just to a sign and $\hat{K}_j = \hat{K}_j^\dagger = \hat{K}_j^{-1}$. So if \hat{c} are fermions then \hat{b} satisfies the commutation and anticommutation relations

$$\begin{aligned} [\hat{b}_i, \hat{b}_j] &= 0, & [\hat{b}_i, \hat{b}_j^\dagger] &= 0, & [\hat{b}_i^\dagger, \hat{b}_j^\dagger] &= 0, \\ \{\hat{b}_i, \hat{b}_j\} &= 0, & \{\hat{b}_i, \hat{b}_j^\dagger\} &= 0, & \{\hat{b}_i^\dagger, \hat{b}_j^\dagger\} &= 0. \end{aligned} \tag{1}$$

Second row could be proven using

$$\hat{b}_j^\dagger \hat{b}_j = \hat{c}_j^\dagger \hat{K}_j^\dagger \hat{K}_j \hat{c}_j = \hat{c}_j^\dagger \hat{c}_j, \quad \hat{b}_j^\dagger \hat{b}_j^\dagger = \hat{c}_j^\dagger \hat{K}_j^\dagger \hat{K}_j \hat{c}_j^\dagger = \hat{c}_j^\dagger \hat{c}_j^\dagger, \quad \hat{b}_j \hat{b}_j = \hat{c}_j \hat{K}_j \hat{K}_j \hat{c}_j = \hat{c}_j \hat{c}_j.$$

And without loss of generality for $j > i$

$$\hat{b}_i \hat{b}_j^\dagger = \hat{c}_i \hat{K}_{i,j} \hat{c}_j^\dagger, \quad \hat{b}_j^\dagger \hat{b}_i = \hat{c}_j^\dagger \hat{K}_{i,j} \hat{c}_i \stackrel{1}{=} -\hat{K}_{i,j} \hat{c}_i \hat{c}_j^\dagger \stackrel{2}{=} \hat{c}_i \hat{K}_{i,j} \hat{c}_j^\dagger, \quad \Rightarrow \quad [\hat{b}_i, \hat{b}_j^\dagger] = 0,$$

with $\hat{K}_{i,j} = \prod_{k=i}^j (1 - 2\hat{n}_k)$. It was used in $\stackrel{1}{=}$ that $\{\hat{c}_i, \hat{c}_j^\dagger\} = 0$ and in $\stackrel{2}{=}$ that \hat{c}_i changes parity for $\hat{K}_{i,j}$. The operators conjugation does not change the calculations, so we have proved (1). We need carefully work with PBS

$$\hat{b}_L^\dagger \hat{b}_1 = \hat{K}_L \hat{c}_L^\dagger \hat{c}_1 \stackrel{3}{=} -\left(\prod_{i=1}^L (1 - 2\hat{c}_i^\dagger \hat{c}_i)\right) \hat{c}_L^\dagger \hat{c}_1 = -(-1)^{\hat{N}} \hat{c}_L^\dagger \hat{c}_1, \quad \hat{N} = \sum_{j=1}^L \hat{c}_j^\dagger \hat{c}_j,$$

where we used in $\stackrel{3}{=}$ that j -site occupied and we could complete to $-(-1)^{\hat{N}}$.

- (c) Summarising, spins are mapped into fermions using

$$\begin{aligned} \hat{\sigma}_x &= \hat{K}_j (\hat{c}_j^\dagger + \hat{c}_j), \\ \hat{\sigma}_y &= \hat{K}_j i (\hat{c}_j^\dagger - \hat{c}_j), \\ \hat{\sigma}_z &= 1 - 2\hat{c}_j^\dagger \hat{c}_j, \end{aligned} \quad \hat{K}_j = \prod_{i=1}^{j-1} (1 - 2\hat{c}_i^\dagger \hat{c}_i).$$

This is the Jordan Wigner transformation of the TFIM

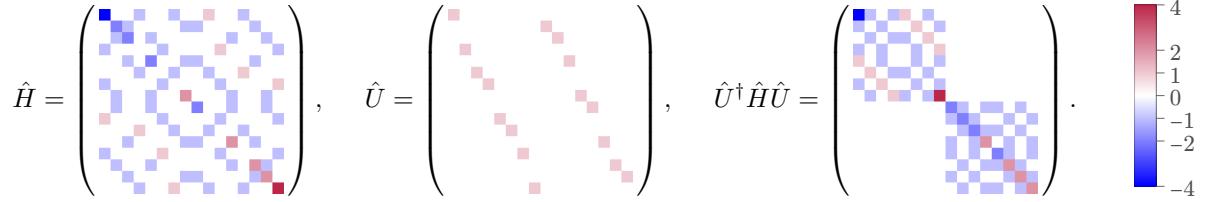
$$\begin{aligned} \hat{H} &= hL - J \sum_{j=1}^{L-1} \left(\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j + \text{h.c.} \right) + 2h \sum_{j=1}^L \hat{c}_j^\dagger \hat{c}_j \\ &\quad + J (-1)^{\hat{N}} \left(\hat{c}_L^\dagger \hat{c}_1 + \hat{c}_L^\dagger \hat{c}_1^\dagger + \text{h.c.} \right). \end{aligned}$$

The number of fermions is not conserved, because of terms $\hat{c}^\dagger \hat{c}^\dagger$, but $[(-1)^{\hat{N}}, \hat{H}] = 0$, so parity is constant. With $(-1)^{\hat{N}} = 1$ we have antiperiodic boundary conditions and periodic otherwise.

2. We could separate Hilbert space as $\mathcal{H} = \mathcal{H}_{\text{even}} \oplus \mathcal{H}_{\text{odd}}$, and conserving parity of fermions \hat{H} as

$$\hat{H} = \hat{P}_0 \hat{H} \hat{P}_0 + \hat{P}_1 \hat{H} \hat{P}_1 = \begin{pmatrix} \hat{H}_0 & 0 \\ 0 & \hat{H}_1 \end{pmatrix}, \quad \hat{P}_{0,1} = \frac{1 \pm (-1)^{\hat{N}}}{2}.$$

Consider $L = 4$, than we could visualize such transform for $J = h = 1$ as



where \hat{U} represents reordering basis from

$$|0000\rangle, |0001\rangle, |0010\rangle, |0011\rangle, |0100\rangle, |0101\rangle, |0110\rangle, |0111\rangle, \\ |1000\rangle, |1001\rangle, |1010\rangle, |1011\rangle, |1100\rangle, |1101\rangle, |1110\rangle, |1111\rangle$$

to

$$|0000\rangle, |0011\rangle, |0101\rangle, |0110\rangle, |1001\rangle, |1010\rangle, |1100\rangle, |1111\rangle, \\ |0001\rangle, |0010\rangle, |0100\rangle, |0111\rangle, |1000\rangle, |1011\rangle, |1101\rangle, |1110\rangle.$$

(a) To diagonalize \hat{H} we could start from Fourier Transform

$$\hat{c}_k = \frac{1}{\sqrt{L}} \sum_j e^{ikj} \hat{c}_j, \quad \hat{c}_j = \frac{1}{\sqrt{L}} \sum_k e^{-ikj} \hat{c}_k.$$

Consider L is even. If we want $\hat{c}_{L+1} = \hat{c}_1$ we have H_1 and

$$\mathcal{K}_{p=1} = \left\{ k = \frac{\pi}{L} 2n \mid n = -\frac{1}{2}L + 1, \dots, 0, \dots, \frac{1}{2}L \right\},$$

otherwise $\hat{c}_{L+1} = -\hat{c}_1$ in H_0 and

$$\mathcal{K}_{p=0} = \left\{ k = \frac{\pi}{L} (2n - 1) \mid n = -\frac{1}{2}L + 1, \dots, 0, \dots, \frac{1}{2}L \right\}.$$

And rewriting in terms of \mathcal{K}_p hamiltonian we have

$$\hat{H}_p = - \sum_{k \in \mathcal{K}_p} (J \cos k + h) \left(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k}^\dagger \hat{c}_{-k} \right) - J \sum_{k \in \mathcal{K}_p} \left(e^{ik} \hat{c}_k^\dagger \hat{c}_{-k}^\dagger + \text{h.c.} \right)$$

(b) It is useful to combine $k = 0$ and $k = \pi$ for $p = 1$

$$\hat{H}_{k=0,\pi} = -2J(\hat{n}_0 - \hat{n}_\pi) + 2h(\hat{n}_0 + \hat{n}_\pi - 2).$$

The remaining terms come into pairs $(k, -k)$, so we could go to the positive k :

$$\mathcal{K}_1^+ = \left\{ k = \frac{\pi}{L} 2n \mid n = 1, \dots, \frac{1}{2}L - 1 \right\},$$

$$\mathcal{K}_0^+ = \left\{ k = \frac{\pi}{L} (2n - 1) \mid n = 1, \dots, \frac{1}{2}L \right\}.$$

The \hat{H} can be expressed as

$$\hat{H}_0 = \sum_{k \in \mathcal{K}_0^+} \hat{H}_k, \quad \hat{H}_1 = \hat{H}_{k=0,\pi} + \sum_{k \in \mathcal{K}_1^+} \hat{H}_k,$$

with

$$\hat{H}_k = -2(J \cos k + h) \left(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k}^\dagger \hat{c}_{-k} \right) - 2iJ \sin k \left(\hat{c}_k^\dagger \hat{c}_{-k}^\dagger - \hat{c}_{-k} \hat{c}_{-k} \right).$$

Introducing $\hat{\Psi}_k^\dagger = (\hat{c}_k^\dagger, \hat{c}_{-k})$ we could simplify \hat{H}_k to the

$$\hat{H} = \hat{\Psi}_k^\dagger H_k \hat{\Psi}_k, \quad H_k = -2J \begin{pmatrix} -\frac{h}{J} + \cos k & i \sin k \\ -i \sin k & \frac{h}{J} - \cos k \end{pmatrix}.$$

Great, we have reduced the Hamiltonian to quadratic form and ready for the *Bogolyubov transform*:

$$\hat{\Psi}_k = U \hat{\Phi}_k, \Rightarrow \hat{H}_k = \hat{\Phi}_k^\dagger D_k \hat{\Phi}_k, \quad D_k = U^\dagger H_k U = \begin{pmatrix} \varepsilon_k & 0 \\ 0 & -\varepsilon_k \end{pmatrix},$$

where $\hat{\Phi}_k^\dagger \stackrel{\text{def}}{=} (\hat{\gamma}_k^\dagger, \hat{\gamma}_{-k})$ – our new operators. Diagonalizing H_k we have

$$U_k = \begin{pmatrix} u_k & -\bar{v}_k \\ v_k & u_k \end{pmatrix} = \frac{1}{\sqrt{\varepsilon_k(\varepsilon_k + z_k)}} \begin{pmatrix} \varepsilon_k + z_k & iy_k \\ iy_k & \varepsilon_k + z_k \end{pmatrix}, \quad \boxed{\varepsilon_k = 2J\sqrt{(\cos k - \frac{h}{J})^2 + \sin(k)^2}} \quad (2)$$

where we introduced new parameters

$$u_k = \frac{\varepsilon_k + z_k}{\sqrt{\varepsilon_k(\varepsilon_k + z_k)}}, \quad v_k = \frac{iy_k}{\sqrt{\varepsilon_k(\varepsilon_k + z_k)}}, \quad z_k = 2(h - J \cos k), \quad y_k = 2J \sin k.$$

We could show that still

$$\{\hat{\gamma}_k, \hat{\gamma}_k^\dagger\} = \{\bar{u}_k \hat{c}_k + \bar{v}_k \hat{c}_{-k}^\dagger, u_k \hat{c}_k^\dagger + v_k \hat{c}_{-k}\} = |u_k|^2 + |v_k|^2 = 1,$$

so $\hat{\gamma}$ is a fermion. **Calculate commutators? But they are fermions!**

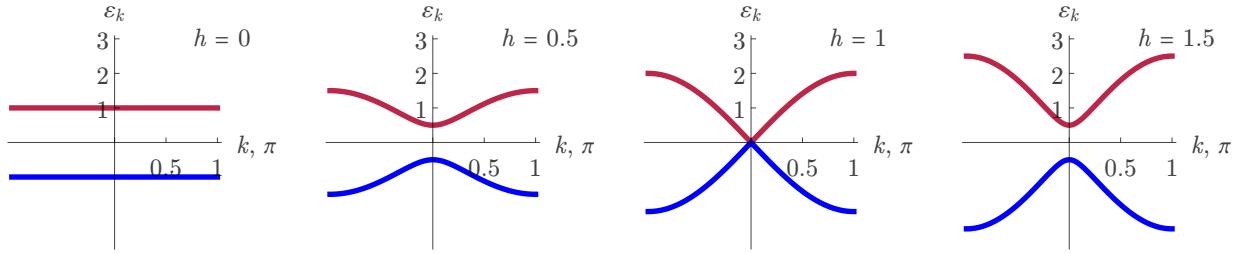


Figure 1: TFIM dispersion with different magnetic fields h with $J = 1$

3. (a) Ground state we could find in \hat{H}_0 such that $\hat{\gamma}_k |gs\rangle = 0 \forall k$. As in BCS theory we could start from some state (not orthogonal $|gs\rangle$), apply $\hat{\gamma}_k$ and normalize, coming to the

$$|gs\rangle = \frac{\prod_k \hat{\gamma}_{-k} \hat{\gamma}_k}{\|\prod_k \hat{\gamma}_{-k} \hat{\gamma}_k |0\rangle\|} |0\rangle = \prod_{k \in \mathcal{K}_0^+} (u_k + v_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger) |0\rangle, \quad E_0 = - \sum_{k \in \mathcal{K}_0^+} \varepsilon_k,$$

with $|0\rangle \sim |\downarrow \dots \downarrow\rangle$ – vacuum for the original fermions $\hat{c}_k |0\rangle = 0 \forall k$. If we want to continue exist in separated Hilbert space, than elementary excitation should save parity

$$\hat{\gamma}_{k_1}^\dagger \hat{\gamma}_{k_2}^\dagger |gs\rangle = \hat{c}_{k_1}^\dagger \hat{c}_{k_2}^\dagger \prod_{k \neq |k_1|, |k_2|}^{K_0^+} (\bar{u}_k - \bar{v}_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger) |0\rangle.$$

Going to the even amount of fermions we could apply even amount of $\hat{\gamma}_k$ to the $|gs\rangle$.

- (b) Gap between minimal exitation and $|gs\rangle$ is $\varepsilon_{k=0}$, and gap in ε_k disappear at $h/J = 1$ (fig. 1). Interesting to plot all \hat{H} eigenvalues and see what is happening in the same values of h (fig. 2).

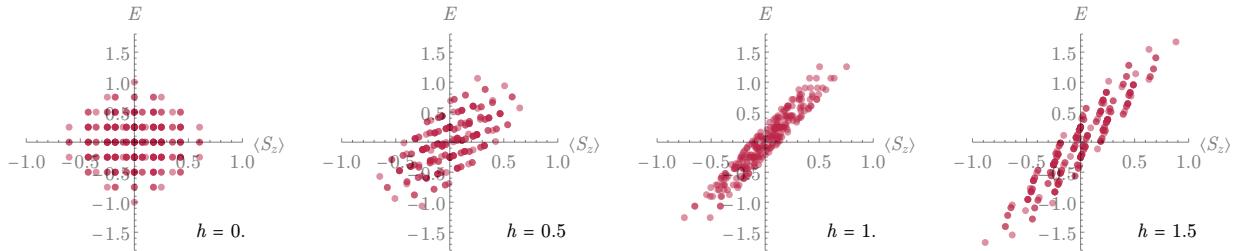


Figure 2: Eigenvalues of \hat{H} as a function of $\langle S_z \rangle$

4. Consider ξ as

$$f(r) = \langle \sigma_j^z \sigma_{j+r}^z \rangle \propto e^{-r/\xi},$$

so we could estimate it numerically (fig. 3). We have finite L that strongly affects ξ estimation, but definitely something interesting happens at $h = h_c = 1$.

We know that

$$\frac{1}{E_{\text{gap}}} \propto \frac{1}{\varepsilon_{k=0}} \propto \xi^z \propto (h - h_c)^{-\nu z},$$

and from (2) at $k = 0$ we have $E_{\text{gap}} \propto h - 1$, than $h_c = 1$ and $\nu z = 1$.

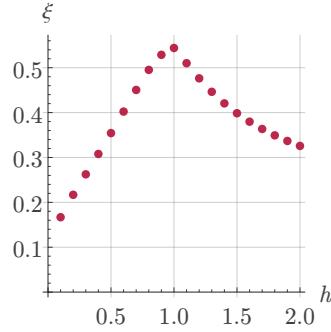


Figure 3: Correlation radius ξ as a function of external magnetic field h at $L = 20$, ground state

4.1 Feynman Path Integral of the Harmonic Oscillator

Consider propagator as

$$K \stackrel{\text{def}}{=} \langle q_f | e^{-i\hat{H}T} | q_i \rangle,$$

that we could rewrite in terms of the Feinman's integral

$$K = \int e^{iS[q(t)]} \mathcal{D}q(t),$$

with in particular action for the harmonic oscillator

$$S[q(t)] = \int_0^T \frac{m}{2} (\dot{q}^2 - \omega^2 q^2) dt \quad (3)$$

with boundary conditions $q(0) = q_i$ and $q(T) = q_f$.

(a) Writing the path as $q(t) = q_c(t) + y(t)$, due to $\delta S[q_c(t)] = 0$ we could rewrite S as

$$S[q(t)] = \int_0^T \frac{m}{2} ((\dot{q}_c + \dot{y})^2 - \omega^2 (q_c + y)^2) dt = S[q_c(t)] + S[y(t)] + \int_0^T m (\dot{q}_c dy - \omega^2 q_c y) dt = S[q_c(t)] + S[y(t)].$$

It was used that Euler-Lagrange equation $\partial_x L - \frac{d}{dt} \partial_{\dot{x}} L = 0$ leads to classical equation of motion $\ddot{q}_c = -m\omega^2 q_c(t)$:

$$\int_0^T m \dot{q}_c dy = y(t) \dot{q}_c \Big|_0^T - \int_0^T m y \ddot{q}_c dt = \int_0^T m \omega^2 y q_c dt.$$

Thus we could factorise K

$$K = e^{iS[q_c(t)]} F(T), \quad F(T) = \int e^{iS[y(t)]} \mathcal{D}y(t).$$

(b) Solving $\ddot{q}_c = -m\omega^2 q_c(t)$ with boundary conditions $q(0) = q_i$ and $q(T) = q_f$ we get

$$q_c(t) = A \cos(\omega t) + B \sin(t), \Rightarrow \begin{cases} q_i = B \\ q_f = A \sin(\omega T) + B \cos(\omega T) \end{cases} \Rightarrow A = \frac{q_f - q_i \cos(\omega T)}{\sin(\omega T)}, \quad B = q_i,$$

and substituting into the action (3)

$$S[q_c(t)] = \frac{m\omega}{2 \sin(\omega T)} ((q_i^2 + q_f^2) \cos(\omega T) - 2q_i q_f).$$

(c) The fluctuations can be expressed as a Fourier series

$$y(t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi t}{T}\right),$$

we go to the integration over $\prod_n a_n$. It is useful to calculate

$$\int_0^T \dot{y}^2 dt = \frac{T}{2} \sum_{n=1}^{\infty} \left(\frac{\pi n}{T}\right)^2 a_n^2, \quad \int_0^T y^2 dt = \frac{T}{2} \sum_{n=1}^{\infty} a_n^2.$$

So we could find F as

$$F(T) \propto \int \exp\left(-\sum_{n=1}^{\infty} \alpha_n a_n^2\right) \prod_n da_n = \prod_{n=1}^{\infty} \sqrt{\frac{\pi}{\alpha_n}}, \quad \alpha_n = \frac{m}{2i\hbar} \frac{T}{2} \left(\frac{\pi n}{T}\right)^2 \left(1 - \frac{\omega^2 T^2}{n^2 \pi^2}\right).$$

Ignoring all factors without ω , we have

$$F(T) = C \prod_{n=1}^{\infty} \left(1 - \frac{\omega^2 T^2}{n^2 \pi^2}\right)^{-1/2} = C \sqrt{\frac{\omega T}{\sin(\omega T)}},$$

with some constant C that could be find from the free particle case $\omega \rightarrow 0$

$$\lim_{\omega \rightarrow 0} F(T) = C = \sqrt{\frac{m}{2\pi i\hbar T}}, \quad \Rightarrow \quad F(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}}.$$

(d, e) Now we could calculate the partition function $Z = \text{tr } e^{-\beta \hat{H}}$ after a Wick rotation to imaginary times $T = -i\beta$

$$Z = \int \langle x | e^{-\beta \hat{H}} | x \rangle dx = \int e^{iS[q_c(-i\beta)]} F(-i\beta) dx \stackrel{(1)}{=} \frac{1}{2 \sinh(\frac{1}{2}\omega\beta)},$$

where in $\stackrel{(1)}{=}$ we calculated Gaussian integral

$$\int \exp(-\alpha x^2) dx = \sqrt{\frac{\pi}{\alpha}}, \quad \alpha = \frac{i m \omega (1 - \cos(\omega T))}{\sin(\omega T)}.$$

4.2 Grassmannian Algebra

We know, that for the Grassmann number η

$$\int \eta d\eta = 1, \quad \int d\eta = 0.$$

1. Interesting to note, that for $f(\eta) = a + b\eta$ ($a, b \in \mathbb{C}$) we have

$$\{\eta, \partial_\eta\}f(\eta) = \{\eta, \int d\eta\}f(\eta) = f(\eta).$$

Enough to calculate

$$\eta \int d\eta f(\eta) = b\eta, \quad \eta \partial_\eta f(\eta) = b\eta, \quad \int d\eta \eta f(\eta) = a, \quad \partial_\eta \eta f(\eta) = a.$$

2. As a next step we calculate

$$\exp \left(\sum_j c_j \eta_j \right) = 1 + \sum_j c_j \eta_j + \sum_{j,k} c_j c_k \eta_j \eta_k = 1 + \sum_j c_j \eta_j + \sum_{j>k} c_j c_k (\eta_j \eta_k + \eta_k \eta_j) = 1 + \sum_j c_j \eta_j,$$

with $c_j \in \mathbb{C}$. Actually it is the same as proof that $\sum_j c_j \eta_j$ is still Grassmann number by calculating anticommutative relations.

