Statistical Physics and Condensed Matter Theory I: Final exam

Tuesday 25 October 2016, 18:00 - 21:00, SP H0.08

- Please write **legibly** and **be explicit** in your answers. I cannot give you points for things I can't/don't see !
- Please **use separate sheets for each question**, and put your **name, student number and study programme** on each of them.
- There is a collection of useful formulas at the end, which you can use **without rederivation**. Class notes and books are **not** allowed.
- This exam consists of 2 problems. You should do **both of them**.
- Sub-questions marked with * are particularly challenging. Consider solving them only once you're finished with the rest.
- **Be smart**: if you're stuck on a (sub-)question, don't lose too much time, you can always move on to the next one (the questions are for the most part formulated in order to make this possible).
- The points add up to 110, that's 10% bonus for you from the start.

1. Heisenberg antiferromagnet in a crystal field (35 pts)

Consider the general spin S one-dimensional Heisenberg antiferromagnet in the presence of a so-called crystal field term:

$$H = J \sum_{m=1}^{N} \mathbf{S}_m \cdot \mathbf{S}_{m+1} + D \sum_m (S_m^z)^2$$

For definiteness, we consider an even number of sites N and impose periodic boundary conditions $\mathbf{S}_{m+N} = \mathbf{S}_m$.

a) (5 pts)

What is the effect of the crystal field term when $S = 1/2$?

b) (5 pts)

For generic S, what are the classical ground states for $D < 0$? For $D > 0$? Are they also quantum ground states?
Hint: think of Néel ordering in various directions, and how H acts on states you're thinking of.

c) (10 pts)

From now on, we assume $S \gg 1$ and $D < 0$. Since antiferromagnetic configurations will be preferred, before applying the Holstein-Primakoff transformation, we rotate the spins on one sublattice (say the even sites) by π around the x-axis, $S_{2n}^x = \tilde{S}_{2n}^x$, $S_{2n}^y = -\tilde{S}^y{}_{2n}$, $S_{2n}^z = -\tilde{S}_{2n}^z$, $S_{2n+1}^{x,y,z} = \tilde{S}_{2n+1}^{x,y,z}$ to yield the equivalent Hamiltonian

$$H = -J \sum_{m=1}^{N} \left[\tilde{S}_m^z \tilde{S}_{m+1}^z - \tilde{S}_m^x \tilde{S}_{m+1}^x + \tilde{S}_m^y \tilde{S}_{m+1}^y \right] + D \sum_m \left(\tilde{S}_m^z \right)^2 .$$

Applying Holstein-Primakoff, show that this allows to write down the Hamiltonian (to leading nontrivial order in $1/S$) in Fourier modes

$$H = -N(J-D)S^2 + JS \sum_k \left[(1 - D/J)\ 2\ a_k^\dagger a_k + \cos k\ (a_{-k} a_k + a_k^\dagger a_{-k}^\dagger) \right] + O(S^0).$$

d) (10 pts)

Still for $D < 0$, diagonalize this Hamiltonian to leading nontrivial order in $1/S$. What is the spin-wave spectrum ?
Hint: you need to explicitly perform a Bogoliubov transformation (see 'Useful formulas').

e) (5 pts)

What happens to the spectrum as $k \to 0$? Contrast this result to that in the case of the pure antiferromagnet ($D = 0$), in which $\varepsilon_k = 2JS|\sin k|$.

