TFY4210 Quantum Theory of Many-Particle Systems Solution sketch for Exam V18.

1: Quick questions

(a) A single particle operator is an operator that can be written as a sum of operators acting on a single coordinate in the many-particle wavefunction, i.e.

$$H = \sum_i h(x_i). \tag{1}$$

The operator in second quantization is given by

$$H = \sum_{\alpha\beta} \langle \alpha | h | \beta \rangle c_\alpha^\dagger c_\beta. \tag{2}$$

(b) The wavefunction $\phi(x_1, x_2, y_1, y_2)$ is symmetric in the x'es and antisymmetric in the y's. There are no specific requirements with respect to the interchange of an x with a y, if such an interchange is even possible.

(c) Both the band insulator and the Mott insulator have a gap in the excitation spectrum, i.e. it costs a finite amount of energy to excite the system from the ground state. For the band insulator, this gap can be understood in terms of the non-interaction dispersion relation and the Pauli principle. For the Mott insulator, the gap is caused by particle-particle interaction.

(d) According to Noethers theorem, a continuous symmetry is associated with a conserved quantity. The generator of the symmetry is this conserved quantity.

(e) To obtain the Lehmann representation of a Greens function, one starts with the definition and evaluates the averages in the energy eigenstate basis. The completeness relation is often sandwiched between operators to replace the operator time dependence with some exponential factors $e^{iE_n t}$.

(f) Analytic continuation is a method to obtain a retarded Greens function from a Matsubara Greens function in the frequency domain by replacing the Matsubara frequency $i\omega_n$ according to $i\omega_n \to \omega + i\eta$.

(g) The Bogoliubov approximation consists of replacing the creation and annihilation operators of the macroscopically occupied state of the BEC with the (spontaneously broken) expectation value, $a_0, a_0^\dagger \to \sqrt{N_0}$.

(h) The Landau criterion can be derived by relating the energy of the superfluid with a single excitation in the labframe and the restframe of the superfluid using a Galilei transformation.

2: Su-Schrieffer-Heeger model

The Fourier transformation is given by

$$d_i = \frac{1}{\sqrt{L}} \sum_k e^{ikx_i} d_k, \tag{3}$$

where d_i can represent both a_i and b_i. Here, x_i is the position of the unit cell, and therefore represents the same position both for a_i and b_i.

We then get

$$\begin{aligned}
\sum_i (a_i^\dagger b_i + \text{h.c.}) &= \frac{1}{L} \sum_i \sum_{kq} (e^{-i(k-q)x_i} a_k^\dagger b_q + \text{h.c.}) \\
&= \sum_k (a_k^\dagger b_k + a_k b_k^\dagger) \qquad (4) \\
\sum_i (b_i^\dagger a_{i+1} + \text{h.c.}) &= \frac{1}{L} \sum_i \sum_{kq} (e^{-ikx_i} e^{iqx_{i+1}} b_k^\dagger a_q + \text{h.c.}) \\
&= \frac{1}{L} \sum_i \sum_{kq} (e^{-i(k-q)x_i} e^{iqa} b_k^\dagger a_q + \text{h.c.}) \\
&= \sum_k (e^{ika} b_k^\dagger a_k + e^{-ika} a_k^\dagger b_k) \qquad (5)
\end{aligned}$$

Introducing $\psi_k^\dagger = (a_k^\dagger, b_k^\dagger)$, we now get

$$H = \sum_k \psi_k^\dagger H_k \psi_k = -\sum_k \psi_k^\dagger \begin{pmatrix} 0 & \alpha + \beta e^{-ika} \\ \alpha + \beta e^{ika} & 0 \end{pmatrix} \psi_k. \tag{6}$$

Introducing a unitary transformation

$$\psi_k = \begin{pmatrix} a_k \\ b_k \end{pmatrix} = P_k \begin{pmatrix} c_k \\ d_k \end{pmatrix} = P_k \phi_k, \tag{7}$$

the new operators c_k and d_k automatically satisfy fermionic commutation relations. The Hamiltonian takes the form

$$H = \sum_k \phi_k^\dagger P_k^\dagger H_k P_k \phi_k \tag{8}$$

Choosing P_k to diagonalize H_k, the Hamiltonian becomes diagonal in the new operators c_k and d_k, where the single particle excitation energies are given by the eigenvalues of H_k. We then get

$$\begin{aligned}
0 = \det \begin{pmatrix} \omega_k & \alpha + \beta e^{-ika} \\ \alpha + \beta e^{ika} & \omega_k \end{pmatrix} &= \omega_k^2 - (\alpha + \beta e^{ika})(\alpha + \beta e^{-ika}) \\
&= \omega_k^2 - (\alpha^2 + \beta^2 + 2\alpha\beta \cos ka) \qquad (9)
\end{aligned}$$