3. Finally, we could find integral

$$\int d\bar{\eta} d\eta e^{-C\bar{\eta}\eta} = \int d\bar{\eta} d\eta \left(1 - C\bar{\eta}\eta + \frac{C^2}{2} \bar{\eta}\eta\bar{\eta}\eta + \dots \right) = C \int d\bar{\eta} \left(\int d\eta \eta\bar{\eta} \right) = C,$$

with $C \in \mathbb{C}$. It was used that $\bar{\eta}\eta\bar{\eta}\eta = -\bar{\eta}^2\eta^2 = 0$.

5.1 Complex analysis

Consider Gaussian integral

$$I_1 = \int_{-\infty}^{\infty} e^{-iax^2} dx,$$

with $\alpha \in \mathbb{R}^+$. We could use that

$$I_2 = \int_{-\infty}^{\infty} e^{-bx^2} dx = \sqrt{\frac{\pi}{a}}.$$

Define $\mathcal{C}_1 = \{z = e^{i\frac{\pi}{4}x} : x \in \mathbb{R}\}$, $\mathcal{C}_2 = \{z = x : x \in \mathbb{R}\}$ and $\mathcal{C}_R^\pm = \{z = \pm Re^{i\varphi} : \varphi \in [0, \pi/4]\}$. Applying Cauchy integral theorem for holomorphic functions to the $\mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_R^+ \cup \mathcal{C}_R^-$ we have

$$-I[\mathcal{C}_1] + I[\mathcal{C}_2] + I[\mathcal{C}_R^+] + I[\mathcal{C}_R^-] = 0,$$

with $I[\mathcal{C}_1]e^{-i\frac{\pi}{4}} = I_1$, $I[\mathcal{C}_2] = I_2$.

The $I[\mathcal{C}_R^\pm]$ could be estimated as

$$|I[\mathcal{C}_{R \rightarrow \infty}^\pm]| \leq \lim_{R \rightarrow \infty} \int_0^{\pi/2} e^{-aR^2\varphi} r d\varphi = \lim_{R \rightarrow \infty} \frac{1}{aR} \left(1 - e^{-\frac{1}{2}a\pi r^2}\right) = 0,$$

thus we have

$$I_1 = I[\mathcal{C}_1]e^{-i\frac{\pi}{4}} = I[\mathcal{C}_2]e^{-i\frac{\pi}{4}} = e^{-i\frac{\pi}{4}} \sqrt{\frac{\pi}{a}},$$

that could be generalized as

$$\int_{-\infty}^{\infty} e^{\pm iax^2} dx = e^{\pm i\frac{\pi}{4}} \sqrt{\frac{\pi}{a}}.$$

5.2 Effective action of coupled harmonic oscillators

We could derive the low-energy effective action for a system of two coupled harmonic oscillators, formally described by the classical partition function

$$Z = \int Dx DX \exp \left(i \int dt L(x, X, \dot{x}, \dot{X}) \right),$$

with

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2 + \frac{1}{2}M\dot{X}^2 - \frac{1}{2}M\Omega^2X^2 - gXx.$$

It could be expanded as

$$Z = \int Dx e^{iS_0 + iS_{\text{int}}}, \quad e^{iS_{\text{int}}} = \int DX \exp \left(i \int dt \left[\frac{1}{2}M\dot{X}^2 - \frac{1}{2}M\Omega^2X^2 - gXx \right] \right).$$

Integrating by parts we have Gaussian integral that coul be calculated directly

$$e^{iS_{\text{int}}} = \int DX \exp \left(i \int dt \left[\frac{1}{2}MX(\partial_t^2 + \Omega^2)X - gXx \right] \right) = \mathcal{N} \exp \left(i \int dt \frac{g^2}{2M} x (\partial_t^2 + \Omega^2)^{-1} x \right)$$

with \mathcal{N} as some irrelevant normalizing factor. That leads to some L_{eff}

$$L_{\text{eff}} = \frac{1}{2}m\ddot{x}^2 - \frac{1}{2}mx^2\omega_{\text{eff}}^2, \quad \omega_{\text{eff}} = \omega \sqrt{1 - \alpha^2 \frac{m}{M} \left(\frac{\omega}{\Omega} \right)^2},$$

with $g = \alpha m\omega^2$ and, apparently, $m_{\text{eff}} = m$.

6.1 Thermal Green's functions

The thermal Green's function is defined as

$$G_{ij}(\tau) = -\langle T_\tau \psi_i(\tau) \psi_j^\dagger(0) \rangle$$

The path integral formulation of the Green's function of non-interacting particles is

$$G_{ij}(\tau) = -\frac{1}{Z} \int D(\bar{\psi}, \psi) \psi_i(\tau) \bar{\psi}_j(0) e^{-S[\bar{\psi}, \psi]}, \quad S = \sum_j \int_0^\beta d\tau \bar{\psi}_j (\partial_\tau + \varepsilon_j - \mu) \psi_j = \sum_j s[\bar{\psi}_j, \psi_j]. \quad (4)$$

1. Time ordering. The path integral automatically takes care of the time ordering:

$$G_{ij}(\tau > 0) = -\langle \psi_i(\tau) \psi_j^\dagger(0) \rangle = \text{tr} \left(e^{-(\beta-\tau)H} \psi_i e^{-H\tau} \psi_j^\dagger \right),$$

and than we could repeat the construction of the path integral and get (4). In other case

$$\begin{aligned} G_{ij}(\tau < 0) &= \zeta \langle \psi_j^\dagger(0) \psi_i(\tau) \rangle = \text{tr} \left(\psi_j^\dagger e^{-(\tau)H} \psi_i e^{-(\beta+\tau)H} \right) \\ &= -\frac{\zeta}{Z} \int D(\bar{\psi}, \psi) \bar{\psi}_j(0) \psi_i(\tau) e^{-S[\bar{\psi}, \psi]} = -\frac{\zeta^2}{Z} \int D(\bar{\psi}, \psi) \psi_i(\tau) \bar{\psi}_j(0) e^{-S[\bar{\psi}, \psi]}, \end{aligned}$$

thus we come to the same (4).

2. Green's function as Matsubara sum. After the Fourier transform (unitary)

$$\psi_j(\tau) = \frac{1}{\sqrt{\beta}} \sum_n e^{-i\omega_n \tau} \psi_{jn}, \quad \omega_n = \frac{\pi}{\beta} \begin{cases} 2n+1, & \text{fermions}, \\ 2n, & \text{bosons}, \end{cases} \quad (5)$$

we get

$$G_{ij}(\tau) = -\frac{1}{Z} \frac{1}{\beta} \sum_{n,m} \int D(\bar{\psi}, \psi) e^{-i\omega_n \tau} \psi_{in} \bar{\psi}_{jm} e^{-S[\bar{\psi}, \psi]}, \quad S = \sum_{j,n} \bar{\psi}_{jn} (-i\omega_n + \varepsilon_j - \mu) \psi_{jn}. \quad (6)$$

We could simplify calculations noticing that due to the sign symmetry of the action

$$\int d(\bar{\psi}_j, \psi_j) \psi_{jn} e^{-s[\bar{\psi}_{jn}, \psi_{jn}]} = 0, \quad \Rightarrow \quad G_{i,j \neq i}(\tau) = 0.$$

To the next simplification in $G_{jj}(\tau)$ we could factor

$$I_{nm}^j = \int d(\bar{\psi}_{jn}, \psi_{jn}) d(\bar{\psi}_{jm}, \psi_{jm}) \psi_{jn} \bar{\psi}_{jm} e^{-s[\bar{\psi}_{jn}, \psi_{jn}]} e^{-s[\bar{\psi}_{jm}, \psi_{jm}]} \propto \delta_{nm}$$

again due to the symmetry. It is useful to rewrite I_{nn}^j as

$$I_{nn}^j = \int d(\bar{\psi}_{jn}, \psi_{jn}) \psi_{jn} \bar{\psi}_{jn} e^{-s[\bar{\psi}_{jn}, \psi_{jn}]} \int d(\bar{\psi}_{jn}, \psi_{jn}) e^{-s[\bar{\psi}_{jn}, \psi_{jn}]} = \frac{1}{-i\omega_n + \varepsilon_j - \mu} \int d(\bar{\psi}_{jn}, \psi_{jn}) e^{-s[\bar{\psi}_{jn}, \psi_{jn}]}.$$

It remains to note that «blue»-term helps us to factorize partition function in the (6)

$$Z = \left(\prod_{k \neq j} \int d(\bar{\psi}_k, \psi_k) e^{-\sum_{k \neq j} s[\bar{\psi}_k, \psi_k]} \right) \cdot \left(\prod_{m \neq n} \int d(\bar{\psi}_{jm}, \psi_{jm}) e^{-s[\bar{\psi}_{jm}, \psi_{jm}]} \right) \cdot \left(\int d(\bar{\psi}_{jn}, \psi_{jn}) e^{-s[\bar{\psi}_{jn}, \psi_{jn}]} \right)$$

Finally $G_{ij}(\tau)$ could be expressed as

$$G_{ij}(\tau) = \frac{\delta_{ij}}{\beta} \sum_n e^{-i\omega_n \tau} G_0(j, i\omega_n), \quad G_0(j, i\omega_n) \stackrel{\text{def}}{=} \frac{1}{i\omega_n - \varepsilon_j + \mu}. \quad (7)$$

Substituting ω_n from (5) as usual $G_{ij}(\tau)$ could be rewritten as

$$G_{jj}(\tau > 0) = -\zeta \oint \frac{dz}{2\pi i} \frac{e^{-z\tau}}{z - \xi_j} n_{\text{BF}}(-z), \quad (8)$$

$$G_{jj}(\tau < 0) = -\zeta \oint \frac{dz}{2\pi i} \frac{e^{z\tau}}{-z + \xi_j} n_{\text{BF}}(z), \quad (9)$$

with $\xi_j \stackrel{\text{def}}{=} \varepsilon_j - \mu$ and $n_{\text{BF}}(z) = (e^{\beta z} - \zeta)^{-1}$. Sign of z was chosen to provide convergence. Summing over the outer pole we get

$$\begin{aligned} G_{jj}(\tau > 0) &= \zeta n_{\text{BF}}(-\xi_j) e^{-\xi_j \tau}, \\ G_{jj}(\tau < 0) &= -\zeta n_{\text{BF}}(\xi_j) e^{-\xi_j \tau}. \end{aligned}$$

Combining all this happiness into one expression

$$G_{ij}(\tau) = -\delta_{ij} (\theta(\tau) + \zeta n_{\text{BF}}(\xi_j)) e^{-\xi_j \tau}. \quad (10)$$

In general, it is quite logical to obtain the theta function due to T-ordering, since $\hat{a}\hat{a}^\dagger = 1 + \zeta \hat{a}^\dagger \hat{a}$.

3. The occupation number. The occupation number in a single particle state j is in general given by

$$\begin{aligned} n_j &= \langle \psi_j^\dagger(0)\psi_j(0) \rangle = \zeta \lim_{\tau \rightarrow 0^-} \langle T_\tau \psi_i(\tau)\psi_j^\dagger \rangle = -\zeta \lim_{\tau \rightarrow 0^-} G_{jj}(\tau), \\ &= \zeta \lim_{\tau \rightarrow 0^+} \langle T_\tau \psi_i(\tau)\psi_j^\dagger - 1 \rangle = \zeta \lim_{\tau \rightarrow 0^+} (-G_{jj}(\tau) - 1) \end{aligned}$$

Expanding (10) we get

$$n_j = -\zeta \lim_{\tau \rightarrow 0^-} G_{jj}(\tau) = \zeta^2 n_{\text{BF}}(\xi_j) \lim_{\tau \rightarrow 0^-} e^{-\xi_j \tau} = n_{\text{BF}}(\xi_j).$$

4. The generating functional. The generating functional for correlation functions is defined as

$$\mathcal{Z}[\bar{J}, J] = \int D(\bar{\psi}, \psi) \exp \left(-S[\bar{\psi}, \psi] - \sum_j \int_0^\beta d\tau (\bar{J}_j \psi_j + \bar{\psi}_j J_j) \right).$$

These can be obtained as functional derivatives of $\mathcal{Z}[\bar{J}, J]$, where the source fields are set to zero after the evaluation:

$$\langle T_\tau \psi_{in} \psi_{jm} \rangle = \frac{\zeta}{\mathcal{Z}[0, 0]} \frac{\delta^2 \mathcal{Z}[\bar{J}, J]}{\delta \bar{J}_{in} \delta J_{jm}} \Big|_{J, \bar{J}=0}.$$

It remains to calculate

$$\begin{aligned} \mathcal{Z}[\bar{J}, J] &= \int D(\bar{\psi}, \psi) \exp \left(- \sum_{j,n} \bar{\psi}_{jn} (-G_0^{-1}(j, i\omega_n)) \psi_{jn} + \sum_{j,n} \left(\bar{J}_{jn} \psi_{jn} + \bar{\psi}_{jn} J_{jn} \right) \right) \\ &= \mathcal{Z}[0, 0] \exp \left(- \sum_{j,n} \bar{J}_{jn} G_0(j, i\omega_n) J_{jn} \right). \end{aligned}$$

Thus for the Green's function $G_{ij}(i\omega_n)$ in Matsubara space

$$G_{ij}(i\omega_n) = -\langle T_\tau \psi_{in} \psi_{jm} \rangle = -\zeta \frac{\delta^2}{\delta \bar{J}_{in} \delta J_{jm}} \exp \left(- \sum_{j,n} \bar{J}_{jn} G_0(j, i\omega_n) J_{jn} \right) \Big|_{\bar{J}=J=0} = \delta_{ij} \delta_{nm} G_0(j, i\omega_n),$$

corresponding to (7).

6.2 Nambu-Goldstone Modes in the Heisenberg Ferromagnet

We consider an isotropic Heisenberg ferromagnet with spin 1/2-particles fixed to the sites of a lattice:

$$\hat{H} = -\frac{1}{2} \sum_{ij} J_{ij} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j,$$

with $J_{ij} > 0$. Let us label the ground states by their orientation in space:

$$|0_{\mathbf{n}}\rangle = \bigotimes_{i=1}^N |i, \mathbf{n}\rangle,$$

with the single site states satisfying $\mathbf{n} \cdot \hat{\mathbf{S}}_j |j, \mathbf{n}\rangle = -\frac{1}{2} |j, \mathbf{n}\rangle$.

1. Orthogonal states. In spherical coordinates the single site state could be found from

$$\mathbf{n} \cdot \hat{\mathbf{S}} = \frac{1}{2} \begin{pmatrix} \cos(\theta) & e^{-i\varphi} \sin(\theta) \\ e^{i\varphi} \sin(\theta) & -\cos(\theta) \end{pmatrix},$$

with eigenstate

$$|0_{\mathbf{n}}\rangle = \frac{\cos(\theta) - 1}{\sqrt{2 - 2 \cos(\theta)}} |\uparrow\rangle + \frac{e^{i\varphi} \sin(\theta)}{\sqrt{2 - 2 \cos(\theta)}} |\downarrow\rangle.$$

We need projection to the $|\downarrow\rangle$, that could be simplified to the

$$|\langle \downarrow | 0_{\mathbf{n}} \rangle| = \left| \frac{2 \sin(\frac{1}{2}\theta) \cos(\frac{1}{2}\theta)}{2 \sin(\frac{1}{2}\theta)} \right| = |\cos(\frac{1}{2}\theta)|.$$

In the thermodynamic limit $N \rightarrow \infty$

$$|\langle 0_{\mathbf{n}_1} | 0_{\mathbf{n}_2} \rangle| = \lim_{N \rightarrow \infty} |\cos(\frac{1}{2}\theta_{\mathbf{n}_1 \mathbf{n}_2})|^N = 0.$$

2. Hamiltonian. We could substitute

$$\hat{S}^x = \frac{1}{2} (\hat{S}^+ + \hat{S}^-), \quad \hat{S}^y = \frac{1}{2i} (\hat{S}^+ - \hat{S}^-), \quad \hat{S}^z = \hat{S}^+ \hat{S}^- - \frac{1}{2},$$

that leads to terms as

$$\begin{aligned}\hat{S}_i^x \hat{S}_j^x &= \frac{1}{4} \left(\hat{S}_i^+ \hat{S}_j^+ + \hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ + \hat{S}_i^- \hat{S}_j^- \right) \\ \hat{S}_i^y \hat{S}_j^y &= \frac{-1}{4} \left(\hat{S}_i^+ \hat{S}_j^+ - \hat{S}_i^+ \hat{S}_j^- - \hat{S}_i^- \hat{S}_j^+ + \hat{S}_i^- \hat{S}_j^- \right) \\ \hat{S}_i^z \hat{S}_j^z &= \hat{S}_i^+ \hat{S}_i^- \hat{S}_j^+ \hat{S}_j^- - \frac{1}{2} \hat{S}_i^+ \hat{S}_i^- - \frac{1}{2} \hat{S}_j^+ \hat{S}_j^- + \frac{1}{4},\end{aligned}$$

so the Hamiltonian

$$\hat{H} = -\frac{1}{2} \sum_{ij} J_{ij} \left(-\frac{1}{2} (\hat{S}_i^+ - \hat{S}_j^+) (\hat{S}_i^- - \hat{S}_j^-) + \hat{S}_i^+ \hat{S}_i^- \hat{S}_j^+ \hat{S}_j^- + \frac{1}{4} \right).$$

3. One-particle Hamiltonian. We can reduce the Hilbert space to the one-particle states $|j\rangle = \hat{S}_j^+ |0\rangle$. Neglecting constant terms, reduced Hamiltonian \hat{H}'

$$H' |i\rangle = -\frac{1}{2} \sum_{kj} J_{kj} \left(-\frac{1}{2} (\delta_{ki}|k\rangle - \delta_{ji}|k\rangle - \delta_{ki}|j\rangle + \delta_{ji}|j\rangle) + \delta_{ji}\delta_{kj}|k\rangle \right) = \frac{1}{2} \sum_j J_{ij} (|i\rangle - |j\rangle)$$

with matrix elements

$$\langle i|\hat{H}|i\rangle = \frac{1}{2} \sum_j J_{ij}, \quad \langle j|\hat{H}|i\rangle = -\frac{1}{2} \sum_j J_{ij}.$$

Assuming $J_{ij} = J(|\mathbf{x}_i - \mathbf{x}_j|)$ consider the plane wave state $|k\rangle = \sum_j e^{i\mathbf{k}\mathbf{x}_j} |j\rangle$:

$$\hat{H}' |k\rangle = \sum_i e^{i\mathbf{k}\mathbf{x}_i} \frac{1}{2} \sum_j J_{ij} (|i\rangle - |j\rangle).$$

To simplify calculations consider

$$\langle m|\hat{H}'|k\rangle = \sum_i e^{i\mathbf{k}\mathbf{x}_i} \frac{1}{2} \sum_j J_{ij} (\delta_{mi} - \delta_{mj}) = e^{i\mathbf{k}\mathbf{x}_m} \frac{1}{2} \sum_j J_{mj} - \sum_j e^{i\mathbf{k}\mathbf{x}_j} \frac{1}{2} J_{jm} = \frac{1}{2} \sum_j J_{jm} \left(1 - e^{i\mathbf{k}(\mathbf{x}_j - \mathbf{x}_m)} \right) e^{i\mathbf{k}\mathbf{x}_m}.$$