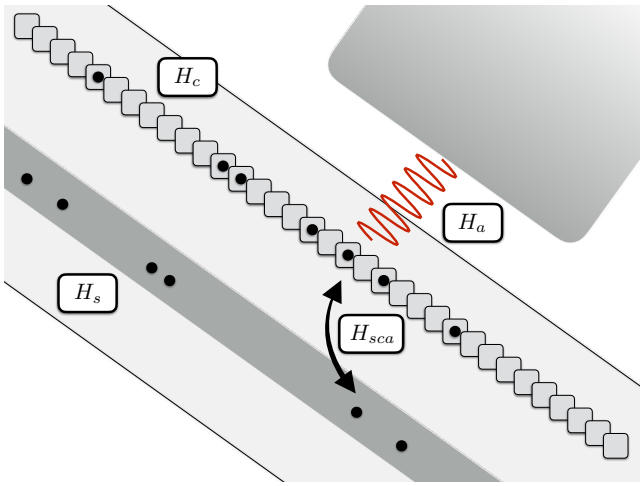

Figure 1: Cartoon of a (too simplified to be realistic) photoemission setup. A 1d chain in which electrons can hop around is represented by Hamiltonian H_c. Next to it is a 1d free-space (continuum) channel represented by H_s. The whole setup is bathed in an electromagnetic field described by H_a. The field can induce hoppings between the chain and channel due to the coupling H_{sca}: an electron in the chain can absorb a photon and be 'promoted' from the chain to the channel, where it can be observed (the reverse is of course also in principle possible, but not relevant to the experiment).

2. Photoemission spectroscopy (75 pts)

One of the obvious first questions to ask about an electronic system is: what are the energy levels available to the electrons? It is thus desirable to have probes which are able to directly 'see' those levels (namely, to directly observe the single-particle spectrum of a system). Electromagnetic waves are commonly used, and the ensuing set of methods is collectively known as spectroscopy.

In this problem, we consider a (cartoonish) setup in which we describe spectroscopy from photoemission, namely the 'emission' of electrons (for simplicity, we ignore spin) from a sample after stimulation by light. The setup is illustrated in Fig. 1.

The Hamiltonian of the chain is taken to only involve nearest-neighbour hopping, and is written using canonical fermionic operators $c_j, c_j^\dagger$ as[1]

$$H_c - \mu N_c = -t\sum_j \left[c_j^\dagger c_{j+1} + \text{h. c.}\right] - \mu \sum_j c_j^\dagger c_j, \qquad \left\{c_j, c_{j'}^\dagger\right\} = \delta_{j,j'}.$$

Performing a Fourier transformation (assuming periodic boundary conditions over N sites, namely site $N+1$ is site 1) for simplicity) using the conventions

$$c_j = \frac{1}{\sqrt{N}}\sum_{k_n} e^{ikj} c_k, \qquad c_k = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{-ikj} c_j, \qquad k_n = \frac{2\pi}{N} n, \quad n = -N/2+1, ..., N/2,$$

we have that $\left\{c_k, c_{k'}^\dagger\right\} = \delta_{k,k'}$ and that the chain Hamiltonian can be written

$$H_c - \mu N_c = \sum_{k_n} (-2t\cos k - \mu) c_k^\dagger c_k \equiv \sum_{k_n} \xi_k c_k^\dagger c_k.$$

For the free-space channel, we rather consider a continuum (no lattice) and directly write its Hamiltonian using momentum-labeled fermionic operators $s(p), s^\dagger(p)$ $(-\infty < p < \infty)$ as

$$H_s = \int_{-\infty}^{\infty} dp\ \varepsilon_s(p) s^\dagger(p) s(p), \qquad \left\{s(p), s^\dagger(p')\right\} = \delta(p-p'),$$

in which $\varepsilon_s(p)$ is here left unspecified (if you insist, $\varepsilon_s(p) = \frac{p^2}{2m}$ but we won't make use of this).

Finally, we keep the light field as simple as it can be, and choose a monochromatic source of fixed frequency ω. Using bosonic operators $a, a^\dagger$ for the photons, its Hamiltonian is simply

$$H_a = \omega a^\dagger a, \qquad \left[a, a^\dagger\right] = 1.$$

[1] We already include the chemical potential here for convenience.

The 'basis' (noninteracting; exactly-solvable) Hamiltonian is thus[2]

$$H_0 = H_c - \mu N_c + H_s + H_a.$$

Note: this exercise is divided into 3 parts. You can start Part II without having finished Part I. Part III is for those who are trying to impress me. If you get stuck, just move on to the next (sub)question.

