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Equilibrium and Non-equilibrium QFT in Many-Body Systems SS 2013

Exercise Sheet 3

(To be handed in on the 11th of June and discussed on the 13th and 14th of June)

3.1 Electron-electron interactions

Consider a system of electrons which interact via the Coulomb interaction $V(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$:

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\sigma\sigma'} \int d^3r \int d^3r'\, \psi^\dagger_\sigma(\mathbf{r}) \psi^\dagger_{\sigma'}(\mathbf{r}')\, \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\, \psi_{\sigma'}(\mathbf{r}') \psi_\sigma(\mathbf{r}) \;, \tag{1}$$

where $c^\dagger_{\mathbf{k}\sigma}, c_{\mathbf{k}\sigma}$ and $\psi^\dagger_\sigma(\mathbf{r}), \psi_\sigma(\mathbf{r})$ are creation and destruction operators for an electron in momentum eigenstate $|\mathbf{k}\sigma\rangle$ and position eigenstate $|\mathbf{r}\sigma\rangle$, respectively.

a) Show that the Fourier transform of $V(\mathbf{r}-\mathbf{r}')$ w.r.t. $(\mathbf{r}-\mathbf{r}')$ is

$$V_{\mathbf{q}} = \frac{4\pi e^2}{q^2} \;.$$

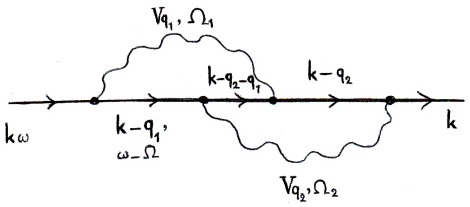
(Note: This is most conveniently shown by solving the Poisson equation for the Coulomb potential in momentum space.)

b) Derive the Hamiltonian H with the interaction term in momentum representation, *i.e.* in terms of $c^\dagger_{\mathbf{k}\sigma}, c_{\mathbf{k}\sigma}$:

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\sigma\sigma'} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c^\dagger_{\mathbf{k}-\mathbf{q},\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'}\, V_{\mathbf{q}}\, c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} \tag{2}$$

c) Draw all Feynman diagrams for the self-energy up to the 3rd order in the interaction $V_{\mathbf{q}}$ and label all lines with the appropriate momentum and energy labels.

d) Write down the mathematical expression for the following Feynman diagram; there is no need to perform the Matsubara summations.

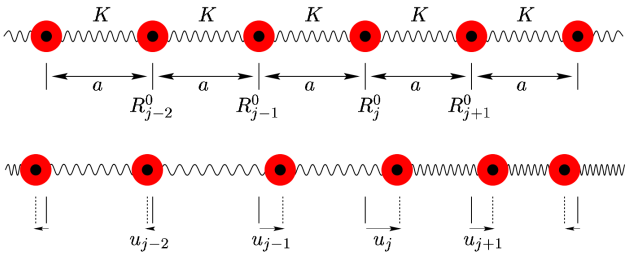


3.2 Phonons I: Free Hamiltonian and Green's Function

Consider a one-dimensional chain of N atoms, each of mass M and coupled to one another via a nearest-neighbour linear coupling of strength K, which in our picture we can think of as balls connected via springs with force constant K. The Hamiltonian describing such a system is

$$H = \sum_{j=1}^{N} \left[\frac{p_j^2}{2M} + \frac{1}{2} K (u_j - u_{j-1})^2 \right] \equiv H_0 + H_{pot} \,, \tag{3}$$

where p_j is momentum of the atom at site j and u_j is the displacement of the atom at site j away from the equilibrium position R_j^0. From this simple model we can study the quantized vibrational modes, or *phonons*.



a) Derive the form of H_{pot} using the harmonic approximation. To do this define a potential energy function $V(\mathbf{r}_i - \mathbf{r}_j)$, where $\mathbf{r}_i = \mathbf{R}_i^0 + \mathbf{u}_j$, and Taylor-expand it in powers of the difference $\mathbf{u}_i - \mathbf{u}_j$. What is the explicit form of K in 1D (which is the case we are considering here)?

