Theoretical Physics 5
Advanced Quantum Mechanics
Winter Semester 2018/2019
Exercise Sheet 3

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return until: 2018-11-12
30 points

The exercise sheets can be found online at `http://www.staff.uni-mainz.de/pschwal/index_1819.html`.
To be handed in until Monday 2018-11-12 (12:30) to the red letterbox 42 (foyer of Staudingerweg 7).

1. **Electrons in a finite volume** **(15 points)**

   The purpose of this exercise is to study the contribution to the Hamilton operator of a gas of N electrons enclosed in a finite cubic volume with edge length L in occupation number representation. As basis states, plane waves $|\vec{k}\rangle$ normalized to the volume L^3,

   $$\psi_{\vec{k}}(\vec{x}) = \langle \vec{x}|\vec{k}\rangle = \frac{1}{L^{3/2}} \exp\left(i\ \vec{k}\cdot\vec{x}\right)$$

   corresponding to quantized momenta $\vec{p} = \hbar\vec{k} = \frac{2\pi\hbar\vec{\nu}}{L}$, $\vec{\nu} \in \mathbb{Z}^3$ can be used. The corresponding creation and annihilation operators are denoted by $\hat{a}^\dagger_{\vec{k}}$ and $\hat{a}_{\vec{k}}$ and satisfy $\{\hat{a}_{\vec{k}}, \hat{a}^\dagger_{\vec{k}'}\} = \delta_{\vec{k}\vec{k}'}$. Spin degrees of freedom are not taken into consideration.

   (a) **(3 points)** Show that

   $$\hat{\phi}(\vec{x}) = \frac{1}{L^{3/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}\, \hat{a}_{\vec{k}}\,.$$

   (b) **(5 points)** The operator 'kinetic energy' in position space is given by $\hat{T} = -\frac{\hbar^2}{2m}\sum_{i=1}^N \Delta_{\vec{x}_i}$. Show that the corresponding operator in occupation number representation can be written as

   $$\hat{T} = \sum_{\vec{k}} \frac{\hbar^2\vec{k}^2}{2m} \hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\,.$$

   (c) **(7 points)** The interaction of the electrons amongst themselves depends only on the distance $|\vec{x}_i - \vec{x}_j|$ and is given in coordinate representation by

   $$\hat{V} = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N} V(|\vec{x}_i - \vec{x}_j|)\,.$$

   Derive the following form in occupation number representation:

   $$\hat{V} = \frac{1}{2L^3}\sum_{\vec{k},\vec{k}',\vec{q}} \tilde{V}(\vec{q}\,)\, \hat{a}^\dagger_{\vec{k}+\vec{q}}\, \hat{a}^\dagger_{\vec{k}'-\vec{q}}\, \hat{a}_{\vec{k}'}\, \hat{a}_{\vec{k}}\,, \qquad \tilde{V}(\vec{q}\,) \equiv \int_{L^3} \mathrm{d}^3x\, V(|\vec{x}|) e^{-i\,\vec{q}\cdot\vec{x}}\,.$$

2. **Para-helium** **(15 points)**

In this exercise we consider the ground state energy of the electron pair in a helium atom with infinitely heavy nucleus. The corresponding two-electron Hamilton operator is given by $H = H_0 + \Delta H$ with

$$H_0 = \frac{(\vec{p}_1)^2}{2m} - \frac{Ze^2}{r_1} + \frac{(\vec{p}_2)^2}{2m} - \frac{Ze^2}{r_2}, \qquad \Delta H = \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}, \quad r_i = |\vec{x}_i| \text{ for } i = 1, 2\,.$$

States in which the electron spins are anti-parallel ($S = 0$, spin-singlet) are called para-helium, whereas ortho-helium denotes states with parallel spin ($S = 1$, spin-triplet).

(a) **(13 points)** Calculate the correction to the ground state energy of para-helium to first order in perturbation theory with respect to the perturbation ΔH. All intergrals have to be solved by hand.

(b) **(2 points)** Calculate the numerical value of the correction.

Hints:

The normalized position-space wave function of the ground state of the single-electron atom with infinitely heavy nucleus with atomic number Z and Hamilton operator

$$H^{(1)} = \frac{(\vec{p})^2}{2m} - \frac{Ze^2}{r} \qquad r = |\vec{x}|$$

is given by

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_B}\right)^{\frac{3}{2}} \exp\left(-\frac{Zr}{a_B}\right),$$

where a_B is the Bohr radius. For the evaluation of the occurring integrals use the multipole expansion of the distance

$$\begin{aligned}\frac{1}{|\vec{x}_1 - \vec{x}_2|} &= \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\alpha)}} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\alpha) \\ &= \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}^*(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2)\end{aligned}$$

with $r_< = \min(r_1, r_2)$ and $r_> = \max(r_1, r_2)$ as well as the orthogonality relation of the spherical harmonics

$$\int \mathrm{d}\Omega\, Y_{l'm'}^*(\theta, \phi) Y_{lm}(\theta, \phi) = \delta_{l'l}\delta_{m'm}\,.$$

To solve the integrals you might use

$$Y_{00}(\theta, \phi) = \frac{1}{\sqrt{4\pi}}$$

in combination with the orthogonality relation mentioned above.