2 Part I: noninteracting electrons

a) (10 pts) The light field is able to excite electrons out of the chain and into the continuum. Such a process involves a photon being absorbed, an electron in the chain being 'destroyed' and re-'created' in the continuum (or the reverse). This coupling can be modeled by adding a term of the form

$$H_{sca} = \gamma \int_{-\infty}^{\infty} dp \sum_k s^\dagger(p) c_k a + \text{h.c.}$$

to our Hamiltonian, in which γ represents some matrix element for the scattering event (for simplicity, we have assumed γ to be independent of p and k).

The observable we are intersted in is the number of particles being scattered into continuum states at momentum p per unit of time. This rate is given in terms of the number density $n_s(p) = s^\dagger(p)s(p)$ as

$$\frac{d}{dt} n_s(p) = i \left[H, n_s(p)\right].$$

Show that this operator is

$$\frac{d}{dt} n_s(p) = -i\gamma \sum_k s^\dagger(p) c_k a + \text{h.c.}$$

b) (10 pts) Let us assume that the light field (generated by a laser or other coherent source) is maintained in the coherent state

$$|\phi\rangle_a = e^{\phi a^\dagger} |0\rangle_a$$

in which $|0\rangle_a$ is the vacuum of a. As far as the electrons are concerned, we can thus use operators averaged over this state of the light field,

$$H_{sc}(t) \equiv \frac{{}_a\langle\phi(t)|H_{sca}|\phi(t)\rangle_a}{{}_a\langle\phi|\phi\rangle_a} \quad \text{and} \quad R(p,t) \equiv \frac{{}_a\langle\phi(t)|\frac{d}{dt}n_s(p)|\phi(t)\rangle_a}{{}_a\langle\phi|\phi\rangle_a}$$

with $|\phi(t)\rangle_a = e^{-iH_a t}|\phi\rangle_a$. Show that this leads to the following expressions for the effective Hamiltonian for s and c electrons and for the rate (here in the Schrödinger picture)

$$H_{sc}(t) = \gamma\phi e^{-i\omega t} J + \text{h.c.}, \qquad R(p,t) = -i\gamma\phi e^{-i\omega t}\ j(p) + \text{h.c.}$$

in which

$$J \equiv \int_{-\infty}^{\infty} dp\ j(p), \qquad j(p) = \sum_k s^\dagger(p) c_k.$$

[2] Of course, the boson a commutes with fermions, $[a, c_k] = 0 = [a, s(p)]$, and fermions anticommute, $\{c_k, s(p)\} = 0$.

c) (10 pts) Our Hamiltonian now involves only electrons, and reads

$$H(t) = H_{0,sc} + H_{sc}(t), \qquad H_{0,sc} \equiv H_c - \mu N_c + H_s.$$

We will consider zero temperature and place the chain at chemical potential μ. The free-space channel is initially empty, so its state is just the vacuum (its chemical potential is zero). We thus take expectation values over the state

$$|\mu;0\rangle \equiv |\mu\rangle_c \otimes |0\rangle_s, \qquad \langle(...)\rangle_0 \equiv \langle\mu;0|(...)|\mu;0\rangle$$

which is the Fermi sea ground state of chain electrons at chemical potential μ, tensored with the vacuum of free-space channel electrons.

