Bosonization: Worksheet 2

Operators in second quantization and exchange correction

Christophe De Beule (christophe.debeule@gmail.com)

---

1 Current-density operator in second quantization

The current-density operator can be written in first quantization as

$$\hat{\boldsymbol{J}}(\boldsymbol{x}) = \sum_{n=1}^{N} \hat{\boldsymbol{j}}(\boldsymbol{x}, \hat{\boldsymbol{r}}_n), \qquad \hat{\boldsymbol{j}}(\boldsymbol{x}, \hat{\boldsymbol{r}}) = \frac{1}{2}\left\{ \frac{\hat{\boldsymbol{p}}}{m}, \delta(\boldsymbol{x} - \hat{\boldsymbol{r}}) \right\},$$

where $\hat{\boldsymbol{p}} = -i\hbar\nabla_{\boldsymbol{r}}$ and $\boldsymbol{x}$ is a parameter indicating the position. Remember that a one-body operator $\hat{O}_1 = \sum_{n=1}^{N} \hat{o}_n$, is represented in second quantization as

$$\hat{O}_1 = \sum_{\mu,\nu} \langle \mu | \hat{o} | \nu \rangle \, \hat{c}_\mu^\dagger \hat{c}_\nu.$$

(1) Show that the current-density operator in second quantization, in the representation with field operators in position space, is given by

$$\hat{\boldsymbol{J}}(\boldsymbol{x}) = \sum_\sigma \int d^d\boldsymbol{r} \, \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\boldsymbol{j}}(\boldsymbol{x}, \boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}),$$

and work out the integral. Hint: Use periodic boundary conditions.

(2) Write down the current-density operator with field operators in momentum space. Use a resolution of identity and $\langle \boldsymbol{r} | \boldsymbol{k} \rangle = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}/\sqrt{V}$. The final result can be written as

$$\hat{\boldsymbol{J}}(\boldsymbol{x}) = \frac{1}{V} \sum_\sigma \sum_{\boldsymbol{k},\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{x}} \, \frac{\hbar \boldsymbol{k}}{m} \, \hat{c}_{\boldsymbol{k}-\frac{\boldsymbol{q}}{2}\sigma}^\dagger \hat{c}_{\boldsymbol{k}+\frac{\boldsymbol{q}}{2}\sigma}.$$

(3) Calculate the current-density operator in momentum representation,

$$\hat{\boldsymbol{J}}_{\boldsymbol{q}} = \int d^d\boldsymbol{x} \, e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} \hat{\boldsymbol{J}}(\boldsymbol{x}).$$

(4) Find an expression for $\boldsymbol{q} \cdot \hat{\boldsymbol{J}}_{\boldsymbol{q}}$ for the Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} E_{\boldsymbol{k}} \, \hat{c}_{\boldsymbol{k}\sigma}^\dagger \hat{c}_{\boldsymbol{k}\sigma},$$

by Fourier transforming the continuity equation, $\partial_t \hat{\rho}(\boldsymbol{x}, t) + \nabla \cdot \hat{\boldsymbol{J}}(\boldsymbol{x}, t) = 0$, where

$$\hat{\rho}(\boldsymbol{x}) = \sum_\sigma \hat{\psi}_\sigma^\dagger(\boldsymbol{x}) \hat{\psi}_\sigma(\boldsymbol{x}) = \frac{1}{V} \sum_\sigma \sum_{\boldsymbol{k},\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{x}} \, \hat{c}_{\boldsymbol{k}-\boldsymbol{q}\sigma}^\dagger \hat{c}_{\boldsymbol{k}\sigma},$$

and calculating $\hbar \partial_t \hat{\rho}_{\boldsymbol{q}} = i[\hat{H}, \hat{\rho}_{\boldsymbol{q}}]$. Show that you recover the result of (3) when $E_{\boldsymbol{k}} = \frac{\hbar^2 \boldsymbol{k}^2}{2m}$.

2 Spin operators in second quantization

The spin-density operator can be written in first quantization as

$$\hat{\boldsymbol{S}}(\boldsymbol{x}) = \sum_{n=1}^{N} \delta(\boldsymbol{x} - \hat{\boldsymbol{r}}_n)\, \hat{\boldsymbol{s}}_n,$$

where $\hat{\boldsymbol{s}}_n$ are the spin operators of the n-th particle. Find $\hat{\boldsymbol{S}}(\boldsymbol{x})$ and $\hat{\boldsymbol{S}}_{\boldsymbol{q}}$ in second quantization, in the representation with field operators in momentum space. Finally, also calculate the spin operator in second quantization: $\hat{\boldsymbol{S}} = \int d^d\boldsymbol{x}\, \hat{\boldsymbol{S}}(\boldsymbol{x}) = \hat{\boldsymbol{S}}_{\boldsymbol{q}=\boldsymbol{0}}$.

3 Exchange integral

Calculate the exchange integral

$$\Sigma_{\text{ex}}(\boldsymbol{k}) = -\frac{1}{V} \sum_{\boldsymbol{q} \neq 0} V_{\text{ee}}(\boldsymbol{q})\, n_{\boldsymbol{k}-\boldsymbol{q}},$$

where $n_{\boldsymbol{k}-\boldsymbol{q}} = \Theta\left(|\boldsymbol{k}-\boldsymbol{q}| \leq k_F\right)$ is the occupation number at zero temperature and $V_{\text{ee}}(\boldsymbol{q}) = 4\pi e^2/q^2$ is the Fourier transform of the Coulomb potential.

(1) Shift the integrand by $\boldsymbol{k}$ and then use spherical coordinates with the z-axis along $\boldsymbol{k}$. Also get rid of units in the integral by using momenta in units of k_F.

(2) Solve the following integral first,

$$\int_{-1}^{1} \frac{du}{a+bu},$$

where a and b are functions of $k = |\boldsymbol{k}|$ and $q = |\boldsymbol{q}|$. This integral converges only for $a > b$. Check that this is always the case.

(3) The final integral should be over the momentum q/k_F and is a bit tricky. Hint: Keep in mind that $\ln x^2 = 2\ln|x|$ for $x \in \mathbb{R}$.

The final result is given by

$$\Sigma_{\text{ex}}(\boldsymbol{k}) = -\frac{2e^2 k_F}{\pi} F(k/k_F),$$

with

$$F(y) = \frac{1}{2} + \frac{1-y^2}{4y} \ln\left|\frac{1+y}{1-y}\right|,$$

which is shown in the figure below.