We could sum over $\mathbf{x}_n = \mathbf{x}_j - \mathbf{x}_m$ and notice that $J_{jm} = J(|\mathbf{x}_j - \mathbf{x}_m|) = J(|\mathbf{x}_n|)$

$$\langle m|\hat{H}'|k\rangle = \frac{1}{2} \left(\sum_n J_{n0} (1 - e^{i\mathbf{k}\mathbf{x}_n}) \right) e^{i\mathbf{k}\mathbf{x}_m} = E_{\mathbf{k}} \langle m|k\rangle,$$

thus we have proven that $|k\rangle$ is eigenstate with energy $E_{\mathbf{k}}$

$$E_{\mathbf{k}} = \frac{J_0 - J_k}{2}, \quad J_k = \sum_j J(|\mathbf{x}_j|) e^{-i\mathbf{k}\mathbf{x}_j}.$$

For a constant nearest neighbour interaction on a square lattice $E_{\mathbf{k}}$ could be calculated explicitly:

$$J_k = \sum_{\mathbf{x}_j=\pm\mathbf{e}_{x,y}} J(|\mathbf{x}_j|) e^{-i\mathbf{k}\mathbf{x}_j} = 2J (\cos k_x + \cos k_y),$$

and energy

$$E_k = J (2 - \cos k_x - \cos k_y) \stackrel{k \rightarrow 0}{\approx} \frac{J}{2} (k_x^2 + k_y^2).$$

7.1 Operator Identity for Gaussian Theories

General case. To form some intuition, let's start with the proof

$$\langle e^{\sum_j b_j x_j} \rangle = e^{\frac{1}{2} \sum_{i,j} b_i \langle x_i x_j \rangle b_j}, \quad (11)$$

with averaging defined as

$$\langle f \rangle = \frac{1}{Z} \int D(\mathbf{x}) f(\mathbf{x}) e^{-\frac{1}{2} \mathbf{x}^T G^{-1} \mathbf{x}}, \quad D(x) = \prod_n dx_n,$$

with $Z = \sqrt{\det(2\pi G)}$ so that $\langle 1 \rangle = 1$. Both parts of the (11) could be calculated directly:

$$\langle e^{\sum_j b_j x_j} \rangle = \frac{1}{Z} \int D(x) e^{-\frac{1}{2} \mathbf{x}^T G^{-1} \mathbf{x} + \mathbf{b} \mathbf{x}} = \frac{1}{Z} \int D(\mathbf{x}) e^{-\frac{1}{2} (\mathbf{x} - G\mathbf{b})^T G^{-1} (\mathbf{x} - G\mathbf{b})} e^{\frac{1}{2} \mathbf{b}^T G \mathbf{b}},$$

and with $\mathbf{x}' = \mathbf{x} - G\bar{\mathbf{b}}$ and $D(\mathbf{x}') = D(\mathbf{x})$

$$\langle e^{\mathbf{b} \mathbf{x}} \rangle = \frac{1}{Z} \int D(\mathbf{x}') e^{-\frac{1}{2} \mathbf{x}'^T G^{-1} \mathbf{x}' + \frac{1}{2} \mathbf{b}^T G \mathbf{b}} = e^{\frac{1}{2} \mathbf{b}^T G \mathbf{b}} = e^{\frac{1}{2} \sum_{i,j} b_i \langle x_i x_j \rangle b_j},$$

which proved in the previous homework fact that $\langle x_i x_j \rangle = G_{ij}$.

Special case. We want to prove the operator identity

$$\langle e^{i(\varphi(r) - \varphi(0))} \rangle = e^{-\frac{1}{2} ((\varphi(r) - \varphi(0))^2)}. \quad (12)$$

With $b(r') = i\delta(r' - r) - i\delta(r')$:

$$\sum_j b_j \varphi_j = \int b(r') \varphi(r') dr' = i(\varphi(r) - \varphi(0)),$$

and for other part $\sum_{i,j} b_i \langle x_i x_j \rangle b_j = \langle \sum_{i,j} b_i x_i x_j b_j \rangle$, so

$$\sum_{i,j} b_i x_i x_j b_j = \int b(r') \varphi(r') \varphi(r'') b(r'') dr' dr'' = \left(\int b(r') \varphi(r') dr' \right)^2 = -(\varphi(r) - \varphi(0))^2,$$

thus we proved (12) using (11).

Wick's theorem. Note that from (11) are convenient to obtain Wick's theorem **maybe**. Expanding (11) in the Taylor series we have from the LHS

$$\langle e^{\sum_j b_j x_j} \rangle = 1 + \frac{1}{2!} \sum_{i,j} b_i b_j \langle x_i x_j \rangle + \frac{1}{4!} \sum_{i,j,k,l} b_i b_j b_k b_l \langle x_i x_j x_k x_l \rangle + \dots$$

and from the RHS

$$e^{\frac{1}{2} \sum_{i,j} b_i \langle x_i x_j \rangle b_j} 1 + \frac{1}{2} \sum_{i,j} b_i b_j \langle x_i x_j \rangle + \sum_{i,j,k,l} b_i b_j b_k b_l \langle x_i x_j \rangle \langle x_k x_l \rangle + \dots,$$

so collecting terms with proper B^4 we get

$$\langle x_i x_j x_k x_l \rangle = \langle x_i x_j \rangle \langle x_k x_l \rangle + \langle x_i x_k \rangle \langle x_j x_l \rangle + \langle x_i x_l \rangle \langle x_j x_k \rangle.$$

This result is known as Wick's theorem.

7.2 Bogoliubov theory

1. Hamiltonian. Consider a microscopic Hamiltonian for bosons with weak contact interactions:

$$\hat{H} - \mu \hat{N} = \sum_p (\varepsilon_p - \mu) \hat{a}_p^\dagger \hat{a}_p + \frac{\varphi}{2V} \sum_{p,p',q} \hat{a}_{p+q}^\dagger \hat{a}_{p'-q}^\dagger \hat{a}_{p'} \hat{a}_p, \quad (13)$$

where $\varepsilon_p = p^2/2m$ and second term as \hat{V} . For $\varphi = 0$ the groundstate in a grandcanonical description is a coherent state of bosons in the zero-momentum state, i.e. all particles are Bose condensed.

Finite interactions lead to scattering of bosons from the condensate into finite momentum modes and hence a depletion of the condensate fraction. However, if the interactions are weak, one can still assume that the $p = 0$ mode is macroscopically occupied, $\langle a_0^\dagger a_0 \rangle \gg 1$. As $[a_0, a_0^\dagger] = 1$, one can neglect it for a macroscopically occupied $p = 0$ mode and replace a_0, a_0^\dagger by their expectation value $\sqrt{N_0}$, the number of bosons in the condensate. Thus our small parameter is $(N - N_0)/N_0$. One can therefore approximate all other modes to be small $a_p \ll \sqrt{N_0}$ and therefore neglect all terms in the interaction part of above Hamiltonian which contain more than two creation/annihilation operators with $p \neq 0$.

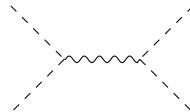


Figure 4: Interaction of condensate particles

The leading term of the expansion involves interactions solely between the stationary particles (particles of the condensate) as in fig. 4 (the dashed line corresponds to condensed particles)

$$\hat{V}_0 = \frac{\varphi}{2V} \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0.$$

There are no terms that contain only one creation or annihilation operator for non-condensate particles due to the conservation of momentum.

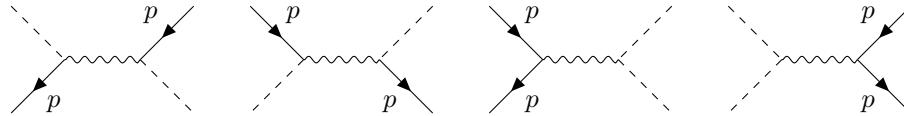


Figure 5: Interaction of condensate particle and non-condensate particle

The next four expansion terms each contain one operator of creation and one operator of annihilation above the non-condensate particles (fig. 5):

$$\hat{V}_2 = \frac{\varphi}{2V} \sum_{p \neq 0} \left(\hat{a}_p^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_p + \hat{a}_p^\dagger \hat{a}_0^\dagger \hat{a}_p \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_p^\dagger \hat{a}_0 \hat{a}_p + \hat{a}_p^\dagger \hat{a}_0^\dagger \hat{a}_p \hat{a}_0 \right) \stackrel{!}{=} \frac{2\varphi}{V} \hat{a}_0^\dagger \hat{a}_0 \sum_{p \neq 0} \hat{a}_p^\dagger \hat{a}_p,$$

where in $\stackrel{!}{=}$ it was used that $[\hat{a}_0, \hat{a}_p] = 0$.

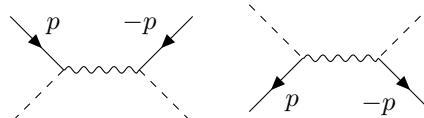


Figure 6: Creation and annihilation of two condensate particles from non-condensate

Two more terms of the expansion contain two creation operators each and two operators for annihilation condensate particles (fig. 6):

$$\hat{V}'_2 = \frac{\varphi}{2V} \sum_{p \neq 0} \left(\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_p \hat{a}_{-p} + \hat{a}_p^\dagger \hat{a}_{-p}^\dagger \hat{a}_0 \hat{a}_0 \right)$$

Let's substitute into the equations $\hat{a}_0 = \hat{a}_0^\dagger = \sqrt{N_0}$ and rewrite it in terms $N = N_0 + \sum_{p \neq 0} \hat{a}_p^\dagger \hat{a}_p$. The quadratic terms in the number of non-condensate particles should be discarded. Thus, the complete Hamiltonian can be represented in the following form:

$$\hat{H} = \frac{N^2}{2V} \varphi + \sum_{p \neq 0} \epsilon_p \hat{a}_p^\dagger \hat{a}_p + \frac{N}{2V} \sum_{p \neq 0} \left(\hat{a}_p^\dagger \hat{a}_{-p}^\dagger + \hat{a}_p \hat{a}_{-p} \right), \quad \epsilon_p = \varepsilon_p + \varphi n. \quad (14)$$

We can assume that the total number of particles is fixed and the number of condensate particles is variable, then we can work with the Hamiltonian in form (14).

2. Bogoliubov transformation. \hat{H} can be diagonalized with a Bogoliubov transformation to a new set of creation and annihilation operators

$$\begin{aligned}\hat{a}_p^\dagger &= u_p \hat{\alpha}_p^\dagger + v_p \hat{\alpha}_{-p}, \\ \hat{a}_p &= u_p \hat{\alpha}_p + v_p \hat{\alpha}_{-p}^\dagger.\end{aligned}\quad (15)$$

The newly introduced $\hat{\alpha}_p$ and $\hat{\alpha}_p^\dagger$ have to obey bosonic commutation relations (canonical transformation):

$$[\hat{a}_p, \hat{a}_p^\dagger] = 1 = u_p^2 (\hat{\alpha}_p \hat{\alpha}_p^\dagger - \hat{\alpha}_p^\dagger \hat{\alpha}_p) + v_p^2 (\hat{\alpha}_{-p}^\dagger \hat{\alpha}_{-p} - \hat{\alpha}_{-p} \hat{\alpha}_{-p}^\dagger) + u_p v_p (\hat{\alpha}_p \hat{\alpha}_{-p} - \hat{\alpha}_{-p} \hat{\alpha}_p + \hat{\alpha}_{-p}^\dagger \hat{\alpha}_p^\dagger - \hat{\alpha}_p^\dagger \hat{\alpha}_{-p}^\dagger) = u_p^2 - v_p^2.$$

That allows for a convenient parametrization of the form $u_p = \cosh \theta_p$, $v_p = \sinh \theta_p$ with¹ $u, v \in \mathbb{R}$. In principle this is the same as substitution of the form $u_p = (1 - A_p^2)^{-1/2}$ and $v_p = A_p(1 - A_p^2)^{-1/2}$.

3. Diagonalization. We find the second relation after substituting (15) into the operator part of the Hamiltonian (14). Equating the coefficients in front of the products $\hat{\alpha}_p^\dagger \hat{\alpha}_{-p}^\dagger$ to zero, we obtain the missing equation:

$$\epsilon_p u_p v_p + \frac{\varphi}{2} (u_p^2 + v_p^2) = 0.$$

Now we find the unknown function A_p

$$A_p = \frac{-\epsilon_p + \sqrt{\epsilon_p^2 - (\varphi n)^2}}{\varphi n}. \quad (16)$$

Here we need to be careful with the sign. Ultimately, the Hamiltonian takes on a diagonal form

$$\hat{H} = \frac{N^2}{2V} \varphi + \sum_{p \neq 0} (\epsilon_p v_p^2 + \varphi n u_p v_p) + \sum_{p \neq 0} E_p \hat{\alpha}_p^\dagger \hat{\alpha}_p, \quad E_p = \sqrt{\epsilon_p^2 - (\varphi n)^2} = \sqrt{\left(\frac{p^2}{2m}\right)^2 + \frac{p^2}{m} \varphi n}, \quad (17)$$

where we substitute u_p , v_p in $E_p = \epsilon_p(u_p^2 + v_p^2) + 2\varphi n u_p v_p$. Note that the ground state $|0\rangle$ of the (17) is simply the vacuum state of Bogoliubov quasi-particles $\hat{\alpha}_p$, $\hat{\alpha}_p^\dagger$.

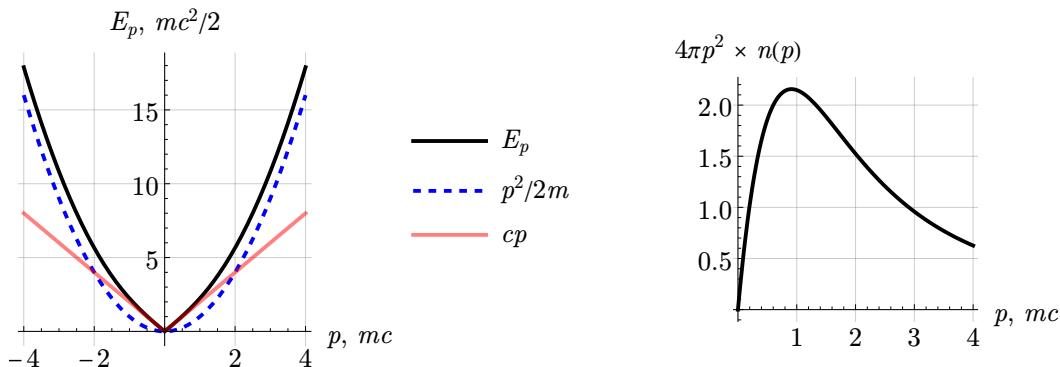


Figure 7: Excitation energy E_p and the momentum distribution function in 3D $4\pi p^2 n(p)$

4. Large canonical ensemble. In zero order ($N_0 \approx N$) we have $\hat{H} - \mu \hat{N} = -\mu N + \frac{N^2}{2V} \varphi$, thus $\Omega_0 = \langle \psi | \hat{H} - \mu \hat{N} | \psi \rangle \rightarrow \min$ and

$$\mu = \varphi n,$$

and we get $\Omega_0 = -\frac{N^2}{2V} \varphi$, so pressure is $P_0 = -\Omega_0/V$ and hydrodynamic speed of sound

$$c^2 = \frac{\partial P_0}{\partial \rho} = V \frac{\partial}{\partial(mN)} \left(-\frac{\Omega_0}{V} \right) = \frac{n\varphi}{m},$$

so we could rewrite E_p as

$$E_p = \sqrt{\left(\frac{p^2}{2m}\right)^2 + (cp)^2}, \quad \Rightarrow \quad E_p = \begin{cases} p^2/2m, & |p| \gg mc, \\ c|p|, & |p| \ll mc. \end{cases} \quad (18)$$

In the long-wave limit, the excitation spectrum has an acoustic character, and the calculated energy deviates from the linear law towards higher energies (fig. 7).

¹We can do this because there are no external fields imposed on the system.

5. Ground state and compressibility. Using (17) and (16) we could calculate the ground state energy

$$\langle 0 | \hat{H} - \mu \hat{N} | 0 \rangle = \Omega_0 = -\mu N + \frac{N^2}{2V} \varphi + \frac{1}{2} \sum_{p \neq 0} (E_p - \epsilon_p). \quad (19)$$

Yes, $\sum_{p \neq 0} (E_p - \epsilon_p)$ diverges as $E_p - \epsilon_p \approx -mn_0^2 \varphi^2 / p^2$ at $p \gg mc$, but for now we will ignore this and find

$$\Omega_0 = -\frac{V}{2\varphi} \mu^2 - \sum_{p > 0} \left(\epsilon_p + \mu - \sqrt{\epsilon_p^2 - 2\epsilon_p \mu} \right)$$

with $N = \mu V / \varphi$, $n = \mu / \varphi$. Isothermal compressibility is equal

$$\kappa = -\frac{1}{V} \frac{\partial^2 \Omega}{\partial \mu^2} = \frac{1}{\varphi} + \frac{1}{V} \sum_{p > 0} \frac{\sqrt{\epsilon_p}}{(\epsilon_p - 2\mu)^{3/2}}, \quad \Rightarrow \quad \lim_{\varphi \rightarrow 0} \kappa = +\infty,$$

corresponding to the limit of the ideal Bose gase.

6. Non-condensate particles. Now we could express explicitly the number of non-condensate particles by *u-v* Bogoliubov transformation $\langle \hat{a}_p^\dagger \hat{a}_p \rangle = \langle \hat{\alpha}_p^\dagger \hat{\alpha}_p \rangle + v_p^2$. Statistical distribution of elementary excitations $\langle \hat{\alpha}_p^\dagger \hat{\alpha}_p \rangle$ with $T \neq 0$ is given by the Bose distribution with $\mu = 0$

$$\langle \hat{\alpha}_p^\dagger \hat{\alpha}_p \rangle = \frac{1}{e^{\beta E_p} - 1}.$$

With $T = 0$ (fig. 7)

$$N(p) = \langle \hat{a}_p^\dagger \hat{a}_p \rangle = v_p^2 = \frac{m^2 c^4}{2E_p \left(E_p + mc^2 + \frac{p^2}{2m} \right)}.$$

The total number of non-condensate particles at $T = 0$ is (3D case)

$$N - N_0 = \frac{V}{(2\pi\hbar)^3} \int_0^\infty 4\pi p^2 dp \langle \hat{a}_p^\dagger \hat{a}_p \rangle = N \sqrt{n} \frac{(m\varphi)^{3/2}}{3\pi^2 \hbar^3},$$

and corresponding quantum depletion of the condensate

$$\frac{N - N_0}{N} = \sqrt{n} \frac{(m\varphi)^{3/2}}{3\pi^2 \hbar^3}.$$

Inserting² $u = \frac{4\pi a}{m} \hbar^2$, $a = 5 \text{ nm}$ and $n = 10^{20} \text{ m}^{-3}$ (typical values for an ultracold atom experiment with ⁸⁷Rb)

$$\frac{N - N_0}{N} \approx 5 \cdot 10^{-2},$$

which justifies the approximation used.

²I am not sure about it, but $[\varphi] = [a/m] \cdot [\hbar]^2$ according to the (13), that's why wrote φ in this way.

