Bosonization: Worksheet 1

Basic concepts of condensed-matter field theory

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

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1 Fourier transform of the Yukawa potential

Calculate the three-dimensional Fourier transform of the Yukawa potential

$$V(\boldsymbol{q}) = \int d^3r \, V(r) \, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}, \qquad V(r) = \frac{e^2}{r} \, e^{-\mu r},$$

and take the limit $\mu \to 0$ to obtain the regularized Fourier transform of the Coulomb potential. Hint: Use spherical coordinates with the z-axis pointing along $\boldsymbol{q}$ to perform the integration.

2 Free electrons

The free electron Hamiltonian can be written as

$$\hat{H}_0 = \sum_{\sigma=\uparrow,\downarrow} \int_V d^dr \, \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V(\boldsymbol{r}) \right] \hat{\psi}_\sigma(\boldsymbol{r}),$$

where $\hat{\boldsymbol{p}} = -i\hbar\nabla$. The field operators obey the anti-commutation relations $\{\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r'})\} = \delta_{\sigma\sigma'}\delta(\boldsymbol{r} - \boldsymbol{r'})$ and $\{\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}_{\sigma'}(\boldsymbol{r'})\} = \{\hat{\psi}_\sigma^\dagger(\boldsymbol{r}), \hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r'})\} = 0$.

(1) Consider the Fourier transform

$$\hat{\psi}_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{c}_{\boldsymbol{k}\sigma},$$

where $\hat{c}_{\boldsymbol{k}\sigma}$ and $\hat{c}_{\boldsymbol{k}\sigma}^\dagger$ are field operators in momentum space. Assume the volume $V = L^d$ is a d-dimensional cube with sides L and use periodic boundary conditions $\hat{\psi}_\sigma(\boldsymbol{r} + L\boldsymbol{e}_i) = \hat{\psi}_\sigma(\boldsymbol{r})$ ($i = 1, \ldots, d$) to find the allowed momenta. Also find an expression for the anti-commutation relations $\{\hat{c}_{\boldsymbol{k}\sigma}, \hat{c}_{\boldsymbol{k'}\sigma'}^\dagger\}$, $\{\hat{c}_{\boldsymbol{k}\sigma}, \hat{c}_{\boldsymbol{k'}\sigma'}\}$, and $\{\hat{c}_{\boldsymbol{k}\sigma}^\dagger, \hat{c}_{\boldsymbol{k'}\sigma'}^\dagger\}$.

(2) For the remainder of this exercise we put $V(\boldsymbol{r}) = 0$. Use the above result to obtain a representation of $\hat{H}_0$ in terms of $c_{\boldsymbol{k}\sigma}$ and $\hat{c}_{\boldsymbol{k}\sigma}^\dagger$.

(3) Calculate the non-interacting ground state energy

$$E_0 = \langle\Omega| \hat{H}_0 |\Omega\rangle,$$

where $|\Omega\rangle = \prod_{|\boldsymbol{k}|\leq k_F,\sigma} \hat{c}_{\boldsymbol{k}\sigma}^\dagger |0\rangle$ is the Fermi sea with k_F the Fermi wave number. Perform the calculation for $d = 1$ and $d = 3$. Hint: $\sum_{\boldsymbol{k}} \overset{L\to\infty}{\longrightarrow} \left(\frac{L}{2\pi}\right)^d \int d^dk$.

3 Lattice version of the interaction Hamiltonian

The interaction Hamiltonian

$$\hat{V}_{ee} = \frac{1}{2} \sum_{\sigma,\sigma'} \int d^dr \int d^dr' \, V_{ee}(\boldsymbol{r} - \boldsymbol{r'}) \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r'}) \hat{\psi}_{\sigma'}(\boldsymbol{r'}) \hat{\psi}_\sigma(\boldsymbol{r}),$$

where $V_{ee}(\boldsymbol{r}-\boldsymbol{r}')$ is the interaction potential, can also be written in terms of Wannier field operators $\hat{c}_{i\sigma}$ and $\hat{c}^\dagger_{i\sigma}$ through a unitary transformation

$$\hat{\psi}_\sigma(\boldsymbol{r}) = \sum_i \phi_{\boldsymbol{R}_i}(\boldsymbol{r})\, \hat{c}_{i\sigma},$$

where the Wannier function $\phi_{\boldsymbol{R}_i}(\boldsymbol{r})$ is localized around the Bravais lattice site $\boldsymbol{R}_i$ and the set of Wannier states $\{|\phi_{\boldsymbol{R}_i}\rangle\}$ form an orthonormal basis of the single-particle Hilbert space. The result is given by

$$\hat{V}_{ee} = \sum_{\sigma,\sigma'} \sum_{ii'jj'} V_{ii'jj'} \hat{c}^\dagger_{i\sigma} \hat{c}^\dagger_{i'\sigma'} \hat{c}_{j'\sigma'} \hat{c}_{j\sigma}.$$

(1) Find an expression for $V_{ii'jj'}$ in terms of the Wannier functions.

(2) Direct terms $V_{ii'ii'} \equiv V_{ii'}$ couple density fluctuations at sites $i \neq i'$. Determine $V_{ii'}$ for a contact potential $V_{ee}(\boldsymbol{r}) = \lambda\delta(\boldsymbol{r})$ and wave functions [1] $\phi_{\boldsymbol{R}_i}(\boldsymbol{r}) = \frac{e^{-(\boldsymbol{r}-\boldsymbol{R}_i)^2/(2\Delta^2)}}{(\Delta\sqrt{\pi})^d}$, for

   (i) an on-site interaction $i = i'$;

   (ii) a nearest-neighbor interaction in a square lattice ($d = 2$) with lattice constant a.

(3) In the limit $\Delta \ll a$, the wave functions are strongly localized on the sites and the on-site interaction $V_{ii} \equiv U/2$, called the Hubbard interaction, is the dominant contribution. Determine the interaction Hamiltonian $\hat{V}_{ee}$ in this approximation.

4 Useful identities

Consider two operators A and B. The Baker-Hausdorff theorem is given by

$$e^{-B}Ae^{B} = \sum_{n=0}^{\infty} \frac{[A,B]_n}{n!} = A + [A,B] + \frac{1}{2}[[A,B],B] + \dots,$$

where $[A,B]_{n+1} \equiv [[A,B]_n, B]$ and $[A,B]_0 \equiv A$. Now define $C \equiv [A,B]$ and assume that C commutes with A and B.

(1) Use the Baker-Hausdorff theorem to show that $e^{-B}Ae^{B} = A + C$.

(2) Consider the operator-valued function $\mathcal{T}(s) = e^{sA}e^{sB}$ ($s \in \mathbb{R}$) and use (1) to write

$$\frac{d\mathcal{T}(s)}{ds} = \mathcal{T}(s)\,\mathcal{P}(s),$$

where $\mathcal{P}(s)$ is to be found. Solve this differential equation by inspection, with the boundary condition $\mathcal{T}(0) = 1$. Use your result to prove

$$e^{A}e^{B} = e^{A+B+C/2} = e^{A+B}e^{C/2},$$

where the last equality follows from $[A+B, C] = 0$.

(3) First use (1) to prove by induction that $e^{-B}A^n e^{B} = (A+C)^n$, and then show that

$$e^{-B}f(A)e^{B} = f(A+C).$$

(4) Use (3) to show that $e^{A}e^{B} = e^{B}e^{A}e^{C}$.

[1] These functions are not strictly Wannier functions because they are not orthogonal. Wannier functions can be constructed from a superposition of Gaussians, but this is beyond the scope of the exercise.