Physics 452:
Assignment 3: Many-body Physics and Low Energy Scattering

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Background and Research Context

The study of ultracold atoms and molecules has revolutionized our understanding of many-body quantum mechanics. By cooling particles to nanokelvin temperatures, researchers can tune interactions using Feshbach resonances and control external potentials with optical lattices.

To navigate this field, you will frequently see we three primary description that connect microscopic scattering and macroscopic collective phenomena.

1. The Energy Functional (Spatial Representation)

Here the system is described by field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$, which annihilate and create a particle at position $\mathbf{r}$. The total energy is given by the Hamiltonian:

$$\hat{H} = \int d^3r \left[\hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right) \hat{\psi}(\mathbf{r})\right] + \frac{1}{2}\int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \quad (1)$$

For a contact interaction $V(\mathbf{r}-\mathbf{r}') = g\delta(\mathbf{r}-\mathbf{r}')$, the interaction simplifies to a local density-density term: $\frac{g}{2}\int d^3r \hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\hat{\psi}$.

2. Momentum Representation

Expanding the field operators in terms of plane waves, $\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\hat{a}_{\mathbf{k}}$, provides the Hamiltonian in momentum space k with kinetic energy ϵ_k, and $\mathcal{V}$ is the volume of the system. This is essential for uniform Bose-Einstein condensation and its excitations:

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_k \hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \frac{1}{2\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \tilde{V}(\mathbf{q})\hat{a}^\dagger_{\mathbf{k}+\mathbf{q}}\hat{a}^\dagger_{\mathbf{k}'-\mathbf{q}}\hat{a}_{\mathbf{k}'}\hat{a}_{\mathbf{k}} \quad (2)$$

3. The Gross-Pitaevskii Equation (Mean-Field)

At temperatures significantly below T_c, we replace the field operator with a classical order parameter $\Psi(\mathbf{r},t)$. Minimizing the energy functional yields the Gross-Pitaevskii Equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t) \quad (3)$$

Question 1: Molecular Potential and Momentum Space Interactions

- **1.1 Fourier Transformation:** Starting from the energy functional, use the expansion $\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\hat{a}_{\mathbf{k}}$ to transform $\hat{H}_{int}$ into momentum space. Show that the interaction takes the form:
$$\hat{H}_{int} = \frac{1}{2\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \tilde{V}(\mathbf{q})\hat{a}^{\dagger}_{\mathbf{k}+\mathbf{q}}\hat{a}^{\dagger}_{\mathbf{k}'-\mathbf{q}}\hat{a}_{\mathbf{k}'}\hat{a}_{\mathbf{k}} \tag{4}$$
where $\tilde{V}(\mathbf{q}) = \int V(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}d^3r$ is the Fourier transform of the potential. Comment on the origin of momentum conservation in the above expression.

- **1.2 Energy of bosons near ground state:** At near zero temperature almost all atoms are in the ground state with ground state population $n_0 \gg n_k \gg 1$, where $n_k = \langle a_k^{+} a_k\rangle$ is the population in an exctied mode with momentum k and $N = \sum_k n_k$ is the total particle number. Write the interaction Hamiltonian in the order of n_0. (Hint: You may assume coherent field $\hat{a}_{\mathbf{k}} \equiv \sqrt{n_k}$ to write the interaction in the decreasing order of n_0 and assume $g_k \equiv \tilde{V}(\mathbf{k})/2\mathcal{V}$.)

- **1.3 Physics picture** Describe the physical processes associated with the leading and next order in n_k and comment on the relative importance of them to the energy of the system.

Question 2: Bogoliubov Excitations and Matrix Diagonalization

Start with the momentum space Hamiltonian described in Question 1, we will derive the Bogoliubov excitation spectrum with the prescription $\hat{a}_0 \to \sqrt{n_0} \gg n_k$.

- **4.1 Hilbert Space Coupling:** Keeping the leading order in n_k in the Hamiltonian, identify the momentum modes $\mathbf{k}$ and $-\mathbf{k}$ that couple due to the interaction term. (Hint: $g_{\mathbf{k}}\hat{a}^{\dagger}_{\mathbf{k}}\hat{a}^{\dagger}_{-\mathbf{k}}\hat{a}_0\hat{a}_0 + H.c.$.)

