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Quantum Field Theory WS 05/06

Exercise 2

1. (a) Show that the Hamiltonian of a second quantized N-particle system with kinetic energy $\hat{T} = \sum\limits_{a=1}^{N} \hat{t}_a$, potential energy $\hat{U} = \sum\limits_{a=1}^{N} \hat{u}_a$ and a two-particle interaction $\hat{V} = \frac{1}{2} \sum\limits_{a,b}^{a \neq b} \hat{v}_{a,b}$ can be written in the form

$$\hat{H} = \sum_{i,j} (t_{ij} + u_{ij}) \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l} v_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \,.$$

   (b) Confirm, for bosons and fermions, that the particle-number operator $\hat{N} = \sum\limits_i \hat{a}_i^\dagger \hat{a}_i$ commutes with the above Hamiltonian.

Remarks:

- The eigenvalue problem of the single-particle operator $\hat{h} = \hat{t}_a + \hat{u}_a$ can be considered solved, $\hat{h}|\varphi_i\rangle = e_i|\varphi_i\rangle$. The operators $\hat{a}_i^{(\dagger)}$ represent bosonic or fermionic creation and annihilation operators that obey the usual commutation or anti-commutation relations, and $\hat{a}_i^\dagger|0\rangle = |\varphi_i\rangle$, $\hat{a}_i|\varphi_i\rangle = |0\rangle$ and $\hat{a}_i|0\rangle = 0$.

2. A model to describe simple metals is the Jellium-Model. It simulates the lattice of ions by a uniformly distributed and positively charged background. The electrons in the system undergo Coulomb interaction amongst each other, and with the ionic background. For N electrons distributed in the volume $V = L^3$ the Hamilton operator of the Jellium-Model reads $\hat{H}_{\text{Jellium}} = \hat{H}_e + \hat{H}_I + \hat{H}_{eI}$, where

$$\begin{aligned}
\hat{H}_e &= \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^{\,2}}{2m} + \frac{e^2}{2} \sum_{i,j}^{i \neq j} \frac{e^{-\alpha|\hat{\vec{r}}_i - \hat{\vec{r}}_j|}}{|\hat{\vec{r}}_i - \hat{\vec{r}}_j|} \\
\hat{H}_I &= \frac{e^2}{2} \frac{N^2}{V^2} \int_V \int_V \mathrm{d}^3R\,\mathrm{d}^3R' \, \frac{e^{-\alpha|\vec{R} - \vec{R}'|}}{|\vec{R} - \vec{R}'|} \\
\hat{H}_{eI} &= -e^2 \frac{N}{V} \sum_{i=1}^{N} \int_V \mathrm{d}^3R \, \frac{e^{-\alpha|\vec{R} - \hat{\vec{r}}_i|}}{|\vec{R} - \hat{\vec{r}}_i|}.
\end{aligned}$$

   (a) Represent the operator $\hat{H}_e$ in second quantized form. Prove that in the thermodynamic limit ($N \to \infty\,, V \to \infty\,, N/V = \text{const}$) the occurring divergence of the energy per particle gets compensated by the background contributions $\hat{H}_I$ and $\hat{H}_{eI}$.

   (b)* Compute the electron density operator $\hat{\rho}(\vec{r}) = \sum\limits_{i=1}^{N} \delta(\vec{r} - \hat{\vec{r}}_i)$ in second quantization and express the second part of $\hat{H}_e$ in terms of the Fourier components

$$\hat{\rho}_{\vec{q}} = \int_V \mathrm{d}^3r \, \hat{\rho}(\vec{r}) \, e^{i\vec{q}\cdot\vec{r}} \,.$$

(turn over)

Remarks:

- Due to the constant lattice potential the electronic one-particle wave functions are plane waves: $|\varphi_{\vec{k},\sigma}\rangle = |u_{\vec{k}}\rangle|u_\sigma\rangle$, with $\langle u_{\vec{r}}|u_{\vec{k}}\rangle = \frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{r})$ and $\hat{\vec{p}}|u_{\vec{k}}\rangle = \vec{k}\,|u_{\vec{k}}\rangle$, and where σ labels the spin degree of freedom. Periodic boundary conditions enforce the wave vectors $\vec{k}$ to be discrete, i.e. $\vec{k} = 2\pi/L(n_x, n_y, n_z)$ with $n_{x,y,z} \in \mathbb{Z}$.
- The factors $\exp(-\alpha|\vec{r} - \vec{r}'|)$, with $\alpha > 0$, have been introduced to cut off integrals. In the final result the limit $\alpha \to 0$ has to be performed.

3. Consider the Hamilton operator of the quantized Klein-Gordon field.

(a) Prove that in the Heisenberg picture the field operator $\hat{\phi}(\vec{x}, t)$ obeys the Klein-Gordon equation,

$$\ddot{\hat{\phi}}(\vec{x}, t) = \left(\vec{\nabla}^2 - m^2\right)\hat{\phi}(\vec{x}, t)\,.$$

(b) Confirm that using the following definitions of the field operator and the conjugate momentum (cf. lecture)

$$\begin{aligned}
\hat{\phi}(\vec{x}, t) &= \int \frac{\mathrm{d}^3k}{\sqrt{(2\pi)^3 2k_0}}\left[\hat{a}(\vec{k})\, e^{i(\vec{k}\cdot\vec{x}-k_0 t)} + \hat{a}^\dagger(\vec{k})\, e^{-i(\vec{k}\cdot\vec{x}-k_0 t)}\right] ,\\
\hat{\pi}(\vec{x}, t) &= \int \frac{\mathrm{d}^3k}{\sqrt{(2\pi)^3 2k_0}}\left[-ik_0\hat{a}(\vec{k})\, e^{i(\vec{k}\cdot\vec{x}-k_0 t)} + ik_0\hat{a}^\dagger(\vec{k})\, e^{-i(\vec{k}\cdot\vec{x}-k_0 t)}\right] ,
\end{aligned}$$

the Klein-Gordon Hamiltonian can be written as

$$\hat{H} = \int \mathrm{d}^3k k_0 \left(\hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) + \frac{1}{2}\left[\hat{a}(\vec{k}), \hat{a}^\dagger(\vec{k})\right]\right) .$$

(c) Calculate the commutators

$$[\hat{a}^\dagger(\vec{q}), \hat{H}] \quad \text{and} \quad [\hat{a}(\vec{q}), \hat{H}]\,.$$