

Quantum Field Theory for Condensed Matter Physics

Exercise 6

(Submission date: 10.01.20)

6.1 Non-equilibrium Dynamics in a Double-well

(5+5+5+5+4+2+4=30 points)

We consider a Bose gas in a double-well potential $V_{\text{ext}}(\mathbf{r})$ as sketched in Figure 1. In terms of the bosonic fields $\psi(\mathbf{r}, t), \psi^*(\mathbf{r}, t)$, the action S for a trapped, atomic Bose gas with a contact interaction reads

$$S[\psi, \psi^*] = \int d^3r dt [\psi^*(\mathbf{r}, t) G_0^{-1}(\mathbf{r}, t) \psi(\mathbf{r}, t) - \frac{\tilde{g}}{2} \psi^*(\mathbf{r}, t) \psi^*(\mathbf{r}, t) \psi(\mathbf{r}, t) \psi(\mathbf{r}, t)], \quad (1)$$

where the coupling parameter $\tilde{g} = 4\pi\hbar^2 a_s/m$ is proportional to the s -wave scattering length a_s , and the inverse free Green function is $G_0^{-1}(\mathbf{r}, t) = i\partial_t - (-\hbar^2\nabla^2/2m + V_{\text{ext}}(\mathbf{r}))$. If the density of the atoms and the characteristic length of the trap are such that, on average, the atoms are very far apart compared to the scattering length, then the so-called *two-mode approximation* can be applied to resolve the spatial dependence of the field $\psi(\mathbf{r}, t)$, i.e.

$$\psi(\mathbf{r}, t) \approx \psi_s(\mathbf{r})\phi_s(t) + \psi_a(\mathbf{r})\phi_a(t), \quad (2)$$

with time-dependent amplitudes $\phi_{s,a}(t)$. The wavefunctions $\psi_{s,a}(\mathbf{r})$ are the two lowest-lying eigenfunctions of $V_{\text{ext}}(\mathbf{r})$. They extend over both wells, with eigenenergies $\varepsilon_{s,a}$ and even (odd) parity, respectively. It is useful to define the symmetric and antisymmetric superpositions $\psi_{1,2}(\mathbf{r}) = [\psi_a(\mathbf{r}) \pm \psi_s(\mathbf{r})]/\sqrt{2}$, since they are localized in the left or right well (s. Fig. 1).

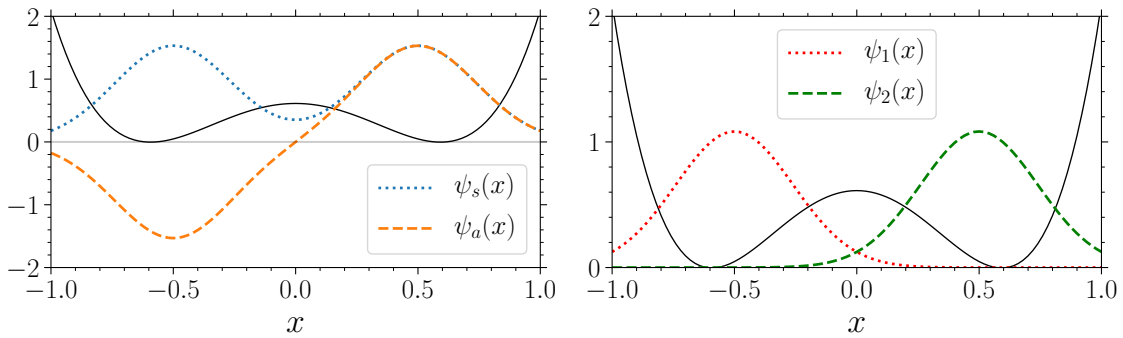


Figure 1: Sketch of the x -components of the eigenfunctions $\psi(\mathbf{r}) = \psi(x)\psi(y)\psi(z)$ of a symmetric, separable double-well potential $V_{\text{ext}}(\mathbf{r}) = V(x) + V(y) + V(z)$. The potential along the x -direction, $V(x)$, is indicated as a solid (black) line.