8.1 Effective action of a condensate in a double well

The following Hamiltonian is a simple model of a condensate in two wells:

$$H = -\frac{g}{2} \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{4} \sum_j n_j(n_j - 1), \quad (20)$$

with $j \in \{1, 2\}$. Consider a system with in total $2N$ particles. After normal ordering $[a_i, a_j^\dagger] = \delta_{ij}$

$$H(a^\dagger, a) = -\frac{g}{2} \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{4} \sum_j a_j^\dagger a_j^\dagger a_j a_j.$$

Non-interacting case. Let's start with $U = 0$ and operator canonical transformation (Fourier transform)

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$

which automatically satisfies the commutation relations $[a_j, a_j^\dagger] = \sin(\alpha)^2 + \cos(\alpha)^2 = 1$. Substituting into the Hamiltonian, we find the condition for diagonalization

$$\cos(\alpha)^2 - \sin(\alpha)^2 = 0, \quad \stackrel{\alpha=\pi/4}{\Rightarrow} \quad a_{1,2} = \frac{1}{\sqrt{2}}(b_1 \pm b_2),$$

and the Hamiltonian

$$H = -\frac{g}{2} \sum_{\langle i,j \rangle} a_i^\dagger a_j = \frac{g}{2} b_1^\dagger b_1 - \frac{g}{2} b_2^\dagger b_2, \quad (21)$$

with ground state $|0, 2N\rangle_b$. Define $|n, 2N-n\rangle_b \stackrel{\text{def}}{=} |n, 2N-n\rangle_b$. Now let's find the δN as

$$\begin{aligned} \delta N &= a_2^\dagger a_2 - a_1^\dagger a_1 = -b_2^\dagger b_1 - b_1^\dagger b_2, \\ (\delta N)^2 &= b_1^\dagger b_1 + b_2^\dagger b_2 + 2b_2^\dagger b_1^\dagger b_1 b_2 = 2N + 4nN - 2n^2. \end{aligned}$$

We immediately see that in the ground state

$$\langle \delta N^2 \rangle_{\text{gs}} = 2N. \quad (22)$$

Note that the temperature correction will be

$$\frac{1}{N} \langle \delta N^2 \rangle = 2 \coth\left(\frac{1}{2}\beta g\right) \approx 2 + 4e^{-\beta g}.$$

To calculate this we can start with the partition function

$$Z = \sum_{n=0}^{2N} e^{-\beta E_n} = \frac{e^{\beta g(N+1)} - e^{-\beta gN}}{e^{\beta g} - 1},$$

with $E_n = -g(N-n)$, and find $\langle n \rangle$ and $\langle n^2 \rangle$ through

$$\langle N-n \rangle = \frac{1}{\beta} \frac{1}{Z} \frac{\partial Z}{\partial g} = T \partial_g \ln Z, \quad \langle (N-n)^2 \rangle = \frac{1}{\beta^2} \frac{1}{Z} \frac{\partial^2 Z}{\partial g^2}.$$

Imaginary-time action. The imaginary-time action associated with this Hamiltonian in the coherent state representation

$$S = \int_0^\beta d\tau \bar{\psi} \partial_\tau \psi + H(\bar{\psi}, \psi) = \int_0^\beta d\tau \bar{\psi} \partial_\tau \psi - \frac{g}{2} \sum_{\langle i,j \rangle} \bar{\psi}_i \psi_j + \frac{U}{4} \sum_j \bar{\psi}_j \bar{\psi}_j \psi_j \psi_j.$$

Consider the density-phase representation given by

$$\psi_1 = \sqrt{N + \frac{\delta N}{2}} e^{i\varphi_1}, \quad \psi_2 = \sqrt{N - \frac{\delta N}{2}} e^{i\varphi_2}.$$

The action than

$$S \stackrel{\text{def}}{=} \int_0^\beta d\tau \mathcal{L}(\varphi, \theta) = \int_0^\beta d\tau 2Ni\dot{\theta} + \frac{\delta N}{2}i\dot{\varphi} - g\sqrt{N^2 - \left(\frac{\delta N}{2}\right)^2} \cos \varphi + 2\frac{U}{4} \left(\frac{\delta N}{2}\right)^2 + \frac{U}{2}N^2, \quad (23)$$

with $\varphi = \varphi_1 - \varphi_2$ and $\theta = \frac{1}{2}(\varphi_1 + \varphi_2)$. We can find the physical observables that are canonical conjugates to φ and θ

$$P_\varphi = \frac{\partial \mathcal{L}}{i\partial \dot{\varphi}} = \frac{\delta N}{2}, \quad P_\theta = \frac{\partial \mathcal{L}}{i\partial \dot{\theta}} = 2N,$$

with i factor from Wick rotation $\tau \rightarrow -it$ (it seems to me).

We can immediately see from Noether's theorem how symmetry in θ leads to conservation of $P_\theta = 2N = \text{const.}$ And indeed $\mathcal{L}(\theta) = \mathcal{L}(\theta + \text{shift}) - U(1)$ symmetry. On the other hand $\mathcal{L}(\varphi) \neq \mathcal{L}(\varphi + \text{shift})$, which corresponds to non-conservation of the $P_\varphi = \delta N$.

Effective action. Expanding the action to quadratic order in the particle number fluctuations $\delta N/N$ and the relative phase φ and neglecting constant terms

$$S_{\text{eff}}(\varphi, P_\varphi) = \int_0^\beta d\tau i P_\varphi \partial_\tau \varphi + \frac{1}{2} g N \varphi^2 + \frac{1}{2} (U + g/N) P_\varphi^2.$$

The fluctuations of the relative particle number between the wells $(\delta N)^2$ could be found as previous through the partition function Z

$$Z = \int D[\varphi, P_\varphi] e^{-S_{\text{eff}}(\varphi, P_\varphi)}, \quad \langle P_\varphi^2 \rangle = \frac{1}{Z} \int D[\varphi, P_\varphi] P_\varphi^2 e^{-S_{\text{eff}}[\varphi, P_\varphi]} = -\frac{2}{\beta Z} \partial_U Z = -\frac{2}{\beta} \frac{\partial \ln Z}{\partial U},$$

so in what follows we only look at factors containing U . Integrating by parts

$$\int_0^\beta d\tau P_\varphi i \partial_\tau \varphi = P_\varphi i \varphi \Big|_0^\beta - \int_0^\beta d\tau \varphi i \partial_\tau P_\varphi,$$

and $D[\varphi]$ could be calculated as gaussian integral

$$Z \propto \int D[P_\varphi] \exp \left(\int_0^\beta d\tau \left(-\frac{(\partial_\tau P_\varphi)^2}{2gN} + \frac{1}{2} (U + g/N) P_\varphi^2 \right) \right),$$

that could be calculated in Matsubara representation $2P_\varphi = \delta N = \frac{1}{\sqrt{\beta}} \sum_k e^{i\omega_k \tau} \delta N_k$

$$Z \propto \int D[\delta N_k] \exp \left(-\frac{1}{8} \sum_k \left(\frac{\omega_k^2}{gN} + U + \frac{g}{N} \right) \delta N_k \delta N_{-k} \right).$$

Since the fluctuation δN is real, then $\delta N_{-k} = \overline{\delta N}_k$, and

$$Z \propto \prod_k \left(\frac{\omega_k^2}{gN} + U + \frac{g}{N} \right)^{-1/2} \Rightarrow \langle \delta N^2 \rangle = \frac{4}{\beta} \sum_k \left(\frac{\omega_k^2}{gN} + U + \frac{g}{N} \right)^{-1},$$

with $\omega_k = 2\pi k/\beta$. After summation as

$$\sum_{k=-\infty}^{\infty} \frac{1}{k^2 + x^2} = \frac{\pi}{x} \frac{1}{\coth(\pi x)}, \quad \Rightarrow \quad \langle \delta N^2 \rangle = 2N \frac{\coth(\frac{1}{2}\beta g F_U)}{F_U},$$

with $F_U = \sqrt{1 + NU/g}$, in full accordance with formula (22).

Low fluctuations. The expansion in $\delta N/N$ is justified with $|\delta N|/N \ll 1$ or $\coth(\frac{1}{2}\beta g F_U)/NF_U \ll 1$. Note that temperature increases fluctuations and decreases interaction. Thus we could rewrite (23) as

$$S_{\text{eff}}(\varphi, P_\varphi) = \int_0^\beta d\tau P_\varphi i \partial_\tau \varphi - gN \cos(\varphi) + \frac{1}{2} UP_\varphi^2,$$

where we neglected P_φ^2/N term.

Equations of motion. The real-time effective action is

$$S_{\text{eff}}[\varphi, P_\varphi] = i \int_0^T dt \mathcal{L} = i \int_0^T dt (P_\varphi \partial_t \varphi + gN \cos(\varphi) - \frac{1}{2} UP_\varphi^2).$$

Classical equations of motion could be obtained from Euler–Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0, \quad \Rightarrow \quad \dot{\varphi} = UP_\varphi, \quad \Rightarrow \quad \ddot{\varphi} = -gNU \sin(\varphi).$$

The current between the wells is $\partial_t \delta N/2 = \partial_t P_\varphi = -gN \sin \varphi$, limited by gN .

Oscillation frequency. With $\varphi_0 \ll 1$ we could limit $|\varphi|$ and rewrite equations as

$$\ddot{\varphi} = gNU \varphi, \quad \Rightarrow \quad \varphi = \varphi_0 \cos(\sqrt{gNU} t),$$

so oscillation frequency is \sqrt{gNU} . Fluctuations are also small as $P_\varphi = \dot{\varphi}/U$. Non-interacting bosons oscillation could be found from (21) with $|\psi(t)\rangle = \sum_{n=0}^{2N} \alpha_n e^{ig(N-n)t} |n, 2N-n\rangle$, we obtain

$$\langle \delta N(t) \rangle = \langle \psi(t) | -b_2^\dagger b_1 - b_1^\dagger b_2 | \psi(t) \rangle = \langle \psi(t) | \sum_{n=1}^{2N-1} \sqrt{n(2N-n-1)} \alpha_n e^{ig(N-n)t} |n, 2N-n\rangle e^{-igt} = \sum_n \dots e^{-igt},$$

so oscillation frequency is g .

8.2 Vortex Excitation in a Superfluid

10.1 Phase Space Argument for the Life Time of Quasi-particles

1. Exact expression. Consider the Coulomb interaction in second quantization between electrons:

$$\hat{V} = \frac{1}{2\mathcal{V}} \sum_{\sigma\sigma'} \sum_{kk'q} V(q) c_{k+q,\sigma}^\dagger c_{k'-q,\sigma'}^\dagger c_{k',\sigma'} c_{k,\sigma},$$

\mathcal{V} is the volume. Taking into account only scattering processes that involve two particles, we could derive an expression for the inverse life time $1/\tau_k$ of the state³ $|i\rangle = |k_1, \sigma_1\rangle \stackrel{n}{=} c_{k_1, \sigma_1}^\dagger |\Omega\rangle$, where $|\Omega\rangle$ denotes the state, where all states below Fermi surface are occupied.

With Fermi's Golden Rule (fig. 8b)

$$\frac{1}{\tau_{k_1}} = 2\pi \sum_f |\langle f | \hat{V} | k, \sigma \rangle|^2 \delta(\varepsilon_i - \varepsilon_f), \quad |f\rangle \stackrel{n}{=} c_{k_1-Q, \sigma_1}^\dagger c_{k_2+Q, \sigma_2}^\dagger c_{k_2, \sigma_2} |\Omega\rangle.$$

Thus life time could be expressed from the matrix elements

$$\langle i | \hat{V} | f \rangle = \frac{1}{2\mathcal{V}} \sum_{\sigma\sigma'} \sum_{k'q} \mathcal{N}_{i,f} V(q) \langle \Omega | c_{k_1, \sigma_1} c_{k+q, \sigma}^\dagger c_{k'-q, \sigma'}^\dagger c_{k', \sigma'} c_{k, \sigma} c_{k_1-Q, \sigma_1}^\dagger c_{k_2+Q, \sigma_2}^\dagger c_{k_2, \sigma_2} |\Omega\rangle,$$

with normalizing factor

$$\mathcal{N}_{i,f} = ((1 - n_{k_1, \sigma_1})(1 - n_{k_1-Q, \sigma_1})(n_{k_2, \sigma_2})(1 - n_{k_2+Q, \sigma_2}))^{-1/2},$$

since $\langle c^\dagger c \rangle = n$ and $\langle cc^\dagger \rangle = 1 - n$.

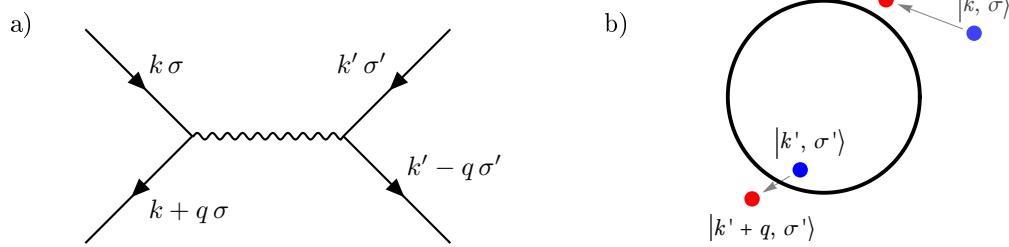


Figure 8: Scattering process

To calculate this matrix element we need just to decide how to distribute $|k_1, \sigma_1\rangle, |k_2, \sigma_2\rangle, |k_1 - Q, \sigma_1\rangle, |k_2 + Q, \sigma_2\rangle$ over the $|k, \sigma\rangle, |k', \sigma'\rangle, |k' - q, \sigma'\rangle, |k + q, \sigma\rangle$ (fig. 8a). There are only two different ways to do this (sign could be found as in the Wick's theorem):

$$\begin{aligned} \langle i | \hat{V} | f \rangle_1 &= \frac{\mathcal{N}_{i,f}}{2\mathcal{V}} \sum_{k, k', q} \sum_{\sigma_1, \sigma_2} V(q) \delta_{\sigma_1, \sigma} \delta_{\sigma_2, \sigma'} \delta(k_1 - k - q) \delta(Q - q) (1 - n_{k_1}) n_{k_2} (1 - n_{k_1-Q}) (1 - n_{k_2+Q}) \\ &= \frac{\mathcal{N}_{i,f}}{2\mathcal{V}} V(Q) (1 - n_{k_1, \sigma_1}) n_{k_2, \sigma_2} (1 - n_{k_2+Q, \sigma_2}) (1 - n_{k_1-Q, \sigma_1}), \end{aligned}$$

and

$$\langle i | \hat{V} | f \rangle_2 = \dots = -\frac{\mathcal{N}_{i,f}}{2\mathcal{V}} V(k_1 - k_2 - Q) \delta_{\sigma_1, \sigma_2} (1 - n_{k_1, \sigma_1}) n_{k_2, \sigma_2} (1 - n_{k_2+Q, \sigma_2}) (1 - n_{k_1-Q, \sigma_1}).$$

Due to symmetry, each term will appear twice, which means

$$\langle i | \hat{V} | f \rangle = \frac{\mathcal{N}_{i,f}}{\mathcal{V}} V(Q) (1 - \delta_{\sigma_1, \sigma_2}) (1 - n_{k_1, \sigma_1}) (1 - n_{k_1-Q, \sigma_1}) (n_{k_2, \sigma_2}) (1 - n_{k_2+Q, \sigma_2}) = \frac{1 - \delta_{\sigma_1, \sigma_2}}{\mathcal{V} \mathcal{N}_{i,f}} V(Q).$$

As expected, we found that only particles with different spins are scattered.

Let's move on to integration

$$\frac{1}{\tau_{k_1}} = 2\pi \sum_f |\langle f | \hat{V} | k, \sigma \rangle|^2 \delta(\varepsilon_i - \varepsilon_f) = \frac{2\pi}{\mathcal{V}^2} \int \frac{d^3 k_2}{(2\pi)^6} \frac{d^3 Q}{(2\pi)^6} |V(Q)|^2 \mathcal{N}_{i,f}^{-2} \delta(\varepsilon_i - \varepsilon_f) \sum_{\sigma_2} (1 - \delta_{\sigma_1, \sigma_2}),$$

with $\varepsilon_i - \varepsilon_f = \varepsilon_{k_1} - \varepsilon_{k_1-Q} - \varepsilon_{k_2+Q} + \varepsilon_{k_2}$.

2. Approximate calculation. By anticipating the result for the screening of the Coulomb interaction, we can assume that $V(Q) \approx V(0) = \text{const}$. It is convenient to use (with $\xi = \varepsilon - \varepsilon_F$ and $d\mathbf{k} = d\cos\theta d\varphi$)

$$\int \frac{d^3 k}{(2\pi)^3} = \int \frac{d\mathbf{k}}{4\pi} \int d\xi N(\xi) = N(0) \int \frac{d\mathbf{k}}{4\pi} \int d\xi.$$

We consider system at $T = 0$:

$$(1 - n_{k_1, \sigma_1})(1 - n_{k_1-Q, \sigma_1})(n_{k_2, \sigma_2})(1 - n_{k_2+Q, \sigma_2}) = \theta(\xi_{k_1}) \theta(-\xi_{k_2}) \theta(\xi_{k_1-Q}) \theta(\xi_{k_2+Q}).$$

³Here and further $\stackrel{n}{=}$ means that we ignore normalization factor, that appears in $\mathcal{N}_{i,f}$.

Substituting this into the expression for the lifetime, we find

$$\frac{1}{\tau_{k_1}} \approx \frac{2\pi}{V^2} |N(0)|^2 V(0)^2 \int d\xi_{k_2} \int \frac{d\mathbf{k}_{k_2}}{4\pi} \int d\xi_Q \int \frac{d\mathbf{k}_Q}{4\pi} \theta(\xi_{k_1}) \theta(-\xi_{k_2}) \theta(\xi_{k_1-Q}) \theta(\xi_{k_2+Q}) \delta(\varepsilon_{k_1} - \varepsilon_{k_1-Q} - \varepsilon_{k_2+Q} + \varepsilon_{k_2}).$$

Let's define $k_f = k_1 - Q$. As in the fig. 8b we take $\xi_{k_1} > 0$ and $\xi_{k_2+Q} > 0$

$$\delta(\varepsilon_{k_1} - \varepsilon_{k_f} - \varepsilon_{k_1+k_2-k_f} + \varepsilon_{k_2}) = \frac{1}{2\varepsilon_F} \delta \left(1 + \tilde{\mathbf{k}}_1 \cdot \tilde{\mathbf{k}}_2 - \tilde{\mathbf{k}}_1 \cdot \tilde{\mathbf{k}}_f - \tilde{\mathbf{k}}_2 \cdot \tilde{\mathbf{k}}_f \right),$$

with $\tilde{\mathbf{k}} = \mathbf{k}/k$. Rewriting the integral for the last time

$$\frac{1}{\tau_{k_1}} \approx \frac{2\pi}{V^2} |N(0)|^2 V(0)^2 \int_{-\xi_{k_1}}^0 d\xi_{k_2} \int_0^{\xi_{k_1}-\xi_{k_2}} d\xi_{k_f} \int \frac{d\mathbf{k}_{k_2}}{4\pi} \int \frac{d\mathbf{k}_Q}{4\pi} \frac{1}{2\varepsilon_F} \delta \left(1 + \tilde{\mathbf{k}}_1 \cdot \tilde{\mathbf{k}}_2 - \tilde{\mathbf{k}}_1 \cdot \tilde{\mathbf{k}}_f - \tilde{\mathbf{k}}_2 \cdot \tilde{\mathbf{k}}_f \right),$$

so finally

$$\frac{1}{\tau_{k_1}} \propto (\varepsilon_{k_1} - \varepsilon_F)^2.$$

10.2 Microscopic Basis of the Fermi-liquid Theory

Fermi liquid theory only holds if the ground state of the interacting system is connected adiabatically to the non-interacting Fermi sea. One can treat this as turning on the interactions adiabatically. The ground state $|\text{gs}\rangle$ of the full system and the excitation state $|\mathbf{k}, \sigma\rangle$ can then be written as

$$|\text{gs}\rangle = U |\Omega\rangle, \quad |\mathbf{k}, \sigma\rangle = U |\mathbf{k}, \sigma\rangle = U c_{\mathbf{k}, \sigma}^\dagger |\Omega\rangle.$$

The time evolution operator in the interaction picture can be expressed as a time-ordered exponential

$$U = T \left\{ e^{-i \int_{-\infty}^0 \hat{V}(t) dt} \right\}.$$

The quasi-particle creation operator (№3) could be expressed from the

$$|\mathbf{k}, \sigma\rangle = a_{\mathbf{k}, \sigma}^\dagger |\text{gs}\rangle = U c_{\mathbf{k}, \sigma}^\dagger |\Omega\rangle = U c_{\mathbf{k}, \sigma}^\dagger U^{-1} |\varphi\rangle, \quad \Rightarrow \quad a_{\mathbf{k}, \sigma}^\dagger = U c_{\mathbf{k}, \sigma}^\dagger U^{-1}.$$

For Fermi liquid theory to be valid, one need to add requirement on the wavefunction renormalization constant

$$Z_k = |\langle \mathbf{k}, \sigma | c_{\mathbf{k}, \sigma}^\dagger | \text{gs} \rangle|^2 = |\langle \text{gs} | a_{\mathbf{k}, \sigma} c_{\mathbf{k}, \sigma}^\dagger | \text{gs} \rangle|^2.$$

Expressing $c_{\mathbf{k}, \sigma}^\dagger$ as a series in the quasi-particle operators

$$\begin{aligned} c_{\mathbf{k}, \sigma}^\dagger &= U^\dagger a_{\mathbf{k}, \sigma}^\dagger U \approx \left(1 + i \int_{-\infty}^0 \hat{V}(t) dt \right) a_{\mathbf{k}, \sigma}^\dagger \left(1 - i \int_{-\infty}^0 \hat{V}(t) dt \right) = a_{\mathbf{k}, \sigma}^\dagger + i \int_{-\infty}^0 [\hat{V}(t), a_{\mathbf{k}, \sigma}^\dagger] dt + O(V^2) \\ &= \sqrt{Z_k} a_{\mathbf{k}, \sigma}^\dagger + \text{higher order} \end{aligned}$$

If we want to $c_{\mathbf{k}, \sigma}^\dagger \approx a_{\mathbf{k}, \sigma}^\dagger$, then (№4) $0 < \sqrt{Z_k} < 1$.