Using the Kubo formula, show that the scattering rate we are looking for is given by

$$\bar{R}(p,t) = \bar{R}_0 - i\gamma^2|\phi|^2 \int_{-\infty}^{\infty} dt' \mathcal{C}_{\rm ret}^{j(p),J^\dagger}(t-t')e^{-i\omega(t-t')} + \text{h.c.}$$

where

$$\mathcal{C}_{\rm ret}^{j(p),J^\dagger}(t-t') \equiv -i\theta(t-t')\langle\Big[j^I(p,t), {J^I}^\dagger(t')\Big]\rangle_0$$

with operators in the interaction representation based on $H_{0,sc}$, *i.e.* $O^I = e^{iH_{0,sc}t}Oe^{-iH_{0,sc}t}$.

d) (10 pts) Show (most easily using a direct calculation, expressing any time dependence directly on the operators) that this retarded Green's function equals

$$\mathcal{C}_{\rm ret}^{j(p),J^\dagger}(t-t') = i\theta(t-t')\sum_k e^{i[\varepsilon_s(p)-\xi_k](t-t')}\bar{n}_k$$

in which $\bar{n}_k \equiv {}_c\langle\mu|c_k^\dagger c_k|\mu\rangle_c = n_F(\xi_k) = \frac{1}{1+e^{\beta\xi_k}}$ is the expectation value of the number of electrons in mode k in the chain (you don't have to rederive this last result).

e) (5 pts) Using this result in the Kubo formula, and using an η-regulator to ensure convergence of the time integral (*i.e. replacing* $e^{i\omega t} \to e^{i\omega t-\eta|t|}, \eta \to 0^+$), and remembering that $\lim_{\eta\to 0^+}\frac{1}{\pi}\frac{\eta}{x^2+\eta^2} = \delta(x)$, show that $\bar{R}(p,t)$ is in fact time-independent and equal to

$$\bar{R}(p) = 2\pi\gamma^2|\phi|^2\sum_k \delta(\omega - \varepsilon_s(p) + \xi_k)\bar{n}_k.$$

For your information: you can now clearly see the usefulness of photoemission spectroscopy. It gives direct access to the energy levels and their occupation.

f)* (5 pts) Going to infinite lattice size $N \to \infty$, the momentum sum $\sum_k(...)$ becomes $N\int_{-\pi}^{\pi} dk(...)$, and the scattering rate per site

$$\bar{r}(p) \equiv \lim_{N\to\infty}\frac{\bar{R}(p)}{N} = 2\pi\gamma^2|\phi|^2\int_{-\pi}^{\pi} dk\delta\left(\omega - \varepsilon_s(p) + \xi(k)\right)\bar{n}(k).$$

Using the δ-function rule

$$\delta(f(x)) = \sum_{x_0 \text{ zero of } f}\frac{1}{|f'(x_0)|}\delta(x-x_0),$$

obtain an explicit expression for $\bar{r}(p)$, in which you have explicitly evaluated $\bar{n}(k)$. Provide as accurate a sketch as you can for this rate, given the form of $\xi(k)$ obtained above, and assuming $\varepsilon_s(p) = p^2/2m$.

2 Part II: interacting electrons

Let us now turn on interactions between electrons when they are on the chain. Specifically, we will modify our H_c to include a Hubbard repulsion term, which is counted if two electrons are on neighbouring sites:

$$H_c - \mu N_c = -t \sum_j \left[c_j^\dagger c_{j+1} + \text{h. c.} \right] - \mu \sum_j c_j^\dagger c_j + U \sum_j n_j n_{j+1}.$$

II.a) (5 pts) Write the Hubbard interaction term in Fourier space, using the conventions in I.a.

II.b) (5 pts) Let us focus first on the free case $U = 0$. The coherent state path integral representation of the partition function $Z^{(0)}$ and free effective action[3] of the free system are

$$\mathcal{Z}^{(0)} = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S_0[\bar{\psi},\psi]}, \qquad S_0[\bar{\psi}, \psi] = \sum_{kn} \bar{\psi}_{kn} \left[-i\omega_n + \xi_k \right] \psi_{kn}.$$

By directly performing the Grassmann integrations, show that the free ($U = 0$) Green's function is

$$\mathcal{G}^{(0)}_{k,n} \equiv \langle \bar{\psi}_{kn} \psi_{kn} \rangle_0 = \frac{1}{i\omega_n - \xi_k} \quad \text{where we denote} \quad \langle (...) \rangle_0 = \frac{1}{\mathcal{Z}^{(0)}} \int \mathcal{D}(\bar{\psi}, \psi)(...) e^{-S_0[\bar{\psi},\psi]}.$$