b) Show that, by performing a Fourier transformation, (3) can be diagonalized in the form

$$H = \sum_k \left[\frac{1}{2M} p_k p_{-k} + \frac{1}{2} M \omega_k^2 u_k u_{-k} \right] \,, \tag{4}$$

where u_k and p_{-k} are conjugate variables. What is the explicit form of ω_k?

c) Using the linear combination

$$u_k = \sqrt{\frac{\hbar}{M\omega_k}} \frac{1}{\sqrt{2}} \left(b_{-k}^\dagger + b_k \right)$$
$$p_k = \sqrt{M\hbar\omega_k} \frac{i}{\sqrt{2}} \left(b_{-k}^\dagger - b_k \right) \,,$$

where $b_k^\dagger$ and b_k are the phonon creation and annihilation operators respectively, write (4) in the final, second quantized form

$$H = \sum_k \hbar\omega_k \left(b_k^\dagger b_k + \frac{1}{2} \right) \,. \tag{5}$$

Note that $[b_{k_1}, b_{k_2}^\dagger] = \delta_{k_1,k_2}$.

d) We now consider the linear combinations

$$A_k \equiv \left(b_k + b_{-k}^\dagger\right)$$
$$A_k^\dagger \equiv \left(b_k^\dagger + b_{-k}\right) .$$

Calculate the *phonon* propagator $D_k^0(\omega_n)$. Do this by first writing down the Green's function in imaginary time

$$D_k^0(\tau - \tau') \equiv -\left\langle T_\tau \left\{ A_k(\tau) A_k^\dagger(\tau') \right\} \right\rangle \tag{6}$$

where T_τ is the time-ordering operator in imaginary time, and $\langle \dots \rangle$ denotes the usual averaging over the imaginary time partition function, and performing a Fourier transform with respect to τ. You can set $\tau' = 0$ before the Fourier transform without loss of generality. Differentiate between the cases $\tau > 0$ and $\tau < 0$.

Hint: Use the relations

$$b_k(\tau) = e^{-\Omega_k \tau} b_k$$
$$b_k^\dagger(\tau) = e^{\Omega_k \tau} b^\dagger ,$$

where $\Omega_k = \hbar\omega_k$.

2.3 Atomic limit of the Hubbard Model

We consider the *fermionic* Hubbard model ($U > 0$, chemical potential μ),

$$H = \sum_{\substack{<ij> \\ \sigma}} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i \widehat{n}_{i\uparrow}\, \widehat{n}_{i\downarrow} , \tag{7}$$

in the limit where the hopping matrix element t_{ij} vanishes, i.e., where all sites are decoupled from each other ("atomic limit") and only the local interaction term remains. We want to calculate the (retarded) Green's function on site j, $G_{j\sigma}^R(\omega)$, for this case. Convince yourself that, for $t_{ij} = 0$, $G_{j\sigma}(\omega)$ is diagonal in position and in spin space.

a) Starting from the general definition of the Green's function

$$G_{j\sigma}^R(t, t') = -i\Theta(t)\langle\{c_{j\sigma}(t), c_{j\sigma}^\dagger(t')\}\rangle , \tag{8}$$

where $\langle \dots \rangle$ denotes the thermal average and quantum mechanical expectation value, derive the equation of motion for $G_{j\sigma}^R(t, t')$ w.r.t. t.

b) This equation of motion contains an average of the form, $\langle\{\widehat{n}_{j-\sigma} c_{j\sigma}(t),\ c_{j\sigma}^\dagger(t')\}\rangle$. Use the fact that *in the atomic limit* the on-site particle number $\hat{n}_{j-\sigma}$ is a conserved quantity (i.e., $\widehat{n}_{j-\sigma}$ may be replaced by its eigenvalue when acting on an eigenstate of H) to evaluate this avarage. Then show by Fourier transforming the equation of motion to the frequency domain that

$$G_{j\sigma}^R(\omega) = \frac{1 - \langle \widehat{n}_{j-\sigma} \rangle}{\omega + \mu + i\eta} + \frac{\langle \widehat{n}_{j-\sigma} \rangle}{\omega + \mu - U + i\eta} . \tag{9}$$

c) Interpret this result physically. Sketch the density of states of the fermionic Hubbard model in the atomic limit.