The spectral function (fig. 9)

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} G^{\text{ret}}(k, \omega) = \sum_{\lambda} |M_{\lambda}|^2 \delta(\omega - \xi_{\lambda}), \quad |M_{\lambda}|^2 = |\langle \lambda | c_{\mathbf{k}, \sigma}^\dagger | \text{gs} \rangle|^2$$

exhibits a sharp quasiparticle peak at ξ_k

$$A(k, \omega) = Z_k \delta(\omega - \xi_k) + \dots$$

with $Z_k > 0$. Thus momentum distribution $\langle \hat{n}_{k\sigma} \rangle$ has a jump at the Fermi momentum

$$\langle \hat{n}_{k\sigma} \rangle = \langle \text{gs} | c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} | \text{gs} \rangle = \int A(k, \omega) n_f(k, \omega) d\omega = \int Z_k \delta(\omega - \varepsilon_k) \theta(\varepsilon_f - \varepsilon_k) d\omega + \dots = Z_k \theta(\varepsilon_F - \varepsilon_k) + \dots$$

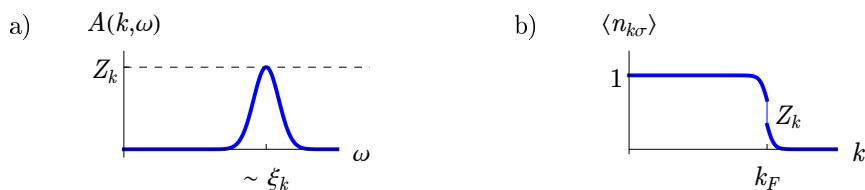


Figure 9: a) The spectral function. b) The momentum distribution.

QMB - HW 10 WS2022/2023

January 18, 2023

1 Green's function and density of states

First of all, let us establish a connection between the retarded Green's function $G^{\text{ret}}(\mathbf{k}, \omega)$ and the density of states of the system $\rho(\omega)$. Show that for **free particles**,

$$\rho(\omega) = -\frac{1}{\pi} \text{Im} \sum_{\mathbf{k}} [G^{\text{ret}}(\mathbf{k}, \omega)]$$

How can we express $\rho(\omega)$ in terms of the spectral function $A(\mathbf{k}, \omega)$?

The free fermion Hamiltonian:

$$\hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} \hat{c}_k^\dagger \hat{c}_k$$

The retarded green's function is the retarded (two-point) correlation for the creation and annihilation operators of the same state:

$$G^{\text{ret}} = C^r(t_1 - t_2) = -i\Theta(t_1 - t_2) \left\langle \left\{ c_k(t_2), c_k^\dagger(t_1) \right\} \right\rangle$$

or

$$G^{\text{ret}} = C^r(t) = -i\Theta(t) \left\langle \left\{ c_k(t), c_k^\dagger(0) \right\} \right\rangle$$

We have seen the imaginary-time cousin of this function before - see the lecture notes sec 2.4.4 for review.

The required Green's function has a very simple form:

$$C^r(\omega) = \frac{1}{\omega - E_{\mathbf{k}}}$$

To derive this, we need the Lehman representation the Green's function assumes the form:

- Fourier transform the real-time retarded Green's function:

$$C^r(\omega) = -i \int_{-\infty}^{\infty} dt e^{i\omega t - \mu|t|} C^r(t) = -i \int_0^{\infty} dt e^{i\omega t - \mu|t|} \left\langle \left\{ c_k(t), c_k^\dagger(0) \right\} \right\rangle$$

μ is introduced to ensure convergence, and later we will take $\lim_{\mu \rightarrow 0}$.

2. Then we substitute for the expectation value

$$\left\langle \left\{ c_k(t), c_k^\dagger(0) \right\} \right\rangle = \frac{1}{Z} \text{Tr} \left[\rho_H \left\{ c_k(t), c_k^\dagger(0) \right\} \right] = \frac{1}{Z} \sum_n e^{-\beta E_n} \left\langle n \left| \left\{ c_k(t), c_k^\dagger(0) \right\} \right| n \right\rangle$$

where ρ_H is the free-fermion equilibrium density function and $|n\rangle$ are the system's eigenstates. So far all of this was completely general. In our case $\rho_H(\beta) = e^{-\beta \hat{H}}$ and we emphasize $n = \{n_i\} \in \{0, 1\}^N$ to denote the multi-particle state $|n\rangle = \prod_{n_i} c_i^{\dagger n_i} |0\rangle$.

3. Time evolution of operators is given by

$$c_k^\dagger(t) = e^{i\hat{H}t} c_k^\dagger e^{-i\hat{H}t}$$

Therefore each element in the sum is actually

$$\begin{aligned} \sum_n e^{-\beta E_n} \left\langle n \left| \left\{ c_k^\dagger(t), c_k(0) \right\} \right| n \right\rangle &= \sum_n e^{-\beta E_n} \left(\left\langle n \left| c_k(t) c_k^\dagger(0) \right| n \right\rangle + \zeta \left\langle n \left| c_k^\dagger(0) c_k(t) \right| n \right\rangle \right) = \\ &= \sum_n e^{-\beta E_n} \left(\left\langle n \left| e^{i\hat{H}t} c_k e^{-i\hat{H}t} c_k^\dagger(0) \right| n \right\rangle + \zeta \left\langle n \left| c_k^\dagger(0) e^{i\hat{H}t} c_k e^{-i\hat{H}t} \right| n \right\rangle \right) = \\ &= \sum_n e^{-\beta E_n} \left(e^{iE_n t} \left\langle n \left| c_k e^{-i\hat{H}t} c_k^\dagger(0) \right| n \right\rangle + \zeta e^{-iE_n t} \left\langle n \left| c_k^\dagger(0) e^{i\hat{H}t} c_k \right| n \right\rangle \right) = \end{aligned}$$

next we insert resolutions of the identity $\sum_m |m\rangle \langle m|$ to get read from the other time evolution operators

$$\begin{aligned} C^r(t) &= \sum_n e^{-\beta E_n} \left\langle n \left| \left\{ c_k^\dagger(t), c_k(0) \right\} \right| n \right\rangle = \\ &= \sum_n e^{-\beta E_n} \sum_m \left(e^{iE_n t} \left\langle n \left| c_k e^{-i\hat{H}t} \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle + \zeta e^{-iE_n t} \left\langle n \left| c_k^\dagger \right| m \right\rangle \left\langle m \left| e^{i\hat{H}t} c_k \right| n \right\rangle \right) = \\ &= \sum_n e^{-\beta E_n} \sum_m \left(e^{i(E_n - E_m)t} \left\langle n \left| c_k \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle + \zeta e^{-i(E_n - E_m)t} \left\langle n \left| c_k^\dagger \right| m \right\rangle \left\langle m \left| c_k \right| n \right\rangle \right) = \\ &= \sum_n e^{-\beta E_n} \sum_m e^{i(E_n - E_m)t} \left\langle n \left| c_k \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle + \zeta \sum_n \sum_m e^{-\beta E_m} e^{-i(E_m - E_n)t} \left\langle m \left| c_k^\dagger \right| n \right\rangle \left\langle n \left| c_k \right| m \right\rangle = \\ &= \sum_n \sum_m \left(e^{-\beta E_n} e^{i(E_n - E_m)t} \left\langle m \left| c_k^\dagger \right| n \right\rangle \left\langle n \left| c_k \right| m \right\rangle + \zeta e^{-\beta E_m} e^{-i(E_m - E_n)t} \left\langle m \left| c_k^\dagger \right| n \right\rangle \left\langle n \left| c_k \right| m \right\rangle \right) = \\ &= \sum_n \sum_m \left(e^{-\beta E_n} e^{i(E_n - E_m)t} + \zeta e^{-\beta E_m} e^{-i(E_m - E_n)t} \right) \left\langle n \left| c_k \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle \\ C^r(t) &= \frac{1}{Z} \sum_n \sum_m \left(e^{-\beta E_n} + \zeta e^{-\beta E_m} \right) \left\langle n \left| c_k \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle e^{i(E_n - E_m)t} \end{aligned}$$

Now perform the time integration:

$$\begin{aligned} C^r(\omega) &= -i \frac{1}{Z} \sum_n \sum_m \left\langle n \left| c_k \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle \int_0^\infty dt e^{i\omega t - \mu|t|} \left(e^{-\beta E_n} e^{i(E_n - E_m)t} - \zeta e^{-\beta E_m} e^{-i(E_m - E_n)t} \right) = \\ &= i \frac{1}{Z} \sum_n \sum_m \left\langle n \left| c_k \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle \left[\frac{e^{-\beta E_n}}{i\omega - \mu + i(E_n - E_m)} - \frac{\zeta e^{-\beta E_m}}{i\omega - \mu + i(E_n - E_m)} \right] = \\ &= \frac{1}{Z} \sum_n \sum_m \left[\frac{e^{-\beta E_n}}{\omega + i\mu + (E_n - E_m)} - \frac{\zeta e^{-\beta E_m}}{\omega + i\mu + (E_n - E_m)} \right] |\left\langle m \left| c_k^\dagger \right| n \right\rangle|^2 \end{aligned}$$

Note $\langle n | c_k | m \rangle = (\langle m | c_k^\dagger | n \rangle)^*$ and $\langle m | c_k^\dagger | n \rangle = (\langle n | c_k | m \rangle)^*$.

We can evaluate the elements $|\langle m | c_k^\dagger | n \rangle|^2$. The state $|n\rangle$ must have no \mathbf{k} particles, Therefore adding such a particle changes the energy $E_m = E_n + E_{\mathbf{k}}$. If $|n\rangle$ contained a \mathbf{k} particle, that $c_{\mathbf{k}}^\dagger$ annihilates it.

$$\begin{aligned} C^r(\omega) &= \frac{1}{Z} \sum_{n,n_k=0} \left[\frac{e^{-\beta E_n} - \zeta e^{-\beta(E_n+E_k)}}{\omega + i\mu - E_k} \right] = \frac{1}{Z} \sum_{n,n_k=0} \frac{e^{-\beta E_n} (1 - \zeta e^{-\beta E_k})}{\omega + i\mu - E_k} = \\ &= \frac{1}{Z} \frac{1}{\omega + i\mu - E_k} (1 + e^{-\beta E_k}) \sum_{n,n_k=0} e^{-\beta E_n} \end{aligned}$$

The sum over m we can replace by $\sum_{m,m_k=0} e^{-\beta E_m} = \prod_{\vec{m},m_k=0} (1 + e^{-\beta E_{\vec{m}}})$. Hence we notice that we found the partition function Z :

$$Z = \sum_{\vec{m}} e^{-\beta E_{\vec{m}}} = \prod_{\vec{m}} (1 + e^{-\beta E_{\vec{m}}}) = (1 + e^{-\beta E_{\mathbf{k}}}) \prod_{\vec{m},m_k=0} (1 + e^{-\beta E_{\vec{m}}})$$

Now we arrived at the result we initially claimed:

$$C^r(t) = \frac{1}{Z} \frac{1}{\omega + i\mu - E_{\mathbf{k}}} (1 + e^{-\beta E_{\mathbf{k}}}) \sum_{n,n_k=0} e^{-\beta E_n} = \frac{1}{Z} \frac{1}{\omega + i\mu - E_{\mathbf{k}}} Z = \frac{1}{\omega - E_{\mathbf{k}} + i\mu} = G^{ret}(\mathbf{k}, \omega)$$

Now using Dirac's identity

$$\lim_{\mu \rightarrow 0^+} \frac{1}{\omega - E_k + i\mu} = -i\pi\delta(\omega - E_k) + P\frac{1}{x}$$

(Note this identity is meaningful strictly only under integration - it is valid for distributions).

We find the spectral function

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} C^r(\omega) = \delta(\omega - E_k)$$

To conclude the question, we remember that the density of states is defined as

$$\rho(\omega) = \sum_n \delta(\omega - \omega_n)$$

where ω_n are the eigenenergies of the system, so we found what we were looking for:

$$\rho(\omega) = -\frac{1}{\pi} \text{Im} \sum_k C^r(\omega) = \sum_k A(\mathbf{k}, \omega)$$

2 Properties of the spectral function

We want to show that the spectral function $A(\mathbf{k}, \omega)$ can be interpreted as a probability distribution over ω . For this, A must satisfy two conditions:

1. Normalization: $\int d\omega A(\mathbf{k}, \omega) = 1$.
2. Positivity: $A(\mathbf{k}, \omega) \geq 0$.

Positivity is guaranteed by $A(\mathbf{k}, \omega) = \delta(\omega - E_k)$ having a positive coefficient. for the case without interactions the normalization follows immediately:

$$\int d\omega A(\mathbf{k}, \omega) = \int d\omega \delta(\omega - E_k) = 1$$

With interaction the result still holds. The spectral function is then

$$A(\mathbf{k}, \epsilon) = \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle (e^{-\beta E_m} - \zeta e^{-\beta E_n}) \delta(\omega + E_n - E_m)$$

Where the states $|n\rangle, |m\rangle$ and energies E_n, E_m are the eigenstates and eigenenergies of the total (interacting) Hamiltonian.

$$\begin{aligned} \int d\epsilon A(\mathbf{k}, \epsilon) &= \int d\epsilon \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle (e^{-\beta E_m} - \zeta e^{-\beta E_n}) \delta(\omega + E_n - E_m) = \\ &= \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle (e^{-\beta E_m} - \zeta e^{-\beta E_n}) \delta(\omega + E_n - E_m) = \\ &= \frac{1}{\pi} \sum_{n,m} e^{-\beta E_n} \langle n | c_k^\dagger | m \rangle \langle m | c_k | n \rangle - \zeta \frac{1}{\pi} \sum_{n,m} e^{-\beta E_m} \langle n | c_k^\dagger | m \rangle \langle m | c_k | n \rangle = \\ &\quad = \frac{1}{Z} \text{Tr} \left[\rho_H [c_k^\dagger, c_k]_\zeta \right] \end{aligned}$$

For fermionic operators $\{c_k^\dagger, c_k\} = \mathbb{I}$ so $\int d\epsilon A(\mathbf{k}, \epsilon) = \frac{1}{Z} \text{Tr} [\rho_H \mathbb{I}] = \frac{1}{Z} \text{Tr} [\rho_H] = 1$. The result can be shown for any density matrix, not only those of thermal equilibrium. Positivity still holds for the interacting case because all of the terms in the sum are positive (The matrix elements contribute their squared absolute value, the exponents are positive and are summed for fermionic operators).

The spectral function can be used to calculate the expected occupancy $n_{B/F}(\mathbf{k}) = \frac{1}{e^{\beta E_k} - \zeta}$ of the eigenstates:

$$\int d\omega n_{B/F}(\hbar\omega) A(\mathbf{k}, \omega) = \int d\omega n_{B/F}(\hbar\omega) \delta(\omega + E_k) = n_{B/F}(E_k) = \langle n_{B/F}(E_k) \rangle$$

And also in the interacting case:

$$\begin{aligned}
\int d\omega n_{B/F}(\omega) A(\mathbf{k}, \omega) &= \int d\omega \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle (e^{-\beta E_n} - \zeta e^{-\beta E_m}) \delta(\omega + E_n - E_m) n_{B/F}(\omega) = \\
&= \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle (e^{-\beta E_n} - \zeta e^{-\beta E_m}) n_{B/F}(E_m - E_n) = \\
&= \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle e^{-\beta E_m} (e^{-\beta(E_n - E_m)} - \zeta) n_{B/F}(E_m - E_n) = \\
&= \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle e^{-\beta E_m} (e^{\beta(E_m - E_n)} - \zeta) \frac{1}{e^{\beta(E_m - E_n)} - \zeta} = \\
&= \frac{1}{Z} \sum_{n,m} \langle n | c_k | m \rangle \langle m | c_k^\dagger | n \rangle e^{-\beta E_m} = \frac{1}{Z} \sum_m \langle n | c_k^\dagger c_k | n \rangle e^{-\beta E_m} = \langle c_k^\dagger c_k \rangle = n_{B/F}(E_\mathbf{k}) = \langle n_{B/F}(E_\mathbf{k}) \rangle
\end{aligned}$$

This results is applies both for fermions and bosons. Generically the pole will be non-negative, so for the bosonic spectral function will also be a probability amplitudes, but this needs to be verified. Then the frequencies can be thought of as the energy, or the Bohr frequencies associated with the energies of the system's allowed transitions.

The spectral function describes how the systems reacts to the addition of a single particles \hat{c}_k^\dagger . The Hamiltonian couples (or not, depends on its interactions) the particle to the systems eigenstates. So initially the state is $\hat{c}_k^\dagger |\psi(t=0)\rangle$ which is a pure state, and after a certain time of evolution by the full Hamiltonian, the system will be in a super position of eigenstates that is dictated by the spectral function.

3 Just add interactions

The addition of interactions introduces the self energy operator $\Sigma(\omega) = \Sigma' + i\Sigma''$ (note Σ'' is negative). As a result, the simple spectral function with a single pole at E_k will be replaced by a distribution of poles, whose center now shifted to $E_k + \Sigma'$, with a width characterized by Σ'' . The intensity of the singularities decays with the distance from the center. A Fourier transform of the Green's function allows to estimate the excitation's life time:

$$G^{ret}(\mathbf{k}, \omega) = \frac{1}{\omega - E_k - \Sigma} = \frac{1}{\omega - E_k - \Sigma' - i\Sigma''}$$

To do the Fourier transform $G^{ret}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G^{ret}(\mathbf{k}, \omega)$, compute the integral by considering a complex frequency z and a suitable contour integral for $f(z) = \frac{e^{-izt}}{\omega - z}$.

1. First shift $\omega \rightarrow \omega' = \omega - E_k - \Sigma'$. This will brings out a phase factor $e^{-i(E_k + \Sigma')t}$.
2. For $t < 0$, notice the pole is below the real line. Close the contour by parameterizing $z(\theta) = Re^{i\theta}$, $\theta \in [0, \pi]$ on a semi-circular path, and on the real line $z \in [-R, R]$. On the circular path $e^{-izt} = e^{-iR\cos\theta} e^{R\sin\theta t}$

which decays strongly because of the positive $\sin \theta$ and negative time. Therefore the integral on this part is 0, and since the contour closes over no poles the integral on the other part vanishes as well.

3. For $t > 0$, do a similar parametrization, however below the real line. The signs of t and $\sin \theta$ will be exchanged. Now there is a single simple pole with residue $\text{Res} \left[e^{-izt} \frac{1}{z-i\Sigma''} \right] = \lim_{z \rightarrow i\Sigma''} (z - i\Sigma'') f(z) = e^{-i(i\Sigma'')t}$, and $\oint dz e^{-izt} \frac{e^{-izt}}{\omega-z} = 2\pi i \text{Res} \left[e^{-izt} \frac{1}{z-i\Sigma''} \right]$.

To conclude:

$$G^{ret}(t) \propto \Theta(t) i e^{-i(E_k + \Sigma')t} e^{\Sigma''|t|}$$

Since $G(t)$ measures the particles probability to still exist at time t (the amplitude of the single particle state), the exponential decay ($\Sigma'' < 0!$) in G indicates the particle will not survive.

To which order in the Coulomb interaction do need to go to actually see this? Second order is sufficient because there we have a diagram that contains a virtual particle with the same mass as the initial additional particle. In the diagram there will be three propagators, each contributing a factor of i which will not vanish thank to the virtual particle.

12.1 Fermions in one dimension

Consider 1D non-interacting electrons described by the Hamiltonian

$$\hat{H} = \sum_k \xi_k \hat{c}_k^\dagger \hat{c}_k, \quad \xi_k = \varepsilon_k - \mu.$$

We want to compute the Lindhard function χ_0 is the correlation function associated with the response to a change of the chemical potential.