II.c) (5 pts) By direct calculation, show that up to and including terms of first order in U/t, the Green's function of the interacting system can be written[4]

$$\mathcal{G}_{k,n} \equiv \langle \bar{\psi}_{kn} \psi_{kn} \rangle = \frac{1}{i\omega_n - \xi_k - \Sigma_{k,n}}$$

where $\Sigma_{k,n}$ is called the *self-energy*. Give an expression for it to first order in U.

II.d) (5 pts) What is the influence of the Hubbard interaction term, to first order in U/t, on the expectation value of the number of electrons in momentum state k? In other words, calculate

$$\langle n_k \rangle = \frac{1}{\beta} \sum_n \langle \bar{\psi}_{kn} \psi_{kn} \rangle.$$

2 Part III, finale

III.a)* (5 pts) Using the result in II.d, and referring back to I.e-f, give a formula for the scattering rate $\bar{r}(p)$ in the presence of Hubbard interactions (to first order), and sketch it.

[3] Here, we always write the momentum k and Matsubara frequency index n separately.
[4] Hint: $1 + U = \frac{1}{1-U} + \mathcal{O}(U^2)$.

Useful Formulas

Trigonometric and hyperbolic functions

$$\sin(\theta_1+\theta_2)=\sin\theta_1\cos\theta_2+\cos\theta_1\sin\theta_2, \qquad \cos(\theta_1+\theta_2)=\cos\theta_1\cos\theta_2-\sin\theta_1\sin\theta_2,$$
$$\cos^2\theta+\sin^2\theta=1, \qquad \sin^2\theta=\frac{1}{2}(1-\cos 2\theta), \qquad \cos^2\theta=\frac{1}{2}(1+\cos 2\theta),$$
$$\sinh(\theta_1+\theta_2)=\sinh\theta_1\cosh\theta_2+\cosh\theta_1\sinh\theta_2, \quad \cosh(\theta_1+\theta_2)=\cosh\theta_1\cosh\theta_2+\sinh\theta_1\sinh\theta_2,$$
$$\cosh^2\theta-\sinh^2\theta=1, \qquad \sinh^2\theta=\frac{1}{2}(\cosh 2\theta-1), \qquad \cosh^2\theta=\frac{1}{2}(\cosh 2\theta+1).$$

Series expansions

$$e^x=\sum_{n=0}^{\infty}\frac{x^n}{n!}, \qquad \cos x=\sum_{n=0}^{\infty}(-1)^n\frac{x^{2n}}{(2n)!}, \qquad \sin x=\sum_{n=0}^{\infty}(-1)^n\frac{x^{2n+1}}{(2n+1)!},$$
$$(1+x)^\alpha=\sum_{n=0}^{\infty}\left(\begin{array}{c}\alpha\\ n\end{array}\right)x^n=1+\alpha x+\frac{\alpha(\alpha-1)}{2}x^2+..., \qquad \ln(1+x)=\sum_{n=1}^{\infty}(-1)^{n+1}\frac{x^n}{n}$$

Bosonic occupation number states

$$[b,b^\dagger]=1, \qquad |n\rangle=\frac{1}{\sqrt{n!}}(b^\dagger)^n|0\rangle, \qquad b^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle, \qquad b|n\rangle=\sqrt{n}|n-1\rangle.$$

Pauli spin matrices

$$\sigma^x=\left(\begin{array}{cc}0&1\\1&0\end{array}\right), \qquad \sigma^y=\left(\begin{array}{cc}0&-i\\i&0\end{array}\right), \qquad \sigma^z=\left(\begin{array}{cc}1&0\\0&-1\end{array}\right), \qquad \sigma^\pm=\frac{1}{2}(\sigma^x\pm i\sigma^y).$$

