Karlsruher Institut für Technologie | Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie I WS 2012/2013

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1. Diatomic molecule. (15 + 15 = 30 Punkte)

Electrons (spin-1/2 fermions) on certain orbitals in a diatomic molecule are described by the Hamiltonian

$$\hat{\mathcal{H}} = \varepsilon_0 \sum_{i=1}^{2} \sum_{\sigma=\uparrow,\downarrow} \hat{a}^\dagger_{i\sigma}\hat{a}_{i\sigma} + t \sum_{\sigma=\uparrow,\downarrow} \left(\hat{a}^\dagger_{1\sigma}\hat{a}_{2\sigma} + \hat{a}^\dagger_{2\sigma}\hat{a}_{1\sigma}\right) + U \sum_{i=1}^{2} \hat{a}^\dagger_{i\uparrow}\hat{a}^\dagger_{i\downarrow}\hat{a}_{i\downarrow}\hat{a}_{i\uparrow},$$

where $i = 1, 2$ labels the two atoms in the molecule, $\hat{a}^\dagger_{i\sigma}$ and $\hat{a}_{i\sigma}$ are the creation and annihilation operators of electrons with spin projection σ on atom i, t is the hopping matrix element between the atoms. The molecule may be ionised and may have 0, 1, or 2 electrons on the respective orbitals.

(a) Determine the eigenstates and the eigenenergies of the electrons for $t = 0$. Consider different possibilities for the number of electrons.

(b) What is the physical meaning of the energy U? Determine the eigenstates and the eigenenergies of the electrons for $U = 0$.

2. Supersymmetric oscillator. (10 + 15 + 5 = 30 Punkte)

The so-called supersymmetric oscillator is a system of non-interacting spinless bosons and fermions described by the Hamiltonian

$$\hat{\mathcal{H}} = \omega(\hat{b}^\dagger\hat{b} + \hat{f}^\dagger\hat{f}),$$

where $\hat{b}^\dagger$ ($\hat{b}$) and $\hat{f}^\dagger$ ($\hat{f}$) are respectively bosonic and fermionic creation (annihilation) operators.

(a) Find the eigenstates and the eigenenergies of the oscillator, together with their degeneracies.

(b) Operators $\hat{Q} = \sqrt{\omega}\hat{b}^\dagger\hat{f}$ and $\hat{Q}^\dagger = \sqrt{\omega}\hat{b}\hat{f}^\dagger$ convert fermions to bosons and bosons to fermions, respectively. Show that these operators correspond to some symmetries of the Hamiltonian. Rewrite the Hamiltonian in terms of $\hat{Q}$ and $\hat{Q}^\dagger$.

(c) Determine the time dependence of the operators $\hat{Q}(t)$ and $\hat{Q}^\dagger(t)$ in the Heisenberg picture.

3. Bosonic density fluctuations. (10 + 30 = 40 Punkte)

Let us consider a system of N free spinless non-interacting bosons with a quadratic spectrum $\varepsilon_{\mathbf{p}} = \mathbf{p}^2/(2m)$, confined in volume V. In this exercise we assume for simplicity, that momentum $\mathbf{p}$ is a good quantum number. The operator of the density of bosons at point $\mathbf{r}$ reads $\hat{\rho}(\mathbf{r}) = \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})$, where $\hat{\Psi}^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{i\mathbf{pr}} \hat{b}^\dagger_{\mathbf{p}}$, and $\hat{b}^\dagger_{\mathbf{p}}$ is the creation operator of a boson in a state with momentum $\mathbf{p}$. Correspondingly, the operator of the number of bosons in a certain volume $v < V$ reads $\hat{n}_v = \int_v \hat{\rho}(\mathbf{r}) d\mathbf{r}$.

(a) At $T = 0$ evaluate the average number of bosons in volume v by averaging the operator $\hat{n}_v$.

(b) At $T = 0$ calculate the fluctuation of the number of bosons in volume v.