1. Lindhard function. The density response function $\chi_0(q, \omega)$ of a one-dimensional Fermi gas

$$\chi_0(q, t) = -\frac{i}{\hbar} \theta(t) \langle [\hat{\rho}_q(t), \hat{\rho}_{-q}(0)] \rangle,$$

Thus we find for the Fourier transform of the Lindhard function

$$\chi_0(q, \omega) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t) \langle [\hat{\rho}_q(t), \hat{\rho}_{-q}(0)] \rangle = -\frac{i}{\hbar V} \sum_k \int_0^{\infty} dt e^{i(\omega - (\xi_k - \xi_{k+q}))t} [n_{k+q}(1 - n_k) - n_k(1 - n_{k+q})],$$

where we took advantage of the quadratic Hamiltonian of free fermions.

$$\chi_0(q, \omega) = \frac{1}{\hbar V} \sum_k \frac{n_{k+q} - n_k}{\omega - (\xi_k - \xi_{k+q}) + 0i}.$$

Moving on to integration

$$\chi_0(q, \omega) = \frac{1}{V\hbar} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{n_{k+q} - n_k}{\omega - (\xi_k - \xi_{k+q}) + 0i} = \mathcal{P} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{n_{k+q} - n_k}{\omega - (\xi_k - \xi_{k+q})} - i\pi \int_{-\infty}^{\infty} \frac{dk}{2\pi} (n_{k+q} - n_k) \delta(\omega - (\xi_{k+q} - \xi_k)),$$

we get

$$\begin{aligned} \chi_0''(q, \omega) &= \text{Im } \chi_0(q, \omega) = \frac{1}{2} \int_{-\infty}^{\infty} dk (\delta(\omega - (\xi_{k+q} - \xi_k)) - \delta(\omega - (\xi_k - \xi_{k-1}))) n_k \\ &= \frac{m}{2|q|} \int_{-\infty}^{\infty} n_k (\delta(k - k_-) - \delta(k - k_+)) dk = \frac{m}{2|q|} (n_{k_-} - n_{k_+}), \end{aligned}$$

with defined zeros

$$\delta(\omega - (\xi_{k+q} - \xi_k)) = \frac{m}{|q|} \delta(k - k_{\pm}), \quad k_{\pm} = \frac{2m\omega \pm q^2}{2q}.$$

2. Perturbation. The energy absorption rate $\propto \chi_0(q, \omega)$ from the perturbation (q, ω) . At zero temperature $\chi_0(T=0)''$ could be rewritten as

$$\chi_0''(q, \omega) = \frac{m}{2|q|} (\theta(-\xi_{k_-}) - \theta(-\xi_{k_+})), \quad \xi_k = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k_F^2}{2m}, \quad k_{\pm} = \frac{2m\omega + q^2}{2q},$$

which completely defines regions with non-zero absorption. Let's find conditions for the boundaries (in units of k_F and ε_F)

$$\begin{cases} k_F^2 - k_-^2 > 0 \\ k_F^2 - k_+^2 < 0 \end{cases} \Rightarrow \begin{cases} q - \frac{1}{2}q^2 < \omega < q + \frac{1}{2}q^2, & 0 < q < 2 \\ -q + \frac{1}{2}q^2 < \omega < q + \frac{1}{2}q^2, & q > 2 \end{cases}$$

, which, taking into account symmetry $\chi_0''(q) = \chi_0''(-q)$, leads to (fig. 10). Here we see well defined sharp $\omega(q)$ at $q \ll k_F$ (in contrast to 2D/3D case with macroscopic Fermi surface).

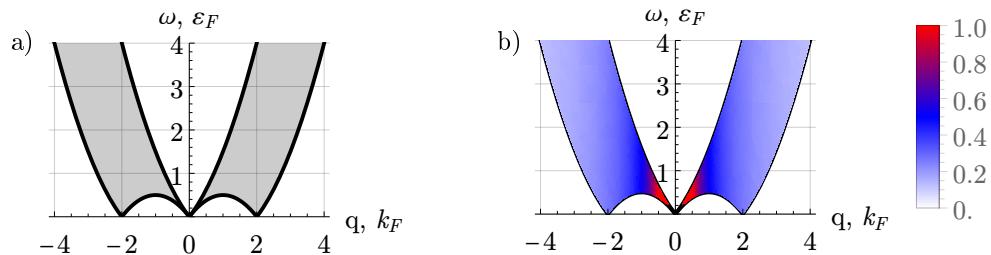


Figure 10: a) Nonzero energy absorption rate regions. b) The density response function χ of the weak interacting system.

3. The sound velocity. The sound velocity of the 1D non-interacting Fermi gas, i.e. the proportionality constant of the linear dispersion at small q

$$v_{\text{sound}} = \frac{\hbar k_F}{m} \frac{\partial}{\partial q} (q - \frac{1}{2}q^2) |_{q=0} = \frac{\hbar k_F}{m} = v_F.$$

4. Width. The width of the region in which energy can be absorbed $\delta\omega(q \ll k_F)$

$$\delta\omega(q \ll k_F) \approx \varepsilon_F (q/k_F)^2,$$

so there is a sharp collective mode in the spectrum in the sense that

$$\lim_{q \rightarrow 0} \frac{\delta\omega(q)}{\omega(q)} = \frac{\varepsilon_F}{k_F^2} \lim_{q \rightarrow 0} \frac{q^2}{v_F q} = 0,$$

and (remembering Luttinger's liquid) operator that create these excitations on top of the ground-state $\hat{\rho}_q$, which is specific to one-dimensional systems.

5. RPA. Now we add a contact interaction u between the Fermions. The density response function $\chi(q, \omega)$ of the interacting system at small q at zero temperature, using the result of the random phase approximation (RPA)

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - u\chi_0(q, \omega)}.$$

To find the pole we need

$$\begin{aligned} \chi'_0(q, \omega) &= \text{Re} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{n_{k+q} - n_k}{\omega - (\xi_{k+q} - \xi_k) + 0i} \\ &= \text{Re} \int_{-k_F-q}^{k_F-q} \frac{dk}{2\pi} \frac{1}{\omega - \frac{1}{2m}(2kq + q^2) + i0} - \text{Re} \int_{-k_F}^{k_F} \frac{dk}{2\pi} \frac{1}{\omega - \frac{1}{2m}(2kq + q^2) + i0} \\ &\approx \frac{1}{\pi} \frac{q^2 v_F}{\omega^2 + v_F^2 q^2}. \end{aligned}$$

Thus ξ has a pole at $1 - u\chi_0 = 0$

$$\omega = \sqrt{1 + \frac{1}{\pi v_F}} v_F = \tilde{v}_{\text{sound}} q, \quad \tilde{v}_{\text{sound}} = v_F \sqrt{1 + \frac{u}{\pi v_F}},$$

with almost the same the sound velocity.

6. On the way to bosonisation. The sound-mode exhausts the f -sum rule

$$\int_{-\infty}^{\infty} \omega S(q, \omega) d\omega = \frac{q^2}{2m},$$

at zero temperature, i.e. all the excitations of a 1D Fermi system are phonons. The imaginary part

$$\chi''(q, \omega) = \frac{\chi''_0}{(1 - u\chi'_0)^2 + u^2(\chi''_0)^2} \stackrel{\chi'' \neq 0}{=} \frac{m}{2|q|} \left(\left(\frac{um}{2q} \right)^2 + \left(1 - \frac{u}{\pi} \frac{q^2 v_F}{q^2 v_F^2 + \omega^2} \right)^2 \right)^{-1}.$$

Thus sum rule

$$\int_{-\infty}^{\infty} \omega S(q, \omega) d\omega = 2 \int_{-\infty}^{\infty} \omega \chi''(q, \omega) \theta(\omega) d\omega = \frac{1}{\pi} \int_0^{\infty} \omega \chi''(q, \omega) d\omega.$$

We could for example assume $q \ll k_F$ and expand in series of ω

$$\omega \chi''(q, \omega) \approx \frac{m\omega}{2q \left(\frac{m^2 u^2}{4q^2} + \left(1 - \frac{u}{\pi v_F} \right)^2 \right)},$$

and

$$\int_{-\infty}^{\infty} \omega S(q, \omega) \approx \int_{-q^2/2}^{q+q^2/2} \frac{\omega}{2q} \left(\frac{u^2}{4q^2} + \left(1 - \frac{u}{\pi} \right)^2 \right) \approx q^2 \left(\frac{u^2}{4q^2} + \frac{u^2}{\pi^2} - \frac{2u}{\pi} + 1 \right)^{-1},$$

with $m = 1$, $v_F = 1$. In general, something like a quadratic.

13.1 Stoner instability

Consider a 3D Fermi gas with point-like interactions:

$$H = T + V = \sum_{k\sigma} \left(\frac{k^2}{2m_e} - \mu \right) n_{k\sigma} + u \int \psi_\uparrow^\dagger(x) \psi_\downarrow^\dagger(x) \psi_\downarrow(x) \psi_\uparrow(x) d^3x,$$

or, completely in the momentum representation:

$$H = \sum_{k\sigma} \left(\frac{k^2}{2m_e} - \mu \right) n_{k\sigma} + \frac{u}{V} \sum_{k_1, k_2, q} c_{k_1+q, \uparrow}^\dagger c_{k_2-q, \downarrow}^\dagger c_{k_2, \downarrow} c_{k_1, \uparrow},$$

after substitution $\psi_\sigma(x) = V^{-1/2} \sum_k e^{-ikx} c_{k, \sigma}$.

The density of states. The density of states at the Fermi Energy for the non-interacting system

$$2 \int \frac{d^3k}{(2\pi)^3} = \int d\varepsilon D(\varepsilon), \quad \Leftrightarrow \quad D(\varepsilon) = 2 \int \frac{d^3k}{(2\pi)^3} \delta(\varepsilon - \varepsilon_k) = \frac{\sqrt{2}}{\pi^2} m_e^{3/2} \sqrt{\varepsilon},$$

with $\varepsilon_k = \frac{1}{2m_e} k^2$. Considering that $n = \frac{N}{V} = \frac{2}{6\pi^2} k_F^3$, we have

$$D_F \stackrel{\text{def}}{=} D(\varepsilon_F) = \frac{3^{1/3}}{2\pi^{4/3}} m_e \left(\frac{N}{V} \right)^{1/3}.$$

For an interacting gas, as a first approximation, we can simply replace the mass $m \rightarrow m_{\text{eff}}$.

The Hartree-Fock approximation. Consider one parameter family of states $|m\rangle$:

$$\begin{aligned} m &= \frac{1}{V} (N_\uparrow - N_\downarrow) \\ n &= \frac{1}{V} (N_\uparrow + N_\downarrow) \end{aligned}$$

which have a fixed magnetisation m and density n , as trial states to find the magnetisation m which minimises the energy $E(m) = \langle m | H | m \rangle$. For kinetic energy term⁴

$$\langle m | T | m \rangle = \sum_{k,\sigma}^{k_F} \left(\frac{k^2}{2m_e} - \mu \right) n_{k\sigma} = \sum_{\sigma} V \int \frac{d^3k}{(2\pi)^3} \left(\frac{k^2}{2m_e} - \mu \right) \theta(\varepsilon_F(\sigma) - \varepsilon_k) = \frac{1}{m_e} \left(\frac{\pi^4}{V^2} \right)^{1/3} \left(N_\uparrow^{5/3} + N_\downarrow^{5/3} \right) + \frac{1}{2} \mu N,$$

with $N_{\uparrow, \downarrow} = \frac{N}{2} (1 \pm \frac{m}{n})$. And, by Wick's theorem, for interaction energy

$$\langle m | V | m \rangle = \frac{u}{V} \sum_{k_1, k_2, q} \langle c_{k_1+q, \uparrow}^\dagger c_{k_1, \uparrow} \rangle \langle c_{k_2-q, \downarrow}^\dagger c_{k_2, \downarrow} \rangle - \frac{u}{V} \sum_{k_1, k_2, q} \langle c_{k_1+q, \uparrow}^\dagger c_{k_2, \downarrow} \rangle \langle c_{k_2-q, \downarrow}^\dagger c_{k_1, \uparrow} \rangle = \frac{u}{V} \sum_{k_1, k_2} n_{k_1 \uparrow} n_{k_2 \downarrow} = \frac{u}{V} N_\uparrow N_\downarrow.$$

Thus the expression for energy is

$$\begin{aligned} E(m) &= \frac{1}{m_e} \left(\frac{\pi^4}{V^2} \right)^{1/3} \left(\frac{N}{2} \right)^{5/3} \left(\left(1 + \frac{m}{n} \right)^{5/3} + \left(1 - \frac{m}{n} \right)^{5/3} \right) + \frac{uN^2}{4V} \left(1 - \frac{m^2}{n^2} \right) \\ D_F E(m)/V &= \left(\frac{9}{20} + \frac{1}{4} u D_F \right) n^2 + \left(\frac{1 - u D_F}{4} \right) m^2 + \frac{1}{108} \frac{m^4}{n^2} + o(m^4). \end{aligned}$$

It looks like a second-order phase transition in Landau's theory, only with interaction u instead of T – quantum phase transition. Magnetisation

$$m(u) = \pm \sqrt{\frac{27}{2}} \theta(u D_F - 1) n \sqrt{u D_F - 1}.$$

Stoner criterion. The critical value of the dimensionless interaction strength for the gas developing a spontaneous magnetisation $m \neq 0$ within the HF approximation

$$uD_F > 1, \quad \Rightarrow \quad u_{\text{crit}} = \frac{1}{D_F}.$$

The critical exponent

$$m \sim \theta(u - u_{\text{crit}}) \left(\frac{u - u_{\text{crit}}}{u_{\text{crit}}} \right)^\beta,$$

corresponds to the $\beta = 1/2$, as in the classical Ising model – second order phase transition.

⁴Here I don't write $5^{-1} 3^{5/3} 2^{-1/3} \approx 0.99 \approx 1$, but take into account in calculations.

13.2 Bogoliubov rotation and gap equation at zero temperature

Let us consider the BCS Hamiltonian

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{\Omega} \sum_{k,k'} V_{kk'} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger c_{-k\downarrow} c_{k\uparrow},$$

where $\xi_k = \varepsilon_k - \mu$ is the single particle energy with respect to the chemical potential μ . We introduce the creation operators for Bogoliubov quasiparticles, denoted $\gamma_{k\sigma}^\dagger$, via the Bogoliubov rotation

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} \sin \theta_k & -\cos \theta_k \\ \cos \theta_k & \sin \theta_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix}, \quad \tan \theta_k = \frac{\Delta_k}{E_k - \xi_k},$$

where $\Delta_k = -\frac{1}{\Omega} \sum_k V_{kk'} \langle c_{-k\downarrow} c_{k'\uparrow} \rangle$ is the gap function and $E_k = \sqrt{\Delta_k^2 + \xi_k^2}$. It's usefull to have

$$\begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} \sin \theta_k & \cos \theta_k \\ -\cos \theta_k & \sin \theta_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_p & v_p \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix}$$

The Bogoliubov quasiparticles satisfy the usual fermionic anti-commutation relations (1):

$$\begin{aligned} \{\gamma_{k\uparrow}, \gamma_{k'\downarrow}\} &= \sin \theta_k \cos \theta_{-k'} \delta_{k,-k'} - \cos \theta_k \sin \theta_{-k'} \delta_{k,-k'} = 0, \\ \{\gamma_{k\sigma}, \gamma_{k'\sigma'}\} &= \left\{ \sin \theta_k c_{k\uparrow} - \cos \theta_k c_{-k\downarrow}^\dagger, \sin \theta_{k'} c_{k'\uparrow} - \cos \theta_{k'} c_{-k'\downarrow}^\dagger \right\} = 0, \\ \{\gamma_{k\uparrow}, \gamma_{k'\uparrow}^\dagger\} &= \sin \theta_k \sin \theta_{k'} \delta_{kk'} + \cos \theta_k \cos \theta_{k'} \delta_{kk'} = \delta_{kk'}. \end{aligned}$$

Hamiltonian. In the mean-field approximation, the BCS Hamiltonian takes the form

$$H \approx \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_k \left(\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \bar{\Delta}_k c_{-k\downarrow} c_{k\uparrow} + \text{const} \right),$$

introducing operators of the form

$$A_k \stackrel{\text{def}}{=} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger, \quad B_k \stackrel{\text{def}}{=} c_{-k\downarrow} c_{k\uparrow},$$

the mean-field approximation amounts to approximating

$$(A_{k'} - \langle A_{k'} \rangle) (B_k - \langle B_k \rangle) \approx 0,$$

i.e. neglecting fluctuations around the expectation values in quadratic order. The interaction (2)

$$\begin{aligned} V &= \frac{1}{\Omega} \sum_{kk'} V_{kk'} A_{k'} B_k = \frac{1}{\Omega} \sum_{kk'} A_{k'} \langle B_k \rangle + \frac{1}{\Omega} \sum_{kk'} V_{kk'} \langle A'_{k'} \rangle B_k - \frac{1}{\Omega} \sum_{kk'} \langle A_{k'} \rangle \langle B_k \rangle \\ &= - \sum_{k'} \Delta_{k'} A_{k'} - \sum_k \bar{\Delta}_k B_k + \text{const}. \end{aligned}$$

Moving on to quasiparticles, we find (3)

$$\begin{aligned} H &= \sum_k \begin{pmatrix} c_{k\uparrow}^\dagger & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \xi_k & -\Delta_k \\ -\Delta_k & \xi_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} + \text{const} \\ &= \sum_k \begin{pmatrix} \gamma_{k\uparrow}^\dagger & \gamma_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \sin \theta_k & \cos \theta_k \\ -\cos \theta_k & \sin \theta_k \end{pmatrix} \begin{pmatrix} \xi_k & -\Delta_k \\ -\Delta_k & \xi_k \end{pmatrix} \begin{pmatrix} \sin \theta_k & -\cos \theta_k \\ \cos \theta_k & \sin \theta_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix} + \text{const} \\ &\stackrel{?}{=} \sum_k \begin{pmatrix} \gamma_{k\uparrow}^\dagger & \gamma_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \tilde{E}_k & 0 \\ 0 & -\tilde{E}_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix}, \end{aligned}$$

with

$$\tilde{E}_k = \xi_k - 2\xi_k \cos(\theta_k)^2 + 2\Delta_k \sin \theta_k \cos \theta_k = \frac{\xi_k^2 + \Delta_k^2}{E_k} = E_k.$$

With $\Delta_k = \Delta$ we could plot the dispersion relation (fig. 11).

Ground state. The BCS state

$$|gs\rangle = \prod_k \left(\sin \theta_k + \cos \theta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \right) |0\rangle,$$

has zero Bogoliubov quasiparticles (4):

$$\begin{aligned} \gamma_{k\uparrow} |gs\rangle &= \left(\sin \theta_k c_{k\uparrow} - \cos \theta_k c_{-k\downarrow}^\dagger \right) \prod_k \left(\sin \theta_k + \cos \theta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \right) |0\rangle \\ &= \sin \theta_k c_{k\uparrow} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger |0\rangle - \cos \theta_k \sin \theta_k c_{-k\downarrow}^\dagger |0\rangle = 0, \end{aligned}$$

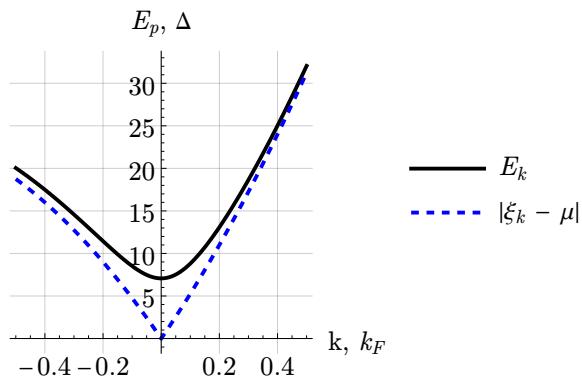


Figure 11: The dispersion relation

so $|gs\rangle$ is ground state of the mean field approximation of H . Actually the $|gs\rangle$ could be observed by

$$|gs\rangle \stackrel{n}{=} \prod_k \gamma_{-k\downarrow} \gamma_{k\downarrow} |0\rangle.$$

In this state

$$E(\theta_k) = \langle gs | H | gs \rangle = \sum_k 2\xi_k \cos^2 \theta_k + \frac{1}{4\Omega} \sum_{kk'} V_{kk'} \sin(2\theta_k) \sin(2\theta_{k'}),$$

and we could find θ_k just by minimizing the energy

$$\frac{\partial}{\partial \theta_q} E(\theta_k) = \frac{1}{\Omega} \cos(2\theta_q) \sum_k V_{qk} \sin(2\theta_k) - 2\xi_q \sin(2\theta_q) = 0.$$

Using this relation we could simplify expression (5)

$$\Delta_k = -\frac{1}{\Omega} \sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle_{gs} = -\frac{1}{2\Omega} \sum_{k'} V_{kk'} \sin(2\theta_{k'}) = -\frac{1}{\Omega} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}},$$

the zero temperature gap equation.

14.1 Specific heat of a BCS superconductor

As we have shown in the previous exercise, in the mean field approximation the BCS Hamiltonian describes non-interacting fermionic Bogoliubov quasiparticles with dispersion E_k . Consequently, their average occupation at inverse temperature β is given by the Fermi-Dirac distribution

$$\langle \hat{\gamma}_{k\sigma}^\dagger \hat{\gamma}_{k\sigma} \rangle = f_k = \frac{1}{e^{\beta E_k(\beta)} + 1}, \quad E_k = \sqrt{\xi_k^2 + \Delta_k^2(\beta)}.$$

Next we assume that $k_B = 1$.

