DESY Theory Group, Hamburg

Tutorials for the Lecture

Quantum Mechanics II

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Tutorial 4

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Home Exercise 11 Matrix element for shielded two-electron Coulomb interaction

In the lecture, we discussed solid-state electrons with one-particle wave functions in the spin-orbit representation

$$\left\langle \vec{r}, \sigma_0 \middle| \vec{k}, \sigma \right\rangle = \delta_{\sigma,\sigma_0} \frac{1}{\sqrt{\mathtt{Vol}}}\, e^{i\vec{k}\cdot\vec{r}} \qquad , \tag{1}$$

where Vol is the volume of a certain fundamental domain in the inverse lattice of wave vectors $\vec{k}$ which are discretized (so called first Brillouin zone).

Take the spin-orbit representation to calculate the matrix element of the shielded pairwise Coulomb interaction between solid-state electrons given by the two-particle operator

$$\Delta\hat{w}_{12} = \frac{e^2}{\left|\hat{\vec{r}}_1 - \hat{\vec{r}}_2\right|} e^{-\alpha\left|\hat{\vec{r}}_1 - \hat{\vec{r}}_2\right|}, \qquad 0 < \alpha \in \mathbb{R}\ . \tag{2}$$

Here, e is the electrical charge. Show that the final result is the one given in the lecture:

$$\begin{aligned} &{}^{(2)}\left\langle \vec{k}_4, \sigma_4 \right| {}^{(1)}\left\langle \vec{k}_3, \sigma_3 \right| \Delta\hat{w}_{12} \left| \vec{k}_2, \sigma_2 \right\rangle^{(1)} \left| \vec{k}_1, \sigma_1 \right\rangle^{(2)} \\ &\qquad = \frac{4\pi e^2}{\mathtt{Vol}} \frac{1}{\alpha^2 + \left|\vec{k}_2 - \vec{k}_3\right|^2} \delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}\delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4} \qquad . \end{aligned} \tag{3}$$

Hint: It turns out to be a good move to introduce distance and center-of-mass position vectors, $\vec{R} := \frac{1}{2}(\vec{r} + \vec{r}')$ and $\vec{\rho} = \vec{r} - \vec{r}'$, where $\vec{r}$ amd $\vec{r}'$ are the two integration variables of the position unity operators to be inserted.

Does the result have a limit $\alpha \to 0$? Interpret the result of the matrix element.

Home Exercise 12 Weakly interacting Bose gas and its dispersion relation

We discuss Helium-4 atoms as a weakly coupled Bose gas (i.e. an ensemble of bosonic degrees of freedom whose density is so low that their interactions are described as a small perturbation to the free case). In the lecture it is shown that the kinetic term and interaction of bosonic one-particle excitations in the momentum (Fourier) space is given by (we work here with finite volumes where the momentum integral becomes a discretized sum)

$$\hat{H} = \sum_{\vec{k}} \epsilon_{\vec{k}} \hat{n}_{\vec{k}} + \hat{W} \qquad , \; \epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2M^*} \qquad , \tag{4}$$

$$\hat{W} = \frac{1}{2} \int_{\texttt{Vol}} d^3V \int_{\texttt{Vol}} d^3V' \, \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|) \hat{\psi}(\vec{r}\,') \hat{\psi}(\vec{r}) \tag{5}$$

Here, M^* is the effective mass of Helium-4 atoms, and, as usual, the Helium-4 number operator is given by $\hat{n}_{\vec{k}} = \hat{b}^\dagger_{\vec{k}} \hat{b}_{\vec{k}}$. Even a weak attractive interaction among bosons leads to Bose-Einstein condensation, the occupation of the lowest state ($\vec{k} = 0$) by a macroscopic number of bosons. Hence, the field operator of the one-particle boson excitations can be decomposed into a quasi-classical condensate part ψ_0 (which also exhibits a specific complex phase) and a part with momentum modes $\vec{k} \neq \vec{0}$, $\Delta\hat{\psi}(\vec{r})$. The latter, however, is small at low temperatures, such that higher than quadratic terms of $\Delta\hat{\psi}$ can be neglected. The explicit form is then:

$$\hat{\psi}(\vec{r}) = \psi_0 + \Delta\hat{\psi}(\vec{r}), \qquad \psi_0 = \sqrt{\frac{n_0}{\texttt{Vol}}}\, e^{i\varphi}, \qquad \Delta\hat{\psi}(\vec{r}) = \sum_{\vec{k} \neq \vec{0}} \frac{1}{\sqrt{\texttt{Vol}}}\, e^{i\vec{k}\cdot\vec{r}}\, \hat{b}_{\vec{k}} \qquad . \tag{6}$$

n_0 is the number of Helium-4 atoms in the condensate, φ is the complex phase of the condensate. `Vol` is again a finite volume, here motivated by the finite size of the Helium-4 vessel, and $\hat{b}_{\vec{k}}$ is the annihilation operator of an Helium-4 atom with momentum $\vec{k}$.