- **4.2 Matrix Representation:** Show that the quadratic part of the Hamiltonian can be written in the basis $(\hat{a}_{\mathbf{k}}, \hat{a}^{\dagger}_{-\mathbf{k}})^T$ as
$$\hat{H}_{\mathbf{k}} = \frac{1}{2}\sum_{\mathbf{k}\neq 0}\begin{pmatrix}\hat{a}^{\dagger}_{\mathbf{k}} & \hat{a}_{-\mathbf{k}}\end{pmatrix}\begin{pmatrix}\epsilon_k + g_k n_0 & g_k n_0 \\ g_k n_0 & \epsilon_k + g_k n_0\end{pmatrix}\begin{pmatrix}\hat{a}_{\mathbf{k}} \\ \hat{a}^{\dagger}_{-\mathbf{k}}\end{pmatrix} \tag{5}$$

- **4.3 Bogoliubov Dispersion:** Rewrite the Hamiltonian by diagonalizing this matrix (ensuring the Bogoliubov transformation $[u, v]$ preserves commutation relations) to find the excitation spectrum $E_k = \sqrt{\epsilon_k(\epsilon_k + 2g_k n_0)}$. Show that for non-interacting gas, $E_k = \epsilon_k = \hbar^2k^2/2m$ shows particle-like excitations. For interacting gas $g_k > 0$, the long wavelength excitations are wave-like phonons ($E_k \approx \hbar ck$) and determine the sound speed c.

Question 3: Dipolar Condensates and Long-Range Interactions

Many atoms or molecules possess a permanent magnetic or electric dipole moment d. When aligned along the z-axis by an external field, we may write tthe interaction potential between two dipoles separated by $\mathbf{r}$ as:
$$V_{dd}(\mathbf{r}) = \frac{d^2}{r^3}(1 - 3\cos^2\theta) \tag{6}$$
where θ is the angle between the relative position vector $\mathbf{r}$ and the z-axis (the polarization axis).

- **3.1 Momentum Space Form:** The effective coupling in momentum space is the Fourier transform of the potential, $g_{dd}(\mathbf{k}) = \tilde{V}_{dd}(\mathbf{k})$. Using the identity for the Fourier transform of a dipole-dipole interaction, show that the momentum-dependent coupling constant takes the form:
$$g_{dd}(\mathbf{k}) = g_{dd}\left(3\cos^2\theta_k - 1\right) \tag{7}$$
where $g_{dd} \propto \frac{4\pi d^2}{3}$ and θ_k is the angle between the momentum vector $\mathbf{k}$ and the polarization axis (z). Derive this result or justify it using the properties of spherical harmonics.

- **3.2 Anisotropy:** Unlike the contact interaction $g_k \equiv g$, which is a constant scalar, $g_{dd}(\mathbf{k})$ is *anisotropic*. In cold collisions of atoms and molecules both scalar and dipolar potential contribute to the coupling constant $g_k = g + g_{dd}(k)$, discuss how the dipolar interactions influence the ground state stability. Specifically:
  - For which directions of $\mathbf{k}$ is the interaction maximally attractive, and for which is it maximally repulsive? At the "magic angle" the interaction V_{dd} vanishes?
  - Use the Bogoliubov spectrum result E_k in Question 2, argue that system becomes unstable when the phonon energy is negative $E_k < 0$. When will this happen in a dipolar gas?

Question 4: The Infinite Wall and Healing Length

Consider a BEC confined in the half-space $x > 0$ by an infinite potential wall at $x = 0$. In the mean-field limit, the wavefunction $\psi(x)$ obeys the time-independent Gross-Pitaevskii equation.

- **4.1 Boundary Conditions:** Show that the boundary conditions for $\psi(x) \to 0$ as $x \to 0$ and $x \to \infty$ for a condensate with bulk density n_0. Solve the 1D GPE with the boundary condition:
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + g|\psi(x)|^2\right]\psi(x) = \mu\psi(x) \tag{8}$$

- **4.2 The Healing Length:** Show that the density $n(x) = |\psi(x)|^2$ reaches its bulk value n_0 over a characteristic length $\xi = \sqrt{\frac{\hbar^2}{2mgn_0}}$. Sketch the resulting density profile.

- **4.3 Kinetic vs interaction energy:** Show that near for $x \ll \xi$ the kinetic energy term dominates the chemical potential, while interaction dominate when $x \gg \xi$. Show that their ratio is exactly $\langle E_k\rangle : \langle gn\rangle = n_0 : n(x)$.

Question 5: Do bosons condense to a single quantum state?