1. The specific heat. Starting from the expression

$$S = -2 \sum_k ((1 - f_k) \ln(1 - f_k) + f_k \ln f_k),$$

for the entropy of a gas of non-interacting fermions, we could find

$$C = T \left. \frac{\partial S}{\partial T} \right|_V = -\beta \left. \frac{\partial S}{\partial \beta} \right|_V = 2\beta \sum_k \ln \left(\frac{f_k}{1 - f_k} \right) \frac{\partial f_k}{\partial \beta}.$$

All that remains is to find

$$\frac{\partial f_k}{\partial \beta} = \left(\frac{1}{2E_k} \frac{d\Delta_k^2}{\beta} + \frac{E_k}{\beta} \right) \frac{\partial f_k}{\partial E_k},$$

thus

$$C = 2\beta \sum_k \left(-\frac{\partial f_k}{\partial E_k} \right) \left(E_k^2 + \frac{\beta}{2} \frac{d\Delta + k^2}{d\beta} \right).$$

2. Nernst's theorem. We can find low-temperature asymptotics to $C(\beta \rightarrow \infty)$

$$C = -2\beta V N(0) \int \frac{\partial f_k}{\partial E_k} \left(E_k^2 + \frac{\beta}{2} \frac{d\Delta^2}{d\beta} \right) d\xi.$$

For low temperatures we can neglect the temperature dependence for the $\Delta_k(\beta \rightarrow \infty) \approx 1.76T_c$ and it is convenient to use the saddle-point method

$$C \approx 2VN(0)\Delta^2 e^{-\beta\Delta} \int e^{-(\beta\xi)^2/2\beta\Delta} d(\beta\xi) = 2\sqrt{2\pi}VN(0)(\beta\Delta)^{5/2} \frac{e^{-\beta\Delta}}{\beta},$$

which corresponds to the desired exponential decay.

$$\frac{C}{C_n} \approx (\beta\Delta)^{5/2} e^{-\beta\Delta}.$$

So $C/C_n = 0.01$ at $\beta\Delta \approx 10$ or $T \approx 0.2T_c$.

3. The specific heat jump. In a second order phase transition the jump in the specific heat just below T_c

$$\Delta C = -\beta^2 \frac{d\Delta^2}{d\beta} \sum_k \left. \frac{\partial f_k}{\partial E_k} \right|_{T_c=0} = 2VN(0)\beta^2 \frac{d\Delta^2}{d\beta} \Big|_{T_c=0} \int \frac{\partial f_k}{\partial E_k} d\xi = \frac{8\pi^2}{7\zeta(3)} N(0) V T_c,$$

with $d\Delta^2/d\beta|_{T_c=0} = 8\pi^2(T_c)^3/(7\zeta(3))$. The universal ratio is

$$\frac{\Delta C}{C_n(T_c)} = \frac{12}{7\zeta(3)} \approx 1.43.$$

4. Compressibility. Consider now the BCS wavefunction at $T = 0$. The BCS ground-state energy is then

$$\Omega_g = \sum_k \left(\xi_k - \sqrt{\xi_k^2 + |\Delta_k|^2} + \frac{|\Delta_k|^2}{2E_k} \right), \quad \Delta_k = \Delta\theta(\hbar\omega_D - |\xi_k|),$$

with Debye temperature $T_D = \hbar\omega_D \gg \Delta$. The zero-temperature isothermal compressibility

$$\kappa = -\frac{1}{V} \frac{\partial^2 \Omega_g}{\partial \mu^2}.$$

More precisely, the difference from the ideal Fermi gas

$$\Delta\kappa = -\frac{1}{V} \frac{\partial^2}{\partial \mu^2} (\Omega_g^{\text{BCS}} - \Omega_g^{\text{FG}}) = -\frac{1}{2V} \frac{\partial^2}{\partial \mu^2} (-N(\varepsilon_F)\Delta^2),$$

with $\Delta|_{T=0} \approx 2\hbar\omega_D \exp\left(-\frac{1}{\alpha N(\varepsilon_F)}\right)$. Due to we live in 3D $N(E) = \frac{\sqrt{2}}{\pi^2} m_e^{3/2} \sqrt{E}$. Thus

$$\Delta\kappa = \frac{\Delta^2}{2V} \left(\frac{1}{\frac{\sqrt{2}}{\pi^2} m_e^{3/2} \alpha^2 \varepsilon_F^{5/2}} - \frac{1}{2\alpha \varepsilon_F^2} - \frac{\frac{\sqrt{2}}{\pi^2} m_e^{3/2}}{2\varepsilon_F^{3/2}} \right) > 0,$$

apparently because of Cooper pairs.

Scientific Essay: Thermalization and Localization

This essay will consider two states of the system: the Ergodic Phase (EP), also known as thermalized, and the Localized Phase (LP). We start with defining these two phases and their experimental observation in 1D and 2D, look at how interaction affects the formation of phases. Then after some numerical calculations⁵ we will try to formulate the main markers of EP and LP, perhaps highlighting the factors influencing their formation. Finally, we will separately consider the issue of the influence of interaction on the growth of entanglement between subsystems. We will also compare Anderson Localization (AL) and Many Body Localization (MBL).

9.1 Intro

Model. We will study the effects of thermalization and localization using the Hubbard model

$$\hat{H} = -J \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j + \text{h.c.}) + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j + \Delta \sum_j \delta_j \hat{n}_j, \quad (24)$$

with V – nearest neighbor interaction, Δ – noise level, $\delta_j \in [-1, 1]$ evenly distributed (fig. 22c). To obtain numerical results, the hard-bosons limit is used (unless explicitly stated otherwise)⁶. This system is convenient in that we can look at various experimental implementations and all phases (EP and LP) of interest to us are implemented in it.

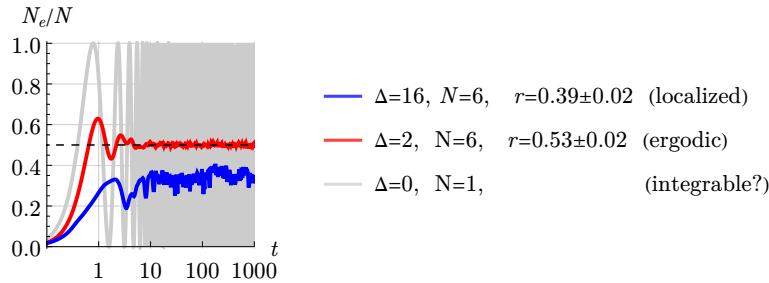


Figure 12: An example of different behavior scenarios for some observable .

Thermalization. Let's start by building some intuition about what could be called thermalization for an isolated quantum system [1]. Let the initial state be given by $|\psi_0\rangle$, then, in the basis of energy eigenstates $|j\rangle$, the evolution

$$|\psi(t)\rangle = \sum_{j=1}^{\mathcal{N}} c_j e^{-i\varepsilon_j t} |E_j\rangle$$

with $c_j = \langle E_j | \psi_0 \rangle$, $\varepsilon_j = \langle j | \hat{H} | j \rangle$ and $\mathcal{N} = \dim H$. For some observable $\hat{A}(t)$ the mean value could be expressed as

$$A(t) = \langle \psi(t) | \hat{A} | \psi(t) \rangle = \sum_{j,k} \bar{c}_k c_j e^{-i(\varepsilon_j - \varepsilon_k)t} \langle k | \hat{A} | j \rangle = \sum_j |c_j|^2 \langle j | \hat{A} | j \rangle + \sum_{k \neq j} c_j \bar{c}_k e^{-i(\varepsilon_j - \varepsilon_k)t} \langle k | \hat{A} | j \rangle. \quad (25)$$

After some time of thermalization t_{th} we would like to see that the observables reach thermal values (independent of the initial conditions) with small fluctuations around (fig. 12, **red curve**)

$$A(t \gg t_{\text{th}}) = A(E) + \text{small fluctuations}, \quad E = \langle \psi_0 | \hat{H} | \psi_0 \rangle.$$

To achieve small fluctuations around the average value, as we see from (25), it is enough to require the smallness of the off-diagonal elements⁷. And so that $A(E)$ does not depend on the initial conditions, we can consider the case when diagonal elements are smooth functions of energy

$$\langle j | \hat{A} | j \rangle = A(\varepsilon_j).$$

Indeed, then for the initial state lying in ΔE such that the spread $\partial_E A(E) \Delta E$ is small, the final result is

$$A(t \gg t_{\text{th}}) \approx \sum_j |c_j|^2 \langle j | \hat{A} | j \rangle \approx A(E).$$

This is how we come to the formulation of the Eigenstate Thermalization Hypothesis (ETH), put forward by Deutsch [2] and Srednicki [3]: if off-diagonal terms $\langle k | \hat{A} | j \rangle$ are small in compared to diagonal and diagonal terms are smooth

⁵Graphs from articles are accompanied by a link to the articles at the beginning, graphs without links are the results of my numerical modeling.

⁶The term $+\frac{1}{2}U \sum_j \hat{n}_j (\hat{n}_j - 1)$ was added to the Hamiltonian with $U \rightarrow \infty$.

⁷Note that the number of diagonal terms is \mathcal{N} and off-diagonal $\mathcal{N}^2 - \mathcal{N}$. If we consider the contribution of each off-diagonal term to be random, then the fluctuations can be estimated as $\sqrt{\mathcal{N}^2} |\langle k | \hat{A} | j \rangle|$, which leads to the requirement of smallness.

functions of energy, then the observed one seems to be thermalized. It is worth making some reservation that for an isolated system a pure state remains pure $\text{tr } \rho^2 = 1$, while for a thermal state $\text{tr } \rho^2 < 1$, which is why we talk about the thermalization of observables⁸. Again, judging by the conditions, it seems that systems and observables A_1, A_2 are possible such that A_1 is thermalized, but A_2 is not.

The main conclusion of this section: sometimes it happens that in some system and for some observable \hat{A} its value $A(t \gg t_{\text{th}})$ reaches a constant with small fluctuations around, most likely this will correspond to the indicated ETH terms.

Localization. The fundamental opposite of thermalization is localization. It happens that the system retains information about the initial conditions even with $t \rightarrow \infty$ (fig. 12, blue curve) and $A = A(\psi_0)$. For example, we can divide the system into two equal subsystems Ω_1, Ω_2 , populate only Ω_1 and monitor the contrast

$$\mathcal{I} = \frac{N_{\Omega_1} - N_{\Omega_2}}{N_{\Omega_1} + N_{\Omega_2}}.$$

So in [4] in 1D the even lattice nodes (fig. 18) were chosen as Ω_1 , and in [5] in 2D the left side of the system was taken as Ω_1 (fig. 13). Just for $\mathcal{I}(t)$ the declared thermal behavior is already visible when $\mathcal{I}(t \gg t_{\text{th}}) \approx 0$, but at some point there is a transition to localization and $\mathcal{I}(t \gg t_{\text{th}}) \approx \text{const} > 0$. This behavior is typical when frozen noise $\Delta > 0$ is added to the system; this effect was first described by Anderson [6] for non-interacting particles (AL). In the case of interaction (MBL), the theoretical description, as far as I know, remains an open task and therefore is of great interest for experiment.

For a single-particle problem, it would be logical to assume that this behavior arises due to the localization of eigenfunctions. Indeed, in fig. 18 the eigenstates of the single-particle 1D Hamiltonian (24) are presented at different noise levels Δ .

9.2 MBL experiment in 2D

Let's consider the experimental implementation of the (24) system in [5] with approximately unity filled Mott insulator of bosonic ^{87}Rb atoms in a single plane of a cubic optical lattice.

To do this, by combining laser beams, we will obtain a certain interference pattern, the antinodes of which, at red detuning, will act as minima of the potential for atoms due to their polarizability (an alternative would be a lattice of optical tweeters). Between these potential minima, atoms will tunnel with a characteristic energy J (as in fig. 22c), which we will use as an energy scale. We can adjust the interaction U between atoms using Feischbach resonances, by turning it up to the value $U = 24J$ we get a system close to hard-bosons. We will apply a global harmonic potential on top of the grating, also by focusing the laser. Let's fill the trap with sufficiently cold atoms, using a microwave knife, leave only the left half filled and wait a little (fig. 13). Noises Δ are added to the system using DMD (alternatively, SLM, AOD or quasi-random potential are used as in [4], more details in [7]), the result is averaged over 50 implementations of δ_j .

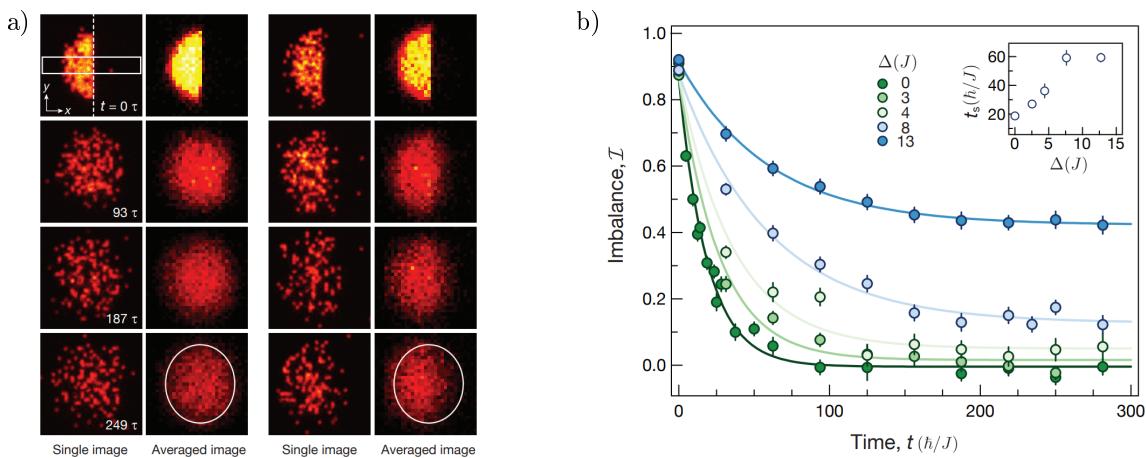


Figure 13: [5] a) Raw fluorescence images (red to yellow corresponds to increasing detected light level) showing the evolution of the initial density step without disorder. The left column shows the evolution with $\Delta = 0$ and the right column $\Delta = 13J$. b) Relaxation dynamics of a density domain wall.

⁸The hope arises that if we divide the system into two subsystems $\Omega_1 \cup \Omega_2$, then $\rho_1 = \text{tr}_{\Omega_2} \rho$ can actually turn out to be thermal, and Ω_2 acts in some sense thermostat for Ω_1 . This assumption will not be developed within the framework of this essay, but I hope to return to this issue later.

It can be seen that in the absence of noise the system reaches a thermal state - thermalization ($\mathcal{I} \rightarrow 0$). With sufficiently strong noise, localization occurs: $\mathcal{I}(t \rightarrow \infty) = \mathcal{I}_\infty > 0$. Assuming the output to \mathcal{I}_∞ to be exponential, we can notice how what is required to reach a steady state increases as the noise level increases.

It can also be seen that $\mathcal{I}_\infty > 0$ appears with $\Delta_c \approx 5.5(4)J$. The article emphasizes that Δ_c will increase as initial filling decreases. The clear difference in critical disorder strengths highlights the strong influence of interactions on the localization.

9.3 MBL experiment in 1D

To demonstrate the EP-LP transition, we can also consider an experiment on the implementation of a one-dimensional system [4] with degenerate Fermi gase of ^{40}K via sympathetic cooling with ^{87}Rb in a magnetic quadrupole and optical dipole trap followed by evaporative cooling.

Now we consider the motion in a quasi-random optical lattice created by two gratings with an incommensurate step, but in general still described by the Hamiltonian close to (24):

$$\hat{H} = -J \sum_{j,\sigma} (\hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \text{h.c.}) + \Delta \sum_{j,\sigma} \cos(2\pi\beta j + \varphi) \hat{n}_{j,\sigma} + U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow},$$

with $\beta \in \mathbb{Q}$ to have quasi-random potential. A general view of the phase diagram is presented in fig. 22b.

Now odd nodes are chosen as Ω_1 and we also study how quickly and to what extent the contrast \mathcal{I} of the population of even and odd nodes will disappear (fig. 14). It can be seen that for $t \approx 15\tau$ the observed \mathcal{I} also reaches a stationary value (fig. 14a), where the dependence $\mathcal{I}(\Delta)$ (fig. 14b) is plotted based on the results of averaging in the yellow region.

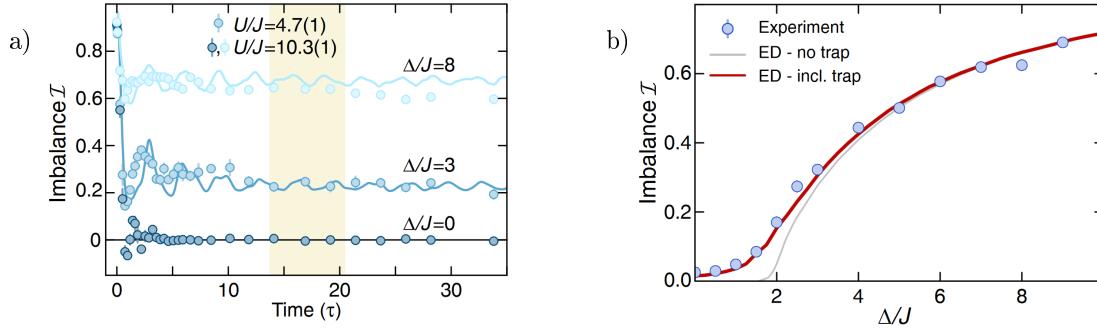


Figure 14: [4] a) Time evolution of an initial charge-density wave . b) Stationary values of the imbalance \mathcal{I} as a function of disorder Δ for non-interacting atoms .

In the paper also measured the stationary value of \mathcal{I} for different interactions U and different noise Δ (fig. 23b), in full accordance with the results of DMRG simulation [8]. It can be seen that LP is preserved in a wide range of interactions. The effect of interactions on the localization gives rise to a characteristic W-shape. It is also worth noting that the interaction leads to a logarithmic increase in the entropy of entanglement of subsystems (DMRG results at fig. 23a) , which we will return to in the corresponding section.

9.4 Numerical model in 2D

I was interested in looking at the behavior of a 2D system for the non-interacting case; a Gaussian packet lying entirely on the left side of the system was chosen as the initial state, and I also monitored the contrast $I(t)$. The presence of a global harmonic potential was described by a term of the form $\sum_j u_j \hat{n}_j$. Evolution was considered through ED (Exact Diagonalization) and expansion of the initial state into its own (fig. 15a). Similarly, at a small noise level the system was thermalized, and at large values it reached a localized state.

In the thermalizing state, the result is statistically significant and does not depend on the initial state (results not presented here). It is interesting to look at the resulting distribution of node population $\langle n_j \rangle_t$, averaged over time, from the energy of this node $\delta_j + u_j$ (fig. 15c). It is also interesting to compare $\langle n_j \rangle_t$ with the resulting thermal distribution $\text{tr } n_j e^{-\beta H}$, I obtained the correlation coefficient

$$\text{corr}(\langle n_j \rangle_t, \text{tr } n_j e^{-\beta H})|_{\Delta=0.5} \approx 0.8, \quad \text{corr}(\langle n_j \rangle_t, \text{tr } n_j e^{-\beta H})|_{\Delta=5} \approx 0.2,$$

which is quite consistent with the ideas of localization and thermalization.

A natural question arises: how exactly can one characterize the localization phase and the ergodic phase (thermalizing) of a system, and what algorithm can be fed with the Hamiltonian. Various metrics are presented in [9], but the best place to start is the r -parameter, which is the focus of the next section.

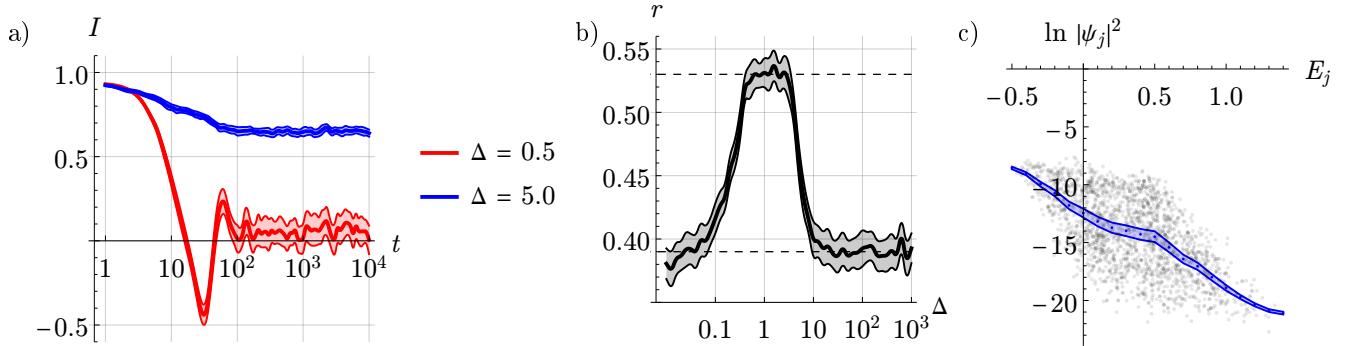


Figure 15: a) Evolution of contrast $I(t)$ averaged over 50 realizations δ_j for two noise levels Δ : thermalization and localization. b) Dependence of r -parameter on the noise level Δ , averaged over 50 realizations of δ_j . c) For a thermalized state, the dependence of the population of the node $|\psi_j|^2$ on the energy of the node $E_j = \delta_j + u_j$, black dots indicate the dependence for a specific implementation δ_j , blue indicates the result of averaging over 50 implementations.