By using Eq. (2) and the fact that the overlap between $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$ is small, the action (1) can be brought to the form

$$S = \int dt \left\{ \sum_{i=1}^2 [\phi_i^* (i\partial_t - \varepsilon_i) \phi_i - \frac{U}{2} |\phi_i^*(t)|^4] - J(\phi_1^* \phi_2 + \phi_2^* \phi_1) \right\}, \quad (3)$$

where $\varepsilon_1 = \varepsilon_2 = (\varepsilon_a + \varepsilon_s)/2$, the tunneling is $2J = \varepsilon_s - \varepsilon_a$, and $U = \tilde{g} \int d^3r |\psi_i^*(\mathbf{r})|^4$, $i = 1, 2$. Note that $J < 0$, since the symmetric state is the ground state of the system. At very low temperatures, the atoms in the trap will form a *Bose-Einstein condensate* (BEC). In the two-mode approximation, this BEC can be described by two complex order parameters. In this exercise, we will investigate the non-equilibrium dynamics of the trapped condensate for different initial conditions.

- a) Derive the time-dependent Gross-Pitaevskii equations for the condensate amplitudes $\Phi_1(t)$ and $\Phi_2(t)$ from Eq. (3). Without loss of generality, you may assume $\varepsilon_1 = \varepsilon_2 = 0$.
- b) Use the polar representation $\Phi_i(t) = \sqrt{N_i(t)} e^{i\varphi_i(t)}$ for the condensate amplitudes in your result from a). Derive four equations for the time-dependent condensate occupations $N_{1,2}(t)$ and phases $\varphi_{1,2}(t)$ by separating real and imaginary parts.
- c) Introduce the following new variables into your equations: the total condensate occupation $N = N_1 + N_2$, the so-called *population imbalance* $z = (N_1 - N_2)/(N_1 + N_2)$, the *relative phase* $\varphi = \varphi_2 - \varphi_1$, and the *total phase* $\Theta = \varphi_1 + \varphi_2$. Give a physical interpretation of the equation for N and discuss the influence of Θ on the dynamics.
- d) Verify that the dynamical problem defined by the differential equations for z and φ can be derived from a classical Hamiltonian $H(z, \varphi) = \frac{NU}{2}z^2 + 2J\sqrt{1-z^2} \cos \varphi$, where z plays the role of the “momentum” canonically conjugate to the “coordinate” φ . Compare this Hamiltonian to that of the *mathematical pendulum*. Which qualitatively different solutions are possible? Sketch the trajectories each of these solutions in the (z, φ) plane. What is the classical-mechanics analogy for the double-well condensate, which comes to mind?
- e) The type of trajectories with unbound φ are called *quantum self-trapped*, because the amplitude z does not oscillate around zero, i.e., the particles are trapped in one side of the double-well potential. They occur when the initial amplitude becomes larger than a critical value z_{crit} . Find z_{crit} by calculating the total energy in the point $(0, \pi)$ and using the analogy to the mathematical pendulum.
- f) Solve the equations in the non-interacting limit, $U = 0$. What is the frequency of the resulting *Rabi oscillations*?
- g) Linearize the equations of motion by assuming $|z| \ll 1$, $|\varphi| \ll 1$. Find the oscillation frequency in terms of J and U . This is the so-called *Bose-Josephson frequency*.
- h) **Optional (10 points):* Solve the system numerically for parameters satisfying $NU/2|J| = 5$ and initial conditions $|z| > |z_{\text{crit}}|$, $\varphi = 0$. What do you observe?

6.2 Transport through a quantum dot

(3+3+2+3+4+3+3=21 points)

We consider the electronic transport through a quantum dot with a finite bias voltage V applied. Two wires are attached to the quantum dot, where each wire is in thermal equilibrium with itself at temperature T . Due to the applied voltage, there is a chemical potential difference $\mu_L - \mu_R = V$ between the left (L) and the right (R) lead. We model the system by a free electron gas in the wires with dispersion $\varepsilon_{k,R/L}$ and the quantum dot by a single fermionic state with energy ε_d . The wires are coupled to the dot by a hopping term. The Hamiltonian reads

$$H = \sum_k (\varepsilon_k - \mu_L) c_{k,L}^\dagger c_{k,L} + \sum_k (\varepsilon_k - \mu_R) c_{k,R}^\dagger c_{k,R} + \varepsilon_d d^\dagger d + J \sum_{k,\alpha=R,L} (c_{k,\alpha}^\dagger d + d^\dagger c_{k,\alpha}).$$