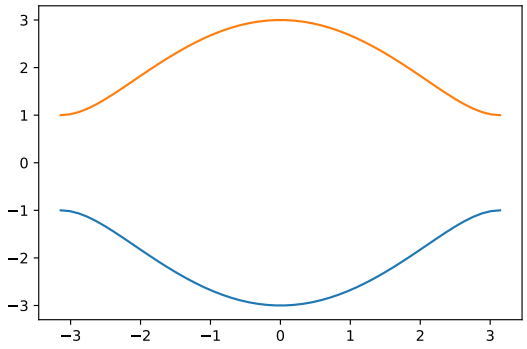

Figure 1: Dispersion relation at $\alpha = 1$ and $\beta = 2\alpha$. The band gap is $2|\alpha - \beta|$.

Hence, the dispersion relation is

$$\omega_k = \pm\sqrt{\alpha^2 + \beta^2 + 2\alpha\beta\cos ka} \tag{10}$$

and the Hamiltonian can be written in the given form.

(b) For some given α and β, ϵ_k varies with the cosine between $\sqrt{\alpha^2 + \beta^2 + 2\alpha\beta} = \alpha + \beta$ at $k = 0$ and $\sqrt{\alpha^2 + \beta^2 - 2\alpha\beta} = |\alpha - \beta|$ at $k = \pm\pi/a$. The dispersion relation is periodic with period $2\pi/a$. We plot the dispersion relation for the (reduced) first Brillouin zone in figure 1.

(c) Since the electrons are spinless and there are $2L$ lattice sites, the total number of states is $2L$. With $N = L$ spinless electrons, half of the states are filled, and at zero termperature, this corresponds to complete filling of the lowest band. To make an excitation, an electron must therefore be lifted to the upper band, and the energy cost of this is the gap size $\Delta = 2|\alpha - \beta|$. At zero temperature, the system is therefore a conductor for $\alpha = \beta$, while a finite hopping anisotropy $|\alpha - \beta|$ gives an insulator. At finite temperature T, we have a conductor when the gap is small compared to the temperature.

(d) Drawing a finite chain, we see that the leftmost and rightmost hopping amplitudes are both α. Hence, when we let $\alpha \leftrightarrow \beta$, the system is slightly changed, since the edge hopping amplitudes are being changed. Setting $\beta = 0$, we decouple the Hamiltonian into pairs of coupled operators, i.e.

$$H = \sum_{i=1}^{L} H_i^{\beta=0} = -\alpha\sum_{i=1}^{L}(a_i^\dagger b_i + b_i^\dagger a_i) = \sum_i (a_i^\dagger, b_i^\dagger)\begin{pmatrix} 0 & -\alpha \\ -\alpha & 0 \end{pmatrix}\begin{pmatrix} a_i \\ b_i \end{pmatrix}, \tag{11}$$

To find the energy eigenvalue, we have to diagonalize each H_i. Using the matrix form above, the eigenvalues ω_i are obtained by

$$0 = \det\begin{pmatrix} \omega_i & \alpha \\ \alpha & \omega_i \end{pmatrix} = \omega_i^2 - \alpha^2 \Rightarrow \omega_i = \pm\alpha. \tag{12}$$

The system therefore has energy eigenvalues $\pm\alpha$ with degeneracy L each.

For $\alpha = 0$, the Hamiltonian still decouples into pairs,

$$H = \sum_{i=1}^{L-1} H_i^{\alpha=0} \tag{13}$$

Now, however, there are only $L-1$ pairs, and the operators for the lattice sites at the edges are not coupled to anything. The states with one particle at the lattice sites on the edges of the sample are therefore eigenstates with eigenvalue 0, and the spectrum is $\omega^{\alpha=0} \in \{0, \pm\beta\}$, where the degeneracy of the eigenvalue 0 is 2 and the degeneracy of $\pm\beta$ is $L-1$ each.

For the bulk dispersion relation, setting either $\beta = 0$ or $\alpha = 0$, we obtain dispersion relation $\pm\alpha$ (or $\pm\beta$). Since the eigenvalue 0 obtained for $\alpha = 0$ is due to an edge effect, it is not captured by the bulk dispersion relation.

