

Advanced quantum mechanics and quantum field theory, FS 2021

Blatt 0

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(to be discussed in the first exercise class; no submission!)

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The purpose of problems 1 and 2 is to train the use of the formalism of second quantization. The anticommutator/commutator relations for fermionic/bosonic operators read

	momentum representation	position representation
fermions	$\{c_{\mathbf{k}'\sigma'}, c_{\mathbf{k}\sigma}^\dagger\} = \delta_{\mathbf{k}'\mathbf{k}}\delta_{\sigma'\sigma}$	$\{\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma^\dagger(\mathbf{r})\} = \delta(\mathbf{r}' - \mathbf{r})\delta_{\sigma'\sigma}$
bosons (spinless)	$[a_{\mathbf{k}'}, a_{\mathbf{k}}^\dagger] = \delta_{\mathbf{k}'\mathbf{k}}$	$[\Phi(\mathbf{r}'), \Phi^\dagger(\mathbf{r})] = \delta(\mathbf{r}' - \mathbf{r})$

All others (like $\{c_{\mathbf{k}'\sigma'}, c_{\mathbf{k}\sigma}\}$, $[a_{\mathbf{k}'}, a_{\mathbf{k}}^\dagger]$, \dots) vanish.

(1) Position and momentum representation

For free electrons, the relation between position and momentum representation reads

$$\Psi_\sigma(\mathbf{r}) = V^{-\frac{1}{2}} \sum_{\mathbf{k}} c_{\mathbf{k}\sigma} e^{i\mathbf{k}\mathbf{r}}.$$

Write the Hamiltonian

$$H = \sum_{\sigma=\pm\frac{1}{2}} \int d^3r \Psi_\sigma^\dagger(\mathbf{r}) \left[\frac{-\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \Psi_\sigma(\mathbf{r})$$

in terms of the $c_{\mathbf{k}\sigma}$, $c_{\mathbf{k}\sigma}^\dagger$.

(2) Tight-binding model in second quantization

A major part of solid-state physics deals with electrons in a periodic potential. As a simplified model we consider fermionic particles moving on a cubic lattice (lattice constant a). The kinetic energy is assumed to have tight-binding form

$$H = -t \sum_{\langle i,j \rangle \sigma} \left[c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right],$$

here, $\sum_{\langle i,j \rangle}$ is the sum over all nearest neighbors (such that each bond appears only once) and \sum_{σ} is the sum over the two spin directions.

- (a) Determine the band structure $\epsilon(\mathbf{k})$ for a d -dimensional cubic lattice ($d = 1, 2, 3$).
- (b) Draw the contours $\epsilon(\mathbf{k}) = \text{const.}$ in the (k_x, k_y) -plane for $d = 2$.

Hint: Diagonalize the Hamiltonian by a Fourier transform, $c_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r}_j) c_{\mathbf{k}\sigma}$, here, \mathbf{r}_j are the coordinates of the lattice sites; N is their total number.

(3) **Variational derivative I**

- (a) Consider the functional $G[f] = \int g(y, f) dy$. Show that

$$\frac{\delta G[f]}{\delta f(x)} = \frac{\partial g(x, f)}{\partial f}.$$

- (b) Now consider the functional $H[f] = \int g(y, f, f') dy$ and show that

$$\frac{\delta H[f]}{\delta f(x)} = \frac{\partial g}{\partial f} - \frac{d}{dx} \frac{\partial g}{\partial f'},$$

where $f' = \partial f / \partial y$.

- (c) For the functional $J[f] = \int g(y, f, f', f'') dy$ show that

$$\frac{\delta J[f]}{\delta f(x)} = \frac{\partial g}{\partial f} - \frac{d}{dx} \frac{\partial g}{\partial f'} + \frac{d^2}{dx^2} \frac{\partial g}{\partial f''},$$

where $f'' = \partial^2 f / \partial y^2$.

(4) **Three-dimensional elastic medium**

For a three-dimensional elastic medium, the potential energy is

$$V = \frac{\mathcal{T}}{2} \int d^3x (\nabla \psi)^2,$$

and the kinetic energy is

$$T = \frac{\rho}{2} \int d^3x \left(\frac{\partial \psi}{\partial t} \right)^2.$$

Here, $\psi(\mathbf{x}, t)$ describes the displacement of the elastic medium at \mathbf{x} at time t , ρ is the mass density, and \mathcal{T} the tension.

Write down the Lagrange density, the action, the Euler-Lagrange equation, and the resulting equation of motion for $\psi(\mathbf{x}, t)$.