Consider a system of N bosons with a novel kinetic energy $E_k = (k^2 - 1)^2$, which possesses two degenerate minima at $k = \pm 1$. Would bosons condense to one or a superposition state of them?

- **5.1 Absolute Ground State:** If atoms are allowed to freely choose any momentum distribution, what is the absolute ground state configuration for the N bosons? Describe if symmetry breaking is involved.

- **5.2 Zero Momentum Constraint:** Now, impose the constraint that the total momentum of the system must be zero ($\sum \mathbf{k}_i = 0$). Determine the ground state configuration under this constraint. Compare the energy of a fragmented state (half the particles at $k = +1$, half at $k = -1$) versus a coherent superposition state.

Problem 6: Feshbach Resonance

Feshbach resonances in collisions of cold atoms occur when two atoms in an open channel collide and couple to a molecular state in a closed channel. Here a channel refers to the internal state of the atoms or molecules. When the total energy of the system is above (below) the dissociation energy of the channel, the channel is considered open (closed).

Consider the system can be prepared in the open channel ψ_o and closed channel ψ_c. The wavefunction is given by $\Psi(r) = \begin{pmatrix} \psi_c(r) \\ \psi_o(r) \end{pmatrix}$, and the Hamiltonian is $H = \frac{p^2}{2\mu}\hat{1} + \mathbf{V}(r)$. Here $\hat{1}$ is the identity matrix and $\mathbf{V}(r)$ is the spin-dependent molecular potential. We assume the closed channel is inaccessible outside the interaction range $r > r_0$ and the short-range potential is attractive:

$$\begin{aligned} \mathbf{V}(r > r_0) &= \begin{pmatrix} \infty & 0 \\ 0 & 0 \end{pmatrix} \\ \mathbf{V}(r < r_0) &= \begin{pmatrix} -V_c & \epsilon \\ \epsilon & -V_o \end{pmatrix} \end{aligned} \tag{9}$$

where ϵ couples the open and closed channels.

- **6.1** We initially prepare free atoms in the open channel with low energy $E = \frac{\hbar^2 k^2}{2\mu} \ll V_c, V_o$. After scattering, the s-wave wavefunction is phase shifted as $r\Psi(r > r_0) = \begin{pmatrix} 0 \\ \sin(kr + \delta) \end{pmatrix}$. Show that:

$$k \cot(kr_0 + \delta) = q_+ \cos^2\alpha \cot(q_+ r_0) + q_- \sin^2\alpha \cot(q_- r_0) \tag{10}$$

  where $\tan 2\alpha = \frac{2\epsilon}{V_c - V_o}$ and $\frac{\hbar^2 q_\pm^2}{2\mu}$ are the eigen-energies at short range. In the limit of zero coupling, the eigen-energies approach V_o and V_c, respectively.

  Hint: Use the continuity of the wavefunction $\Psi(r_0^+) = \Psi(r_0^-)$ and $\Psi'(r_0^+) = \Psi'(r_0^-)$.

  Remark: In cold atoms, weak coupling $\epsilon \ll |V_c - V_o|$ is a very good approximation since spin-spin interactions (typically GHz) are very weak compared to exchange interactions (typically 100 THz).

- **6.2** We may assume that the closed channel supports a bound state at energy $E = E_c$ close to the open channel threshold $E = 0$. Show that the second term contributes to the phase shift resonantly as:

$$k \cot(kr_0 + \delta) \approx k \cot(kr_0 + \delta_{bg}) - \frac{\mu\Gamma/\hbar^2}{E - E_c} \tag{11}$$

  where we have defined the Feshbach coupling strength as $\Gamma \approx 4\alpha^2 V_c$.

  Hint: The existence of the bound state in the square potential suggests $\sin\left(\sqrt{\frac{2\mu}{\hbar^2}(V_c + E_c)}r_0\right) = 0$. *Since the bound state is near the continuum, we can assume $|E_c| \ll V_c$ and rewrite the term $\cot(q_- r_0)$ in terms of $1/(E - E_c)$.*

- **6.3** Show that the scattering length a is linked to boundary conditions in the low energy limit, and we can rewrite:

$$a = a_{bg}\left(1 - \frac{\Delta}{E_c + E^*}\right) \tag{12}$$

  where a_{bg} is the background scattering length far from the resonance, $\Delta = \alpha\Gamma/2$ is the energy width of the resonance, $\alpha = (a_{bg} - r_0)^2/a_{bg}r_0$, and $E^* = (a_{bg}/r_0 - 1)\Gamma/2$ is the self-energy shift of the bound state.