(e) To demonstrate the presence of edge states in a finite system, we first introduce

$$\psi^\dagger = (a_1^\dagger, b_1^\dagger, a_2^\dagger, b_2^\dagger, \ldots, a_L^\dagger, b_L^\dagger) \tag{14}$$

The Hamiltonian can then be written in matrix form $H = \psi^\dagger M \psi$, where

$$M = -\begin{pmatrix} 0 & \alpha & 0 & & & & & \\ \alpha & 0 & \beta & 0 & & & & \\ 0 & \beta & 0 & \alpha & 0 & & & \\ & 0 & \alpha & 0 & \beta & & & \\ & & 0 & \beta & 0 & & & \\ & & & & & \ddots & & \\ & & & & & & 0 & \alpha \\ & & & & & & \alpha & 0 \end{pmatrix}. \tag{15}$$

Introducing new operators c_i and d_i, $i = 1, \ldots L$, and putting these into the column vector ϕ, we may diagonalize the Hamiltonian by a unitary transformation. Choosing some appropriate system size L, we may diagonalize the matrix numerically to obtain the eigenvalues and eigenvectors. If we let $\psi = P\phi$, where P diagonalizes M, columns of P are eigenvectors of M. For a given eigenstate $|n\rangle$,

$$|n\rangle = \phi_n^\dagger |0\rangle = \sum_j (P^\dagger)_{nj}^* \psi_j^\dagger |0\rangle = \sum_j (P)_{jn} \psi_j^\dagger |0\rangle \tag{16}$$

The probability for a particle in state $|n\rangle$ to be at the lattice site corresponding to operator j in ψ is therefore $|P_{jn}|^2$, which is the j-th component of eigenvector n of M. By plotting the eigenvectors, we may therefore demonstrate the presence of edge states.

Full credit is also awarded for simply pointing out that one may find and plot the eigenvectors of M.

3: Spin currents of Heisenberg model

(a) Write the Hamiltonian as $H = H_J + H_h$, where H_J is the Heisenberg term and H_h is the magnetic field term. We assume $h \geq 0$, so that the ground state is given by all spins pointing in the z-direction. We are given that H_J can be written in the form

$$H_J = C_0 + \sum_k \omega_k^{h=0} a_k^\dagger a_k \tag{17}$$

with some constant C_0, and where a_k is a magnon annihilation operator. The magnetic field term can be written as

$$H_h = -h \sum_i S_i^z = -h \sum_i (S - a_i^\dagger a_i) = -NhS + h \sum_k a_k^\dagger a_k, \tag{18}$$

where N is the number of lattice sites. The Hamiltonian then becomes

$$H = C + \sum_k (\omega_k^{h=0} + h) a_k^\dagger a_k, \tag{19}$$

and the dispersion relation is $\omega_k = \omega_k^{h=0} + h$.

With $h = 0$, the Hamiltonian is invariant under any global spin rotation. These form a continuous set of transformations. Furthermore, the ground state consists of all spins pointing in the same direction, and this ground state breaks the continuous rotation symmetry. According to Goldstones theorem, the excitation spectrum must therefore be gapless. By Taylorexpanding the cosine in $\omega_k^{h=0}$, it is clear that $\omega_k^{h=0} \to 0$ for $k \to 0$, consistent with Goldstones theorem.

When we add a magnetic field in the z-direction, the Hamiltonian is only invariant under spin rotations around the z-axis. However, the ground state is also invariant under this transformation, and therefore, there is no spontaneous symmetry breaking. Goldstones theorem does not require a gapless excitation spectrum, and looking at the excitation spectrum, there is a gap of size h.

(b) Since the Heisenberg EoM is $i\dot{S}_i^z = [S_i^z, H]$, we need to find the commutator $[S_l^z, H]$. H consists of two terms. However, since H_h is simply a sum over the z-component of the spin, it commutes with S_l^z. Then

$$\begin{aligned} [S_l^z, H] &= \sum_{i,\delta} [S_l^z, -J\mathbf{S}_i \cdot \mathbf{S}_{i+\delta}] = -J \sum_{i,\delta} [S_l^z, S_i^z S_{i+\delta}^z + (1/2)(S_i^+ S_{i+\delta}^- + S_i^- S_{i+\delta}^+)] \\ &= -(J/2) \sum_{i,\delta} [S_l^z, (S_i^+ S_{i+\delta}^- + S_i^- S_{i+\delta}^+)] \end{aligned} \tag{20}$$