(a) Show that the interaction operator can be written as

$$\hat{W} = n_0\, \tilde{v}(0) \left(N - \frac{1}{2} n_0 \right) + \sum_{\vec{k} \neq \vec{0}} n_0\, \tilde{v}(|\vec{k}|) \cdot \left[\hat{n}_{\vec{k}} + \frac{1}{2} e^{2i\varphi} \hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{-\vec{k}} + \frac{1}{2} e^{-2i\varphi} \hat{b}_{\vec{k}} \hat{b}_{-\vec{k}} \right] + \mathcal{O}(\Delta\hat{\psi}^3) \qquad . \tag{7}$$

where $v(0) \equiv v(|\vec{k}| = 0)$. We use the following convention for the Fourier transform from position to momentum space:

$$\tilde{v}(\vec{q}) = \int_{\texttt{Vol}} \frac{d^3V}{\texttt{Vol}}\, e^{i\vec{q}\cdot\vec{r}} v(\vec{r}) \qquad . \tag{8}$$

What is the physics interpretation of $N - n_0$?

(b) We have shown that the Hamiltonian is of the form

$$\hat{H} = \sum_{\vec{k}} \left[X_{\vec{k}} \hat{n}_{\vec{k}} + Y_{\vec{k}} \hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{-\vec{k}} + Y^*_{\vec{k}} \hat{b}_{-\vec{k}} \hat{b}_{\vec{k}} \right] + C \qquad . \tag{9}$$

What are the coefficients $X_{\vec{k}}$, $Y_{\vec{k}}$ and C? Which relations do $X_{-\vec{k}}$ and $Y_{-\vec{k}}$ fulfill? In sheet 3 we saw that the presence of the anomalous terms containing two creation or annihilation operators breaks phase invariance and particle number conservation.

A proper solution describing also the backreaction of the free Helium-4 atoms onto the Bose-Einstein condensate would be using the mean field formalismus for Eq. (9). We are just determining its spectrum here. For doing so, first show that it can be written as

$$\hat{H} = \hat{H}_{\vec{k}=\vec{0}} + \sum_{\text{positive } \vec{k}\text{-half space}, \vec{k}\neq\vec{0}} \left(\hat{H}_{1,\vec{k}} + \hat{H}_{2,\vec{k}} \right) \tag{10}$$

with

$$\hat{H}_{1,\vec{k}} = X_{\vec{k}} \cdot \left(\hat{n}_{\vec{k}} + \hat{n}_{-\vec{k}} \right) \qquad \hat{H}_{2,\vec{k}} = 2 \left(Y_{\vec{k}} \hat{b}^\dagger_{\vec{k}} \hat{b}^\dagger_{-\vec{k}} + Y^*_{\vec{k}} \hat{b}_{-\vec{k}} \hat{b}_{\vec{k}} \right) \qquad . \tag{11}$$

(c) To derive the spektrum of this Hamiltonian, we restrict ourselves to a single direction $\vec{k} \neq \vec{0}$. In order to diagonalize the Hamiltonian, we take the following linear transformation of creation and annihilation operators:

$$\hat{b}_{\vec{k}} = \alpha_{\vec{k}} \hat{a}_{\vec{k}} + \gamma_{\vec{k}} \hat{a}^\dagger_{-\vec{k}} \qquad \hat{b}^\dagger_{\vec{k}} = \alpha^*_{\vec{k}} \hat{a}^\dagger_{\vec{k}} + \gamma^*_{\vec{k}} \hat{a}_{-\vec{k}} \qquad . \tag{12}$$

Calculate the inverse transformation and derive consistency equations for the coefficients $\alpha_{\vec{k}}$ and $\gamma_{\vec{k}}$ by demanding that the new operators $\hat{a}_{\vec{k}}$ and $\hat{a}^\dagger_{\vec{k}}$ fulfill the commutation relations for bosonic creation and annihilation operators. (Why is this called a canonical transformation?)

Show that the following is a solution of these consistency conditions:

$$\alpha_{\vec{k}} = e^{i\psi_\alpha} |\alpha_{\vec{k}}|, \qquad \gamma_{\vec{k}} = e^{i\psi_\gamma} |\gamma_{\vec{k}}|, \qquad |\alpha_{\vec{k}}| = \frac{1}{\sqrt{1-\lambda^2_{\vec{k}}}}, \qquad |\gamma_{\vec{k}}| = \frac{\lambda_{\vec{k}}}{\sqrt{1-\lambda^2_{\vec{k}}}} \quad , \tag{13}$$

with $0 \leq \lambda_{\vec{k}} \leq 1, \lambda_{\vec{k}} \in \mathbb{R}$.

