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Theory of Superconductivity, Frühjahrsemester 2023

Blatt 0

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	$\{c_{\mathbf{k}'\sigma'}, c^\dagger_{\mathbf{k}\sigma}\} = \delta_{\mathbf{k}'\mathbf{k}}\delta_{\sigma'\sigma}$	$\{\Psi_{\sigma'}(\mathbf{r}'), \Psi^\dagger_\sigma(\mathbf{r})\} = \delta(\mathbf{r}'-\mathbf{r})\delta_{\sigma'\sigma}$
bosons (spinless)	$[a_{\mathbf{k}'}, a^\dagger_{\mathbf{k}}] = \delta_{\mathbf{k}'\mathbf{k}}$	$[\Phi(\mathbf{r}'), \Phi^\dagger(\mathbf{r})] = \delta(\mathbf{r}'-\mathbf{r})$

All others (like $\{c_{\mathbf{k}'\sigma'}, c_{\mathbf{k}\sigma}\}$, $[a^\dagger_{\mathbf{k}'}, a^\dagger_{\mathbf{k}}]$, $\cdots$) vanish.

(1) **Position and momentum representation**
For free electrons, the relation between position and momentum representation reads

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

Write the Hamiltonian

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

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

(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

$$H = -t \sum_{<i,j>\sigma} \left[c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right] ,$$

here, $\sum_{<i,j>}$ is the sum over all nearest neighbors (such that each bond appears only once) and $\sum_\sigma$ 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.