There are now two cases we have to consider, $l = i$ and $l = i+\delta$. Using the spin commutation relation

$$[S^z, S^\pm] = \pm S^\pm \tag{21}$$

given in the formula sheet, we get

$$[S_l^z, H] \;=\; -(J/2)\sum_\delta \left((S_l^+ S_{l+\delta}^- - S_l^- S_{l+\delta}^+) - (S_{l-\delta}^+ S_l^- - S_{l-\delta}^- S_l^+)\right). \tag{22}$$

Moving this commutator to the right hand side of the Heisenberg equation and dividing out the i, we get

$$\dot{S}_l^z + (-iJ/2)\sum_\delta \left((S_l^+ S_{l+\delta}^- - S_l^- S_{l+\delta}^+) - (S_{l-\delta}^+ S_l^- - S_{l-\delta}^- S_l^+)\right) = 0 \tag{23}$$

We may then identify

$$j_\delta(l) = (-iJ/2)(S_l^+ S_{l+\delta}^- - S_l^- S_{l+\delta}^+). \tag{24}$$

First, we note that this is a Hermitian operator since $S_i^+ = (S_i^-)^\dagger$. Furthermore, we see that the operator $S_l^+ S_{l+\delta}^-$ represents the transfer of an up spin from $l+\delta$ to l, i.e. from state $\downarrow\uparrow$ to state $\uparrow\downarrow$, i.e. flow of spin up to the left. The other term represents $\uparrow\downarrow$ goes to $\downarrow\uparrow$, i.e. flow of spin up to the right. Since this is in the opposite direction, this term comes with a relative minus. The operator therefore seems to make sense.

(c) We now want to express the current operator in terms of magnon operators. We then introduce the Holstein-Primakoff bosons. Since we are working within linear spin wave theory, we may neglect all terms that contain three or more creation and annihilation operators. To this order,

$$S_i^+ \simeq \sqrt{2S}a_i, \quad S_i^- \simeq \sqrt{2S}a_i^\dagger, \tag{25}$$

where we Taylor expanded the square root expressions to zeroth order in $a_i^\dagger a_i/2S$. Inserting, we obtain

$$j_\delta(l) = (-iJS)(a_l a_{l+\delta}^\dagger - a_l^\dagger a_{l+\delta}) \tag{26}$$

The total spin current then becomes

$$\begin{aligned} j_\delta &= JS\sum_l i(a_l^\dagger a_{l+\delta} - a_{l+\delta}^\dagger a_l) \\ &= JS\left(\frac{1}{N}\right)\sum_l\sum_{kq}(ie^{-i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}_l}e^{iq_\delta}a_k^\dagger a_q + \text{h.c.}) \\ &= JS\sum_k i(e^{ik_\delta} - e^{-ik_\delta})a_k^\dagger a_k \\ &= \sum_k(-2JS\sin k_\delta)\; a_k^\dagger a_k \end{aligned} \tag{27}$$

When calculating the average current $\langle j_\delta \rangle$, $a_k^\dagger a_k \to \langle a_k^\dagger a_k \rangle$. The average value is a thermal average calculated with respect to the full Hamiltonian. When there is no magnetic field whatsoever, $\langle a_k^\dagger a_k \rangle = \langle a_{-k}^\dagger a_{-k} \rangle$, and the contributions from $\pm k$ in the above sum cancel out to give $\langle j_\delta \rangle = 0$ since $\sin k_\delta$ is antisymmetric in k.

(e) To obtain the spin conductivity, we Fouriertransform the equation $\langle j_\delta \rangle = \sigma \nabla h$ assuming σ is constant. We discretize the gradient by writing it as $\nabla h = h_{i+\delta} - h_i$. Then,

$$\langle j_\delta(\mathbf{q}, \omega) \rangle = \sigma \sum_l e^{-i\mathbf{q}\cdot\mathbf{r}_l} (h_{l+\delta}(\omega) - h_l(\omega)) = \sigma (e^{i\mathbf{q}\cdot\delta} - 1) h^z(\mathbf{q}, \omega) \tag{28}$$

Since we are looking at a static problem and the current is position independent, we may consider $\mathbf{q} \to 0$ and $\omega \to 0$ (like we did for the electric conductivity), and obtain

$$\langle j_\delta(\mathbf{q} \to 0, \omega \to 0) \rangle \simeq \sigma \; i q_\delta \; h^z(\mathbf{q} \to 0, \omega \to 0) \tag{29}$$

This is on the same form as equation (7) in the exam, and by considering the same limit of $\mathbf{q} \to 0, \omega \to 0$ there, we may compare the two expressions and obtain σ.