9.5 Random Matrices

Let's consider the following procedure: for some matrix M , find all eigenvalues λ_j , ordered in ascending order, and determine the r -parameter [10]

$$r \stackrel{\text{def}}{=} \left\langle \frac{\min(\delta_j, \delta_j + 1)}{\max(\delta_j, \delta_{j+1})} \right\rangle_j, \quad \delta_j = \lambda_{j+1} - \lambda_j. \quad (26)$$

We can immediately note several such properties that it is not sensitive to transformations of the form $M \rightarrow \alpha_1 M + \alpha_2 \mathbb{1}$, moreover, as we will notice later, it is not sensitive to many things.

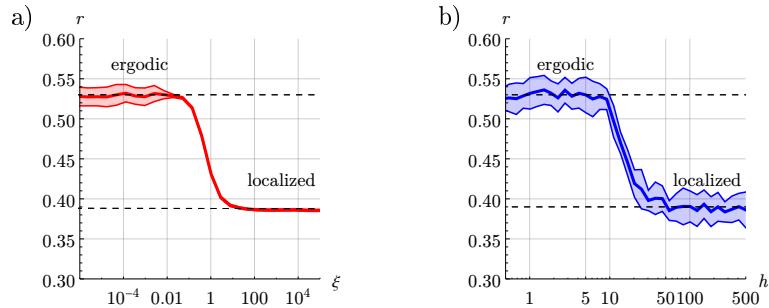


Figure 16: a) Phase transition EP-LP with random matrix. b) Phase transition EP-LP with 1D hard-bosons (24), $h \equiv \Delta$

Now let's take a closer look at the (24) system and the phase transition that occurs when Δ increases. In coordinate representation, noise is simply a random diagonal addition to the Hamiltonian⁹. Thus, for $\Delta \gg J$ (at least in the single-particle case), the Hamiltonian is practically diagonalized (fig. 18). On the other side there is a non-diagonal part, for which J is responsible. The paper [10] proposes to model this phase transition using two random matrices: a random Hermitian M_1 (GOE) and a random diagonal M_2 , thus $M = (1 - k)M_1 + kM_2$. The limiting values $k = 0$ and $k = 1$ characterize chaotic and nonchaotic regimes (thermalizing and localizing). To ensure that the transition does not depend on the parameters $M_{1,2}$, we can scale k as

$$\xi = \frac{1}{D} \frac{k\sigma_2}{(1 - k)\sigma_1},$$

where $\sigma_{1,2}$ are the standard deviation of elements in $M_{1,2}$ respectively and D is the size of the matrix.

We can find $r(\xi)$ for matrices with $D = 200$, $\sigma_1 = \sigma_2 = 1$ (for other values the dependence is the same), averaging the result over 100 implementations (fig. 16a). For comparison, the dependence of $r(\xi)$ is given for a 1D system (24) hard-bosons for noise level h (the same as Δ) on the lattice with $L = 14$ half-fill sites¹⁰ (7 particles). According to

⁹You need to be careful here, because as we will see later, small changes in the diagonal through $V \neq 0$ lead to fundamentally different behavior of the system [11].

¹⁰If we were talking about the Heisenberg model, then this would correspond to a complete spin equal to zero.

[10, 9] the value $r \approx 0.53$ is a marker of the ergodic phase (a characteristic value for GOE), and $r \approx 0.39$ is a marker of the localized phase (the so-called Poisson statistics):

$$r \approx 0.53 - \text{ergodic} \quad r \approx 0.39 - \text{localized}$$

I note that it is the word marker that is used, since these conditions are neither necessary nor sufficient.

A similar dependence will be obtained if we consider as M_1 the connectivity matrix of a random graph (a Hermitian matrix with random elements 0, 1). Considering that on average there are θ non-zero elements per line, we can ask the question about the influence of θ on the formation of the ergodic phase (fig. 17a). If θ is too small, the probability of Hilbert Space Fragmentation [12] is high, which obviously cannot lead to thermalization of the system. Moreover, the system does not thermalize when it is integrated [13].

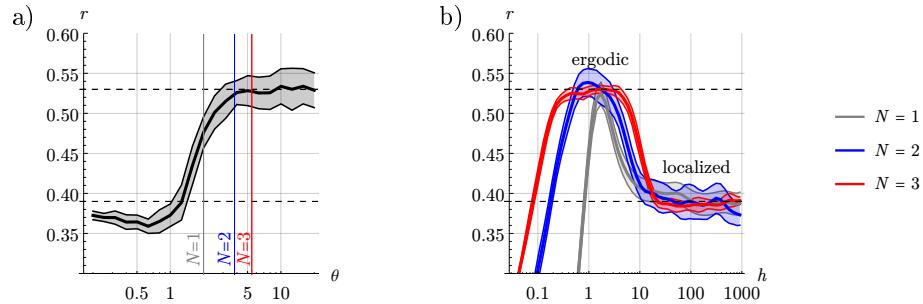


Figure 17: a) The influence of matrix rarefaction θ on phase formation with $\xi = 0.01$. b) Phase transition with 1D hard-bosons with $L = 20$.

I paid such attention to θ and fragmentation, since this in some sense helps to understand why for a small number of particles in the system the ergodic phase (judging by r) practically does not occur (fig. 17). Indeed, with a smaller number of particles ($N = 1, 2, 3$) and the same lattice size $L = 14$, the Hamiltonian is more rarefied (fig. 17a), Hilbert Space Fragmentation occurs (that is the Hamiltonian can be represented in block diagonal form) and, accordingly, thermalization does not occur.

The main conclusion of this section: the r -parameter is quite universal in nature and can be used as a marker of the ergodic phase and localized phase. The EP-LP phase transition can be modeled by random matrices (GOE, random diagonal, random graph adjacency matrix).

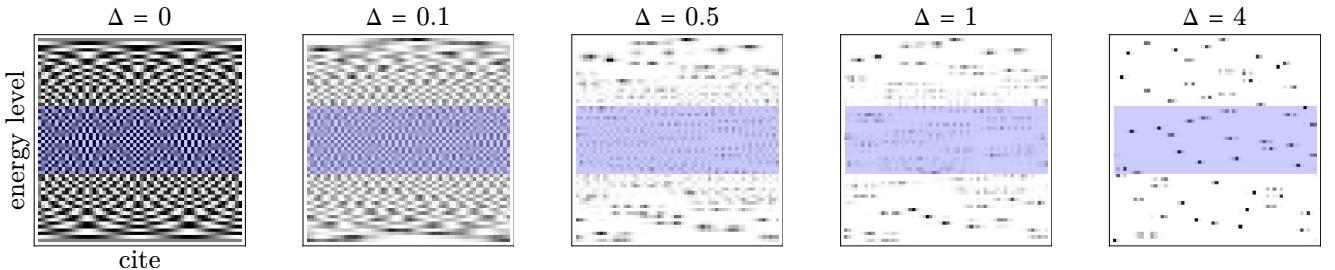


Figure 18: The eigenstates $|\psi_j\rangle$ of the single-particle 1D Hamiltonian (24) onto gratings of length $L = 60$, the color indicates the value $|\psi_j|^2$. It can be seen that localization occurs immediately for the ground state, but in the area highlighted in blue, localization occurs later.

9.6 Numerical model in 1D

As can be seen from fig. 18 localization depends on temperature: for the system under consideration, low-energy states are localized first, and then the middle of the spectrum (the area highlighted in blue in fig. 18). The article [9] specifically examines the occurrence of localization at $\beta = 0$, that is, when in a thermal state all states are equally probable (however, for purity, all metrics will be calculated in the middle third of the spectrum). The system is considered to be a Heisenberg chain with random fields along the z -direction

$$\hat{H} = J \sum_{j=1}^L \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1} + \sum_{j=1}^L h_j \hat{S}_j^z,$$

for zero total spin, which is generally almost equivalent to the Hubbard hard-boson model and $h_j \in [-h, h]$. A phase transition is detected in the system at (or crossover?) at $h = h_c = (3.5 \pm 1) J$. The system is quite exotic in that we see a quantum phase transition at a non-zero temperature, and even in one dimension. To a large extent, this is possible precisely due to the lack of ergodicity in the system.

The article performs Exact Diagonalization (ED) for $J = 8, 10, \dots, 16$. A phase transition is detected (fig. 19a) by the already familiar r -parameter (26). Also, for all results, averaging is carried out over noise realizations.

It is also proposed to consider the decay of the longest wavelength disturbance of the spin density

$$\hat{M} = \sum_j \hat{S}_j^z \exp\left(i \frac{2\pi j}{L}\right).$$

Consider an initial condition that is at infinite temperature, but with a small modulation of the spin density in this mode, so the initial density matrix is $\rho_0 = (\mathbb{1} + \epsilon \hat{M}^\dagger)/Z$. For such an initial condition $\langle \hat{M} \rangle_0 = \text{tr}(\rho_0 \hat{M})$. The long-time average of the spin polarization in this mode is

$$\langle \hat{M} \rangle_t = \frac{\epsilon}{Z} \sum_n \langle n | \hat{M}^\dagger | n \rangle \langle n | \hat{M}^\dagger | n \rangle.$$

They define the fraction of the contribution to the initial polarization that is dynamic and thus decays away (on average) at long time, as

$$f^{(n)} = 1 - \frac{\langle n | \hat{M}^\dagger | n \rangle \langle n | \hat{M}^\dagger | n \rangle}{\langle n | \hat{M}^\dagger \hat{M} | n \rangle}.$$

In the ergodic phase, the system does thermalize, so the initial polarization does relax away and $f \rightarrow 1$. In the localized phase, on the other hand, there is no long-distance spin transport, so $f \rightarrow 0$. Это и наблюдается (fig. 19a).

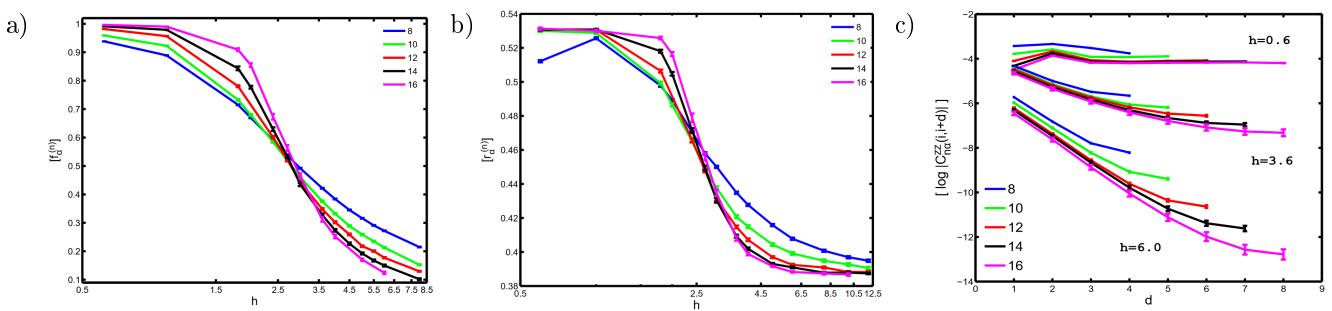


Figure 19: [9] a) The fraction of the initial spin polarization that is dynamic. b) The ratio of adjacent energy gaps (r -parameter). c) The spin-spin correlations in the manybody eigenstates as a function of the distance d .

Another way to detect a phase transition is to see that for large noises the correlations begin to decay exponentially

$$C_n(i, j) = \langle n | \hat{S}_i^z \hat{S}_j^z | n \rangle - \langle n | \hat{S}_i^z | n \rangle \langle n | \hat{S}_j^z | n \rangle,$$

where the average value $\langle \log |C_n(i, i+d)| \rangle_{i,n,h_j}$ is displayed (fig. 19c).

9.7 Entropy growth

The last topic I want to focus on in this essay is the effect of entropy on the growth of entanglement between subsystems. Let us select a subsystem Ω_1 in the system $\Omega = \Omega_1 \cup \Omega_2$. The entropy of the subsystem can be found through the reduced density matrix $\rho_{\Omega_1} = \text{tr}_{\Omega_2} \rho$

$$S(\rho_{\Omega_1}) = -\text{tr} \rho_{\Omega_1} \ln \rho_{\Omega_1},$$

one shows that bipartite entanglement exists between two disjoint subsystems Ω_1 and Ω_2 of Ω with reduced density matrices ρ_{Ω_1} and ρ_{Ω_2} if

$$S(\rho_{\Omega_1}) > S(\rho_{\Omega_1 \cup \Omega_2}) \quad \text{or} \quad S(\rho_{\Omega_2}) > S(\rho_{\Omega_1 \cup \Omega_2}).$$

However, further we will simply monitor the growth of the entropy of the subsystem, which in general most likely indicates the entanglement of the subsystems. We will also work with one-dimensional chain hard-bosons described by the Hamiltonian (24). Let us divide the system into two parts: left and right; as the initial state we will consider half population at even nodes (fig. 20). The growth of entropy in LP is considered. It can be seen that the addition of a weak interaction leads to a statistically significant increase in entropy. In my opinion, this is a rather non-obvious result, since the interaction is a small diagonal addition to the Hamiltonian, which already has random numbers on the diagonals.

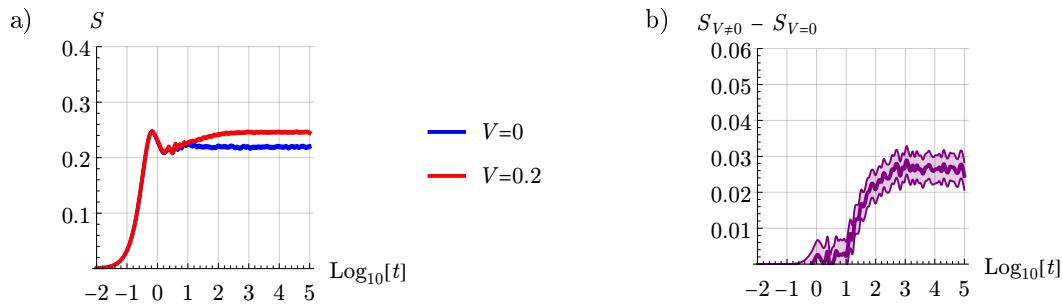


Figure 20: a) Entanglement growth. b) The same data but with subtracted values.

Similar results were obtained in [11]. As in [4] (fig. 23a), a logarithmic increase in entropy is observed (fig. 21a). Since the calculations in the article were carried out through ED, rather small systems were considered, which led to the constant S (fig. 21b), however, an obvious trend can be traced as the size of the system increases.

Thus, at least from the point of view of entanglement and entropy of subsystems, MBL is fundamentally different from AL. The entanglement increases slowly until a saturation time scale, which diverges in the infinite system.

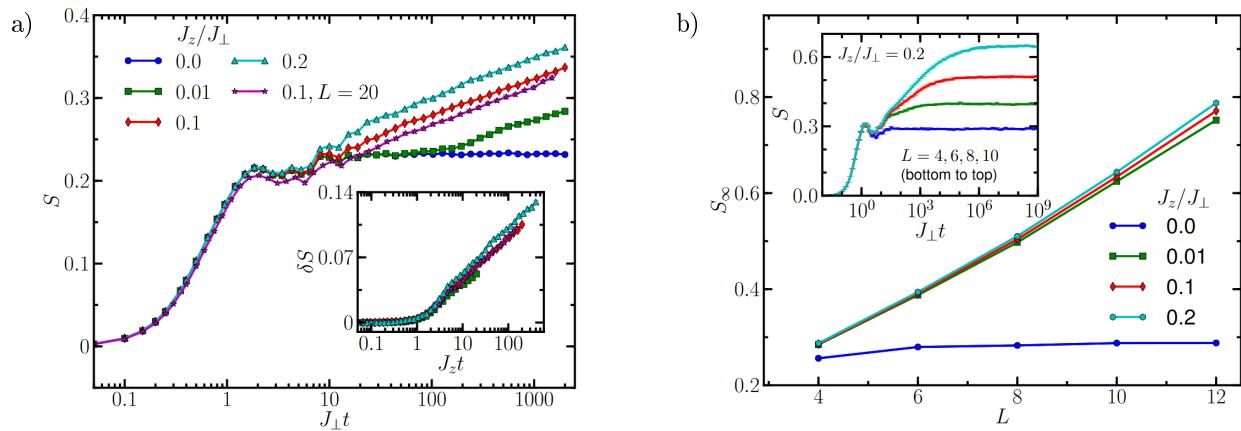


Figure 21: [11] a) Entanglement growth. b) Saturation values of the entanglement entropy as a function of L .

9.8 Conclusion

Experimental implementations and numerical simulations of EP and LP in the Hubbard model (or in 1D Heisenberg model) in 1D and 2D for the non-interacting case (EP-LP:AL) and the interacting case (EP-LP:MBL) are considered. For a many-particle problem, the Hamiltonian is less sparse; Hilbert Space Fragmentation, but thermalization usually occurs. A shift in the critical noise level required for transition to LP was observed due to the presence of interactions between particles. Also, fundamentally different behavior was observed in MBL compared to AL in terms of the growth of entanglement and entropy of subsystems.

9.9 Supplementary Material

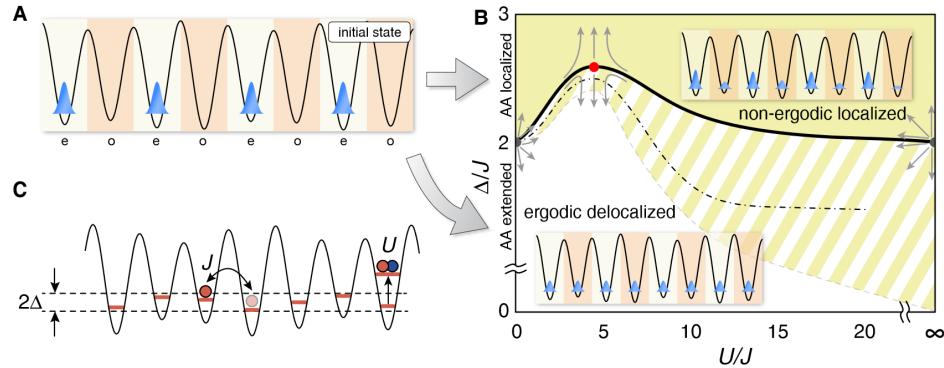


Figure 22: [4] 1D system (24). a) Initial state of the system consisting of a charge density wave, where all atoms occupy even sites only. For an interacting many-body system, the evolution of this state over time depends on whether the system is ergodic or not. b) Schematic phase diagram for the system: in the ergodic, delocalized phase (white) the initial state quickly decays, while it persists for long times in the non-ergodic, localized phase (yellow). c) Schematic showing a visual representation of the three terms in the Hamiltonian (24).

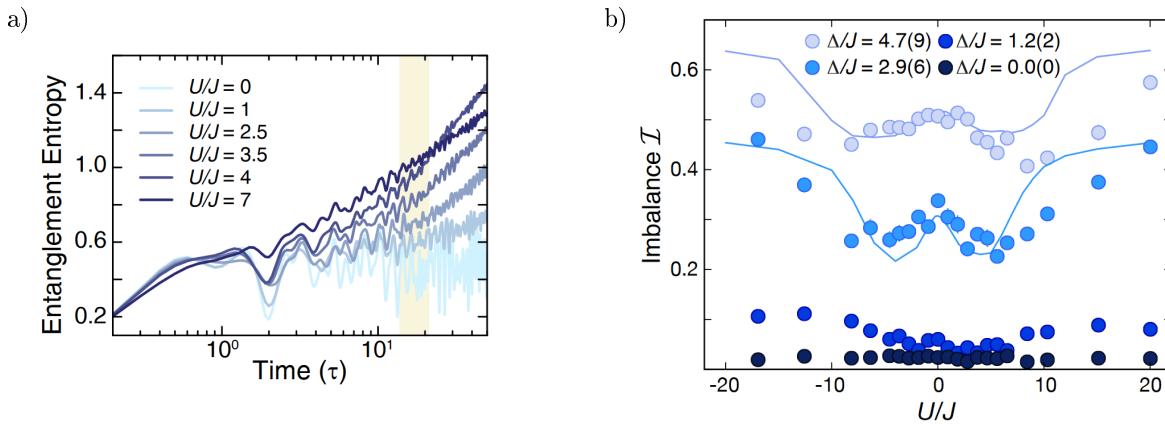


Figure 23: [4] a) DMRG results of the entanglement entropy growth for various interaction strengths and $\Delta = 5J$. For long times, logarithmic growth characteristic of interacting MBL states is visible. b) Cuts along four different disorder strengths. The effect of interactions on the localization gives rise to a characteristic W-shape. Solid lines are the results of DMRG simulations for a single homogeneous tube.

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