Spins on a lattice

$su(2)$ spin algebra (here, $i,j,k=x,y,z$ and m,n denote lattice sites and ε^{ijk} is the completely antisymmetric tensor with $\varepsilon^{ijk}=\pm 1$ for $ijk=$ even/odd permutation of xyz, 0 otherwise).

$$\left[\hat{S}^i_m,\hat{S}^j_n\right]=i\delta_{mn}\varepsilon^{ijk}\hat{S}^k_n.$$

Spin raising and lowering operators: $\hat{S}^\pm_m=\hat{S}^x_m\pm i\hat{S}^y_m$ with

$$\left[\hat{S}^z_m,\hat{S}^\pm_n\right]=\pm\delta_{nm}\hat{S}^\pm_m, \qquad \left[\hat{S}^+_m,\hat{S}^-_n\right]=2\delta_{nm}\hat{S}^z_m.$$

For the $S=1/2$ case, one can use the representation $S^i=\sigma^i/2$, $i=x,y,z$.

Holstein-Primakoff transformation

$$\hat{S}^-_m=a^\dagger_m(2S-a^\dagger_m a_m)^{1/2}, \qquad \hat{S}^+_m=(2S-a^\dagger_m a_m)^{1/2}a_m, \qquad \hat{S}^z_m=S-a^\dagger_m a_m$$

where a_m, $a^\dagger_m$ are bosonic operators obeying the canonical algebra $[a_m,a^\dagger_n]=\delta_{mn}$ (other commutators vanish).

Fourier transformation

$$a_k=\frac{1}{\sqrt{N}}\sum_{m=1}^{N}e^{ikm}a_m, \quad a_m=\frac{1}{\sqrt{N}}\sum_{k\in BZ}e^{-ikm}a_k, \quad [a_k,a^\dagger_{k'}]_\zeta=\left\{\begin{array}{ll}a_ka^\dagger_{k'}-a^\dagger_{k'}a_k, & \text{bosons}\\ a_ka^\dagger_{k'}+a^\dagger_{k'}a_k, & \text{fermions}\end{array}\right.=\delta_{kk'}$$

Bogoliubov transformation (bosons)

The quadratic form

$$\begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

can be diagonalized by the transformation to new variables α_k,

$$\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = \mathbf{U}_k^{-1} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix},$$

with $[\alpha_k, \alpha_{k'}^\dagger] = \delta_{kk'}$. The matrix $\mathbf{U}_k$ is

$$\mathbf{U}_k = \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} = \cosh\theta_k \mathbf{1} + \sinh\theta_k \sigma^x$$

and is such that $\mathbf{U}_k^\dagger = \mathbf{U}_k$ and $\mathbf{U}_k^{-1} = \sigma^z \mathbf{U}_k \sigma^z$ (pseudo-unitarity). Choosing $\gamma_k = \tanh 2\theta_k$ makes the quadratic form matrix diagonal,

$$(\mathbf{U}_k^{-1})^\dagger \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \mathbf{U}_k^{-1} = \frac{1}{\cosh 2\theta_k} \mathbf{1} = \left[1 - \gamma_k^2\right]^{1/2} \mathbf{1}.$$

Bogoliubov transformation (fermions)

The matrix

$$\begin{pmatrix} a & b \\ b & -a \end{pmatrix}$$

(here for $a, b \in \mathbb{R}$) can be diagonalized by the unitary transformation

$$UHU^\dagger = \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}, \qquad U = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}$$

where $\tan 2\theta = \frac{b}{a}$ and $\varepsilon = (a^2 + b^2)^{1/2}$.