(f) The given expression for the response function χ contains a current-spin response function. The continuity equation relates a time derivative of the spin to some spin currents. By using the identity given in the hint, we may write the factor $e^{i\omega t}$ in the integral as

$$e^{i\omega t} = \frac{1}{i\omega} \left(\frac{d}{dt} \right) e^{i\omega t} \tag{30}$$

Notice that this gives the factor (i/ω) present in the Kubo formula. We may then use partial integration to transfer the time derivative to the commutator. Since we have time-translational invariance in the unperturbed Hamiltonian (i.e. not including the magnetic field), we may rewrite the commutator using

$$[j_\delta(\mathbf{q}, t), S^z(-\mathbf{q}, 0)] = [j_\delta(\mathbf{q}, 0), S^z(-\mathbf{q}, -t)]. \tag{31}$$

The time derivative of this commutator becomes a commutator between the current and the time derivative of the spin, and after inserting the continuity equation, we have replaced the z-component of the spin in the commutator with a current, and we therefore get a current-current response function. The boundary term from the partial integration gives a term which corresponds to the constant term in the Kubo formula.

4: Greens functions and impurity scattering

(a) We want to show that $\mathcal{G}(\nu, \nu', \tau + \beta) = \zeta \mathcal{G}(\nu, \nu', \tau)$. We restrict the argument of the Greens function to the interval $(-\beta, \beta)$, and should therefore consider $-\beta < \tau < 0$. Then,

$$\begin{aligned}\mathcal{G}(\nu,\nu',\tau+\beta) &= -\langle T_\tau c_\nu(\tau+\beta)c^\dagger_{\nu'}(0)\rangle = -\langle c_\nu(\tau+\beta)c^\dagger_{\nu'}(0)\rangle \\ &= -(1/Z)\,\mathrm{Tr}\left(e^{-\beta H}e^{H(\tau+\beta)}c_\nu e^{-H(\tau+\beta)}c^\dagger_{\nu'}\right) \\ &= -(1/Z)\,\mathrm{Tr}\left(e^{H\tau}c_\nu e^{-H\tau}e^{-\beta H}c^\dagger_{\nu'}\right) \qquad (32)\end{aligned}$$

Using invariance of the trace under cyclic permutations, we may now rewrite this as

$$\begin{aligned}\mathcal{G}(\nu,\nu',\tau+\beta) &= -(1/Z)\,\mathrm{Tr}\left(e^{-\beta H}c^\dagger_{\nu'}e^{H\tau}c_\nu e^{-H\tau}\right) \\ &= -(1/Z)\,\mathrm{Tr}\left(e^{-\beta H}c^\dagger_{\nu'}(0)c_\nu(\tau)\right) \\ &= -\zeta\langle T_\tau c_\nu(\tau)c^\dagger_{\nu'}(0)\rangle = \zeta\mathcal{G}(\nu,\nu',\tau), \qquad (33)\end{aligned}$$

using the definition of the time ordering operator and that $\tau < 0$.

(b) The Greens function in the imaginary time domain is given by

$$\mathcal{G}(\nu,\nu';\tau) = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n\tau}\mathcal{G}(\nu,\nu';i\omega_n) \qquad (34)$$

Then,

$$\mathcal{G}(\nu,\nu';\tau+\beta) = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n\beta}e^{-i\omega_n\tau}\mathcal{G}(\nu,\nu';i\omega_n) \qquad (35)$$

To satisfy the symmetry relations from subproblem (a), we then need $\exp(-i\omega_n\beta) = \zeta$, which gives

$$i\omega_n = \left\{ \begin{array}{ll} (2n+1)\pi i/\beta, & \zeta = -1 \ \text{(fermions)} \\ 2n\pi i/\beta, & \zeta = +1 \ \text{(bosons)} \end{array} \right\}, \qquad (36)$$

where m is an integer. These are the Matsubara frequencies.