- **6.4** Across the Feshbach resonance what is the scattering amplitude f, matrix S, phase shift δ and reaction matrix K in the open channel?

Problem 7: Bose-Einstein Distribution and Condensation

Consider $N = \sum_{i=0} N_i \gg 1$ ideal bosons with mass m confined within a volume V, where n_i is the population in the i-th eigenstate. Given a grand canonical ensemble with chemical potential μ and temperature T, the probability to find $\alpha = 0, 1, 2, \ldots$ bosons in the state is $p_\alpha \propto e^{-\beta(\alpha E_i - \alpha\mu)}$ where $\beta = \frac{1}{k_B T}$.

- **7.1 Mean Population:** Show that the mean population $\overline{N}_i = \langle \alpha p_\alpha \rangle$ in the state is exactly given by the Bose-Einstein distribution:

$$\overline{N}_i = \frac{1}{e^{\beta(E_i - \mu)} - 1} \tag{13}$$

- **7.2 Transition Condition:** BEC occurs when a sizable fraction of particles occupies the ground state $N_0 = \mathcal{O}(N)$. Show that the BEC transition occurs when μ increases toward the ground state energy E_0.

- **7.3 3D Equation of State:** Consider a 3D box where $E_0 \equiv 0$ and the density of states is $\rho(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$. Show that the equation of state is:

$$n\lambda_{dB}^3 = n_0\lambda_{dB}^3 + g_{3/2}(e^{\beta\mu}) \tag{14}$$

  where $\lambda_{dB} = h(2\pi m k_B T)^{-1/2}$ is the thermal de Broglie wavelength and $g_n(z)$ is the Bose function.

- **7.4 Dimensionality and Traps:** Show that for ideal bosons in a 2D box, BEC occurs only at $T = 0$. Then, determine the critical temperature T_c for N bosons in a 3D isotropic harmonic potential $V(r) = \frac{1}{2}m\omega^2 r^2$.

Problem 8: Coherent Coupling of Quantum Fields

We examine a many-body system coherently oscillating between two quantum fields a and b. The Hamiltonian is given by:

$$\hat{H} = \frac{\Delta}{2}(b^\dagger b - a^\dagger a) - g a^\dagger b - g a b^\dagger \tag{15}$$

where Δ is the energy splitting and $g > 0$ is the coupling constant. The state of the system can be written in Fock state basis as $|\psi\rangle = |n_a, n_b\rangle$, where $n_a, n_b = 0, 1, 2...$ are the particle numbers in the two modes a and b, respectively.

- **8.1 Two-Level Analogy:** Show that for a system containing exactly 1 particle, the dynamics reduces to a two-level system with detuning Δ and Rabi frequency $2g$.

- **8.2 N particle ground state:** What is the ground state for $N = N_a + N_b > 1$ particles and $\Delta = 0$?

- **8.3 Equation of motion:** Away from the grounds state, determine the equation of motion for the number operators $\hat{n_a}$ and $\hat{n_b}$. (Hint: you may use the Heisenberg equation to simplify the calculation.)

- **8.4 Coherent State Dynamics:** For $N \gg 1$ we may approximate the fields as coherent states $\Psi = |C_a\rangle \otimes |C_b\rangle$, where C_a and C_b are complex amplitudes. Show that the equation of motion is

$$i\hbar\partial_t \begin{pmatrix} C_a \\ C_b \end{pmatrix} \approx \frac{1}{2}\begin{pmatrix} \Delta & g \\ g & -\Delta \end{pmatrix}\begin{pmatrix} C_a \\ C_b \end{pmatrix}. \tag{16}$$

  Comment on the "Rabi" oscillations before the two modes and how it is compared to 8.1?

- **8.5 Classical Oscillator Mapping:** Define the fractional population difference $n = (N_b - N_a)/N$ and phase difference $\phi = \phi_b - \phi_a$. Show they follow Hamiltonian equations $\dot{\phi} = \partial_n H_{cl}$ and $\dot{n} = -\partial_\phi H_{cl}$ with:

$$H_{cl} = \Delta n - \sqrt{1 - n^2} \cos \phi. \tag{17}$$

  Is this result consistent with the solution of 8.3 where we do not assume coherent state approximation.