Random walks

Diffusion equation:

$$\left(\frac{\partial}{\partial t} - D\ \nabla^2\right) P(\boldsymbol{r}, t) = 0.$$

In the scaling limit, for a d-dimensional hypercubic lattice, the diffusion constant D is related to the lattice spacing a, step time δt and dimension d by

$$D = \lim_{\substack{a\to 0 \\ \delta t \to 0}} \frac{a^2}{2d\delta t}.$$

The probability per unit volume of being at position $\boldsymbol{r}_1$ at time t_1 given that one was at $\boldsymbol{r}_0$ and time t_0 is given by

$$\begin{aligned} p(\boldsymbol{r}_1, t_1 | \boldsymbol{r}_0, t_0) \equiv \lim a^{-d} P_{\boldsymbol{r}_1, t_1 | \boldsymbol{r}_0, t_0} &= \int_{-\infty}^{\infty} \frac{d^d \boldsymbol{k}}{(2\pi)^d} e^{-(t_1 - t_0) D \boldsymbol{k}^2 + i\boldsymbol{k}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_0)} \\ &= \frac{1}{[4\pi D(t_1 - t_0)]^{\frac{d}{2}}} \exp\left[-\frac{|\boldsymbol{r}_1 - \boldsymbol{r}_0|^2}{4D(t_1 - t_0)}\right]. \end{aligned}$$

Coherent states (bosons: $\zeta = 1$, fermions: $\zeta = -1$)

$$|\phi\rangle \equiv \exp\left[\zeta \sum_i \phi_i a_i^\dagger\right]|0\rangle$$

$$a_i|\phi\rangle = \phi_i|\phi\rangle, \qquad a_i^\dagger|\phi\rangle = \zeta\partial_{\phi_i}|\phi\rangle, \qquad \langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i, \qquad \langle\phi|a_i = \partial_{\bar{\phi}_i}\langle\phi| \qquad \forall i.$$

The norm of a coherent state is

$$\langle\phi|\phi\rangle = \exp\left[\sum_i \bar{\phi}_i\phi_i\right].$$

Coherent states form an (over)complete set of states:

$$\int \prod_i d(\bar{\phi}_i, \phi_i) e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}}$$

with $\mathbf{1}_{\mathcal{F}}$ the identity in Fock space. The measures are $d(\bar{\phi}_i, \phi_i) = \frac{d\bar{\phi}_i d\phi_i}{\pi}$ for bosons, $d(\bar{\phi}_i, \phi_i) = d\bar{\phi}_i d\phi_i$ for fermions.

Campbell-Baker-Hausdorff formula

The general identity called the Campbell-Baker-Hausdorff formula reads:

$$e^{-B}Ae^{B} = \sum_{n=0}^{\infty} \frac{1}{n!}[A, B]_n, \qquad \text{where } [A, B]_n = [[A, B]_{n-1}, B], \quad [A, B]_0 \equiv A.$$

This can be specialized to some simpler particular cases. Let A and B be two quantum operators such that $[A, B]$ commutes with A and B. Then, the following identities hold:

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}, \qquad [A, e^{\lambda B}] = \lambda[A, B]e^{\lambda B}.$$

Another useful one is:

$$\text{if } [A, B] = DB \text{ and } [A, D] = 0 = [B, D], \text{ then } f(A)B = Bf(A + D).$$

This then implies (under the same conditions) that

$$e^A Be^{-A} = Be^D.$$

Grassmann variables

$$\forall i, j, \quad \eta_i\eta_j = -\eta_j\eta_i, \qquad \int d\eta_i = 0, \qquad \int d\eta_i\eta_i = 1.$$

Coherent state path integral representation of the partition function

For a second-quantized Hamiltonian of the form

$$\hat{H}(a^\dagger, a) = \sum_{ij} h_{ij}a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}a_i^\dagger a_j^\dagger a_k a_l,$$

the partition function is

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi}, \psi)e^{-S[\bar{\psi},\psi]}.$$