(c) The diagrams at order 0, 1, and 2 are given in the upper panel of the figure, while the diagrams at order 3 are drawn in the lower panel. The self energy diagrams are marked with a tick. The corresponding expressions are

$$\overline{\mathcal{G}}_{3A}(\mathbf{k},ip_n) = \sum_{k_1,k_2}\mathcal{G}^{(0)}(\mathbf{k})NU(\mathbf{k}-\mathbf{k}_1)\mathcal{G}^{(0)}(\mathbf{k}_1)U(\mathbf{k}_1-\mathbf{k}_2)\mathcal{G}^{(0)}(\mathbf{k}_2)U(\mathbf{k}_2-\mathbf{k})\mathcal{G}^{(0)}(\mathbf{k}) \qquad (37)$$

$$\overline{\mathcal{G}}_{3B}(\mathbf{k},ip_n) = \sum_{k_1}\mathcal{G}^{(0)}(\mathbf{k})NU(\mathbf{k}-\mathbf{k}_1)\mathcal{G}^{(0)}(\mathbf{k}_1)NU(0)\mathcal{G}^{(0)}(\mathbf{k}_1)U(\mathbf{k}_1-\mathbf{k})\mathcal{G}^{(0)}(\mathbf{k}) \qquad (38)$$

(d) Using the Dyson equation is equivalent to including all Feynman diagrams that can be constructed by forming products of the diagrams in the self energy. To obtain diagrams at order $n = 5$, we therefore have to put together diagrams at order 1, 2 and 3. By putting

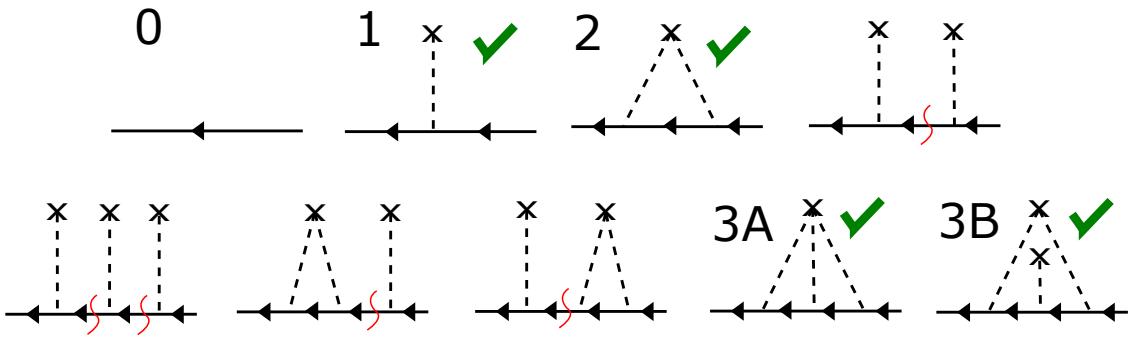

Figure 2: All Feynman diagrams up to order $n = 3$ in the impurity potential. The irreducible diagrams are marked with a tick, while the reducible diagrams are marked with a red line where an electron line can be cut to cut the diagram in two. The irreducible diagrams have been labelled. To obtain the self energy diagram corresponding to an irreducible diagram, one may simply remove the external legs.

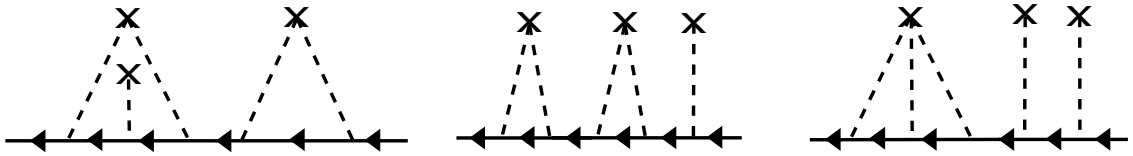

Figure 3: All inequivalent Feynmandiagrams at order $n = 5$ with $m = 3$ impurity crosses that can be constructed from self energy diagrams up to order 3.

together diagrams, the order in the impurity potential is the number of interaction lines, which is obtained by adding the order of the self energy diagrams that we put together. Possible ways to sum 1, 2, 3 up to 5 are

$$3+2, \quad 3+1+1, \quad 2+2+1, \quad 2+1+1+1, \quad 1+1+1+1+1$$

Notice that for $n = 1$ and $n = 2$, there is only one possible self-energy diagram, which then has a fixed number of impurity crosses. We have to self energy diagrams to choose between at order $n = 3$, and have to pick the one which gives 3 impurity crosses in total.

For $3+2$, the diagram Σ^2 has one impurity cross. We then have to combine it with diagram Σ^{3B}, which has two impurity crosses.

For $3+1+1$, the diagram Σ^1 has 1 cross, and with two such diagrams, the last diagram can only have 1 cross. Thus, we need to combine Σ^{3A} with two of the diagrams Σ^1.

For the remaining possibilities, there is no choice. The only possibility with 3 crosses is $2+2+1$. Hence, there are 3 different diagrams satisfying all requirements. These are shown in figure 3.