(d) Now plug in the linear transformation from (c) and diagonalize the Hamiltonian. Derive the dispersion relation (dependence of the one-particle energies on the wave vector). You should arrive at an expression

$$\hat{H}_{\vec{k}} = \tilde{\epsilon}_{\vec{k}} \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} + \text{“}\vec{k} \leftrightarrow -\vec{k}\text{''} + C_{\vec{k}} + C_{-\vec{k}} \quad , \tag{14}$$

where

$$\tilde{\epsilon}_{\vec{k}} = X_{\vec{k}} \left[|\alpha_{\vec{k}}|^2 + |\gamma_{-\vec{k}}|^2 \right] + 2 \left[Y_{\vec{k}} \alpha^*_{\vec{k}} \gamma^*_{-\vec{k}} + \text{c.c.} \right] \qquad , \tag{15}$$

$$0 = X_{\vec{k}} \left(\alpha^*_{\vec{k}} \gamma_{\vec{k}} + \alpha^*_{-\vec{k}} \gamma_{-\vec{k}} \right) + 2 \left(Y_{\vec{k}} \alpha^*_{\vec{k}} \alpha^*_{-\vec{k}} + Y^*_{\vec{k}} \gamma_{-\vec{k}} \gamma_{\vec{k}} \right) \tag{16}$$

Furthermore, for the Bose-Einstein condensate in suprafluid Helium-4 it is justified to assume symmetry under parity (space inversion), $\alpha_{\vec{k}} = \alpha_{-\vec{k}}$, $\gamma_{\vec{k}} = \gamma_{-\vec{k}}$, $\lambda_{\vec{k}} = \lambda_{-\vec{k}}$.

Show that using the definitions $\tilde{Y}_{\vec{k}} = Y_{\vec{k}} e^{-i(\psi_\alpha + \psi_\gamma)}$ and $r_{\vec{k}} = X_{\vec{k}}/(-2\tilde{Y}_{\vec{k}})$, the solution for the one-particle energies is given by

$$\tilde{\epsilon}_{\vec{k}} = \sqrt{\frac{\hbar^4 |\vec{k}|^4}{4(M^*)^2} + \frac{\hbar^2 |\vec{k}|^2}{M^*} n_0 \tilde{v}(|\vec{k}|)} \qquad , \tag{17}$$

and the full diagonalized Hamiltonian has the form

$$\hat{H} = E_0 + \sum_{\vec{k}} \tilde{\epsilon}_{\vec{k}} \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} \qquad E_0 = C + \sum_{\vec{k}} C_{\vec{k}} \qquad . \tag{18}$$

Voluntarily, show that the coefficients C and $C_{\vec{k}}$ are given by

$$C = n_0 \left(N - \tfrac{1}{2} n_0 \right) \qquad\qquad C_{\vec{k}} = \tilde{\epsilon}_{\vec{k}} - X_{\vec{k}} \tag{19}$$

(e) Empirically, for the two cases of vanishing and ultralarge wave vectors, $|\vec{k}| \to 0$ and $|\vec{k}| \to \infty$, the potential of ultracold Helium-4 atoms approaches a constant and falls off quadratically, respectively,

$$\tilde{v}(|\vec{k}|) \overset{|\vec{k}|\to 0}{\longrightarrow} \tilde{v}(0) \equiv \text{const.} \qquad \tilde{v}(|\vec{k}|) \overset{|\vec{k}|\to\infty}{\longrightarrow} \frac{1}{k^2} \qquad . \tag{20}$$

Show that the excitations energies asymptotically behave as

$$\tilde{\epsilon}_{\vec{k}} \overset{|\vec{k}|\to 0}{\longrightarrow} \hbar|\vec{k}| \cdot c_s + \mathcal{O}(k^3) \equiv \hbar|\vec{k}| \cdot \sqrt{\frac{n_0 \tilde{v}(0)}{M^*}} + \mathcal{O}(h^3) \tag{21}$$

$$\tilde{\epsilon}_{\vec{k}} \overset{|\vec{k}|\to\infty}{\longrightarrow} \epsilon_{\vec{k}} + \mathcal{O}(\frac{1}{k^2}) = \frac{\hbar^2 k^2}{2M^*} + \mathcal{O}(\frac{1}{k^2}) \qquad . \tag{22}$$

The quantity c_s is the speed of sound in (supra)fluid Helium-4 and vanishes for a non-interacting ultracold Bose gas.

Draw in a diagram $\tilde{\epsilon}_{\vec{k}}$ (which is directly correlated to the temperature of the system) as a function of the wave vector $|\vec{k}|$. Interpolate between the two asymptotic solutions. Around the minimum one can approximate the curve quadratically, so there harmonic oscillator degrees of freedom exist, which correspond to acoustic oscillations ("rotons" or so called second sound in Helium-4).

(f) Helium-3 is a system of three nucleons and four electrons, so seven spin-1/2 particles. Why would you assume it cannot form a suprafluid phase? How can it nevertheless?