Here, we work directly in the Matsubara frequency (usually labeled by the index n, whose value runs over all integers) representation. The measure is defined as $\mathcal{D}(\bar{\psi}, \psi) = \prod_i \prod_n d(\bar{\psi}_{in}, \psi_{in})$ and $d(\bar{\psi}, \psi) \equiv \beta d\bar{\psi}d\psi$ for fermions and $d(\bar{\psi}, \psi) \equiv \frac{1}{\pi\beta}d\bar{\psi}d\psi$ for bosons (see next subsection for the Gaussian integral). The effective action is

$$S[\bar{\psi}, \psi] = \sum_{ij,n} \bar{\psi}_{in}\left[(-i\omega_n - \mu)\delta_{ij} + h_{ij}\right]\psi_{jn} + T\sum_{ijkl,\{n_i\}} V_{ijkl}\bar{\psi}_{in_1}\bar{\psi}_{jn_2}\psi_{kn_3}\psi_{ln_4}\delta_{n_1+n_2,n_3+n_4}.$$

Gaussian integration over bosonic/Grassmann variables

By definition, in the Matsubara frequency representation of the action, we use

$$\int d(\bar{\psi}_{in}, \psi_{in}) e^{-\bar{\psi}_{in}\varepsilon\psi_{in}} = (\beta\varepsilon)^{-\zeta}$$

with $\zeta = +1$ for bosons and -1 for fermions.

Wick's theorem (fermions)

The expectation value of a product of fermionic fields over a noninteracting theory is given by the sum over all pairings signed by the permutation order. For four fields,

$$\langle\bar{\psi}_a\bar{\psi}_b\psi_c\psi_d\rangle_0 = \langle\bar{\psi}_a\psi_d\rangle_0\langle\bar{\psi}_b\psi_c\rangle_0 - \langle\bar{\psi}_a\psi_c\rangle_0\langle\bar{\psi}_b\psi_d\rangle_0.$$

The first term is the Hartree term, the second is the Fock term.

Relations between Green's functions

retarded from imaginary-time: $\mathcal{C}^{ret}(\omega) = \mathcal{C}^{\tau}(i\omega_n)|_{i\omega_n\to\omega+i\eta}$

advanced from imaginary-time: $\mathcal{C}^{ret}(\omega) = \mathcal{C}^{\tau}(i\omega_n)|_{i\omega_n\to\omega-i\eta}$

Matsubara sums (fermions)

$$\sum_n \ln(\beta\left[-i\omega_n + \xi\right]) = \ln\left[1 + e^{-\beta\xi}\right],$$

$$T\sum_n \frac{1}{i\omega_n - \varepsilon_a + \mu} = \frac{1}{e^{\beta(\varepsilon_a-\mu)}+1} \equiv n_F(\varepsilon_a, \mu).$$

Interaction picture/representation

For the Hamiltonian $H = H_0 + H_I$ in which H_I represents the 'interaction' and H_0 the free (exactly-solvable) model, the interaction picture states and operators are related to the Schrödinger ones by

$$|\psi^I(t)\rangle = e^{iH_0t}|\psi^S(t)\rangle, \qquad \mathcal{O}^I(t) = e^{iH_0t}\mathcal{O}^S e^{-iH_0t}.$$

Linear response theory: the Kubo formula

For the time-dependent Hamiltonian (in the Schrödinger picture)

$$H(t) = H_0 + F(t)\hat{P},$$

with initial condition that the system at $t \to -\infty$ is in state $|\psi_o\rangle$, the time-dependent expectation value of operator $\mathcal{O}$ is given in linear response by the Kubo formula

$$\bar{O}(t) = \langle\psi_0|\hat{O}|\psi_0\rangle + \int_{-\infty}^{\infty} dt' \mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_0}(t-t')F(t') + O(F^2)$$

in terms of the retarded correlation function (computed in state $|\psi_0\rangle$) between the perturbation and observable, this retarded function being defined (for a generic state $|\psi\rangle$) as

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi}(t-t') \equiv -i\theta(t-t')\langle\psi|[\hat{O}^I(t), \hat{P}^I(t')]|\psi\rangle.$$

If your perturbation consists of a sum of terms, the total linear response is of course given by the sum of the individual responses.