- a) We want to compute the current on the left wire, which is the change of the particle density there. Use the Heisenberg equation of motion to show that

$$I_L(t) = - \left\langle \frac{dN_L(t)}{dt} \right\rangle = i \sum_k J \left[\langle c_k^\dagger(t) d(t) \rangle - \langle d^\dagger(t) c_k(t) \rangle \right].$$

- b) We will need some properties of the Green function in the following. First, show that

$$G_{c,d}^<(k; t, t') = i \langle c_k^\dagger(t') d(t) \rangle = -[G_{d,c}^<(k; t', t)]^\dagger.$$

Second, show that for the free electrons in equilibrium, the lesser Green function is given by

$$G_{c,c}^<(k; t, t') = i \langle c_k^\dagger(t') c_k(t) \rangle = i e^{i\varepsilon_k(t-t')} f(\varepsilon_k). \quad (4)$$

Hint: For free electrons, the time dependence of the creation/annihilation operators can be calculated by Heisenberg's equation of motion.

In momentum space, show that $G_{c,c}^<(k; \omega) = 2\pi i f(\omega) \delta(\omega - \varepsilon_k)$.

- c) With the first part of question b), show that we can write

$$I_L(t) = 2J \operatorname{Re} \sum_k G_{c,d}^<(k; t, t).$$

- d) The Green function $G_{c,d}^<$ vanishes without lead-dot coupling J . To incorporate the hopping, we use perturbation theory to first order in J for the countour time ordered Green function. Use Wick's theorem to show that it is given by

$$G_{c,d}(t, t') = J \int_C d\tau G_{d,d}(t, \tau) G_{c,c}(k; \tau, t'). \quad (5)$$

The result is exact when using the full $G_{d,d}$ and the free $G_{c,c}$ Green function. Why?

- e) We now calculate $G_{c,d}^<$. Specify for this the position of (t, t') on the contour and split up the contour integration in forward and backward branches. Replace the contour time ordered Green function on these branches by the appropriate Green functions. Hint: Helpful relations for time ordered $G^T = G^< + G^R$ and anti-time ordered $G^{\bar{T}} = G^< - G^A$ Green functions. The result is

$$G_{c,d}(k; t, t') = J \int d\tau [G_{d,d}^R(t, \tau) G_{c,c}^<(k; \tau, t') + G_{d,d}^<(t, \tau) G_{c,c}^A(k; \tau, t')].$$

We are now interested in a steady state solution. In this case, the Green functions only depend on time differences and therefore just one frequency. We can write in frequency space:

$$I_L = \int \frac{d\omega}{\pi} \text{Re} \sum_k J^2 [G_{d,d}^R(\omega) G_{c,c}^<(k; \omega) + G_{d,d}^<(\omega) G_{c,c}^A(k; \omega)]$$

We can now plug in the the Green function of the wire electrons and use the equilibrium Green function of a free Fermi gas with chemical potential $\mu_{L,R}$.

f) In the steady state we know the currents must satisfy $I_L = -I_R$. Therefore we can write the total current as $I = (I_L - I_R)/2$. Show that the current is given by

$$I = i \frac{J^2}{4\pi} \sum_k \int d\omega [(f_L(\omega)\delta(\omega - \varepsilon_{k,L}) - f_R(\omega)\delta(\omega - \varepsilon_{k,R}))(G_{d,d}^R(\omega) - G_{d,d}^A(\omega)) + (\delta(\omega - \varepsilon_{k,L}) - \delta(\omega - \varepsilon_{k,R}))G_{d,d}^<(\omega)] .$$

The primary difficulty lies now in determining the Green functions of the quantum wire. The self energy can be obtained by considering the possible hopping processes, assuming again the leads being in equilibrium. The result is the Landauer formula

$$I = J^2 \int d\omega [f_L(\omega) - f_R(\omega)] \frac{\rho_L(\omega)\rho_R(\omega)}{\rho_L(\omega) + \rho_R(\omega)} A_{d,d}(\omega). \quad (6)$$

Here $\rho_{L/R}$ is the density of states in the leads and $A_{d,d}(\omega)$ is the interacting spectral function of the quantum dot. The spectral function is defined as the the difference between retarded and advanced Green function.

g) Calculate the current at small voltage, so small difference in the chemical potentials and low temperatures. The spectral function of the quantum dot will be renormalised to

$$A_{d,d}(\omega) = \frac{\Gamma/\pi}{(\omega - \varepsilon_d)^2 + \Gamma^2}.$$