Übung Quantenmechanik 2 WS 2024/25

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1. Coulomb Interaction in second Quantization

The total (Coulomb) interaction operator of an eletron gas in second Quantization is given by

$$\hat{V}_c = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\psi^\dagger_{\sigma_1}(\boldsymbol{r}_1)\psi^\dagger_{\sigma_2}(\boldsymbol{r}_2)\psi_{\sigma_2}(\boldsymbol{r}_2)\psi_{\sigma_1}(\boldsymbol{r}_1) \tag{1}$$

where $\psi^\dagger_{\sigma_1}(\boldsymbol{r}_1)$ is a fermionic quantum field, which creates an electron on position $\boldsymbol{r}_1$, and $\sigma = \pm\frac{1}{2}$.

(a) Why is the factor $\frac{1}{2}$ neccessary to correctly define the Coulomb interaction in this language?

(b) Apply the following Fourier transform

$$\psi^\dagger_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{kr}} f^\dagger_\sigma(\boldsymbol{k}) \qquad \psi_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{kr}} f_\sigma(\boldsymbol{k}) \tag{2}$$

where V, is the volume of the crystal to obtain the Coulomb-Interaction in momentum space.
Hint: Apply the substitution $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1$ and a similar substitution for two momentum variables.

The result you should find is given by

$$\hat{V}_c = \frac{1}{2V}\sum_{\sigma_1\sigma_2}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q}} f^\dagger_{\sigma_1}(\boldsymbol{k}_1) f^\dagger_{\sigma_2}(\boldsymbol{k}_2) f_{\sigma_2}(\boldsymbol{k}_2+\boldsymbol{q}) f_{\sigma_1}(\boldsymbol{k}_1-\boldsymbol{q}) V(\boldsymbol{q}) \tag{3}$$

where

$$V(\boldsymbol{q}) = \frac{e^2}{4\pi\epsilon_0}\int d\boldsymbol{r}\frac{e^{i\boldsymbol{qr}}}{|\boldsymbol{r}|}. \tag{4}$$

(c) Solve the remaining integral $V(\boldsymbol{q})$ in 3 spatial dimensions.
Hint: You will need to multiply a convergence factor $e^{-\kappa|\boldsymbol{r}|}$ with $\kappa > 0$ to the integral and evaluate $\kappa \to 0$ afterwards in order to make the integral converge. Give a physical argument to justify this procedure.

(d) The result you just calculated will be required in order to do perturbation theory for the Coulomb interaction. How can the result be written as a Feynman-Diagram?

2. Bose-Einstein Distribution

From thermodynamics, the grand canonical partition function Z is known to be

$$Z = \operatorname{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right], \tag{5}$$

where μ denotes the chemical potential and the trace over the Hamilton operator $\hat{H}$ and total number operator $\hat{N}$ is taken over the whole many-particle Hilbert space (also known as Fock space) $\mathcal{F}$, i.e.

$$\operatorname{tr}\left[\hat{O}\right] = \sum_i \langle\psi_i|\hat{O}|\psi_i\rangle \tag{6}$$

for any base $\{|\psi_i\rangle\}$ of $\mathcal{F}$.

We can compute thermal averages of any operator $\hat{O}$ as

$$\left\langle\hat{O}\right\rangle = \frac{1}{Z}\operatorname{tr}\left[\hat{O}e^{-\beta(\hat{H}-\mu\hat{N})}\right]. \tag{7}$$

Suppose, that we can find a basis, labeled by the quantum number λ, in which the Hamiltonian is diagonal, i.e.

$$\hat{H} = \sum_\lambda \epsilon_\lambda \hat{n}_\lambda, \tag{8}$$

where $\hat{n}_\lambda$ is a *bosonic* number operator.

(a) Write $\hat{H}$ and $\hat{N}$ in terms of (bosonic) creation and annihilation operators.

(b) Show, that one can write $Z = \prod_\lambda Z_\lambda$ and calculate Z_λ.
Hint: Geometric series

(c) Using Z_λ, calculate the grand canonical potential $\Omega_\lambda = -\frac{1}{\beta}\ln Z_\lambda$. From this calculate $\langle\hat{n}_\lambda\rangle = -\frac{\partial\Omega_\lambda}{\partial\mu}$. Which distribution do you obtain? How does this calculation connect to (7)?

(d) For which values of μ does our result hold?

(e) Repeat the calculation for fermionic creation and annihilation operators. What changes and which distribution do you obtain now?

3. Coulomb Potential in the Klein-Gordon-Equation

Consider a relativistic particle in an electromagnetic field, which is described by the wave function ψ. The respective Klein-Gordon equation reads

$$\left((i\hbar\partial_t - eA_0)^2 - c^2\left(\frac{\hbar}{i}\boldsymbol{\nabla} - \frac{e}{\hbar}\boldsymbol{A}\right)^2 - c^4m^2\right)\psi(\boldsymbol{x},t) = 0 \tag{9}$$

The vector potential $A = (A_0, \boldsymbol{A})$ is chosen to have only a zeroth component ($\boldsymbol{A} = 0$) to be a central potential ($\Phi(|\boldsymbol{x}| = r) = A_0(r)$).

(a) Decouple the differential equation by choosing an Ansatz $\psi(\boldsymbol{x}, t) = R(r)\phi(\varphi, \theta)e^{-i\omega t}$.
Hint: Write down the Laplace operator in spherical coordinates and use

$$\boldsymbol{\nabla}^2 = \Delta = \frac{1}{r^2}\partial_r\left(r^2\partial_r\right) - \frac{1}{\hbar^2 r^2}\boldsymbol{L}^2. \tag{10}$$

Introduce the spherical harmonics as eigenfunctions $\boldsymbol{L}^2$ with $\boldsymbol{L}^2\phi(\varphi, \theta) = \hbar^2 l(l+1)\phi(\varphi, \theta)$.

(b) Show that in the classical limit $E_{\mathrm{kin}} \ll mc^2$ the Schrödinger equation for a central potential is recovered.

(c) The Coulomb potential is given by $\Phi(r) = -eZ/4\pi\epsilon_0 r$. We introduce the following notations

$$\begin{aligned} \alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}, \quad E = \hbar\omega, \quad \sigma^2 = \frac{4\left(m^2c^4 - E^2\right)}{\hbar^2c^2}, \quad \gamma = Z\alpha, \\ \lambda = \frac{2E\gamma}{\hbar c\sigma}, \quad \rho = \sigma r, \quad l'(l'+1) = l(l+1) - \gamma^2 \end{aligned} \tag{11}$$

Use the definitions in (11) to write the differential equation with the dimensionless quantity ρ:

$$\left(-\frac{\partial^2}{\partial(\rho/2)^2} + \frac{l'(l'+1)}{(\rho/2)^2} + 1 - \frac{2\lambda}{(\rho/2)}\right)\rho R(\rho) = 0. \tag{12}$$

(d) Solve equation (12) in the limits $\rho \to 0$ and $\rho \to \infty$.

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