University of Regensburg Summer Term 2018

Quantum Theory of Condensed Matter I

Prof. John Schliemann
Dr. Paul Wenk, M.Sc. Martin Wackerl

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Sheet 4

1. Simple Fermion-Boson Model ..... [5P]

A simple Hamiltonian which contains a coupling between fermions (electrons) and bosons (phonons) is written as

$$H = \epsilon\, c^\dagger c + M(b^\dagger + b)c^\dagger c + \omega b^\dagger b, \tag{1}$$

where the fermion and boson annihilation(creation) operators are represented by $c(c^\dagger)$ and $b(b^\dagger)$, respectively. The Fock-space is spanned by the states $|n_f, n_b\rangle$ where $n_f \in \{0, 1\}$ is the fermion and $n_f \in \{0, 1, 2, \cdots\}$ the boson occupation number. Obviously, the Fock-space decomposes into two subspaces for $n_f = 0$ and $n_f = 1$.

a)(3P) Write down the matrix representation with respect to $|n_f, n_b\rangle$ in both subspaces.

b)(2P) Diagonalize the Hamiltonian analytically by completing the square, i.e., rewrite it in the form

$$H = \tilde{\epsilon}\, c^\dagger c + \omega \tilde{b}^\dagger \tilde{b}. \tag{2}$$

Proof that $\tilde{b}(\tilde{b^\dagger})$ still fulfills the commutator relations and compute the energy eigenvalues.

2. Coulomb Interaction ..... [8P]

Assuming only intra-atomic Coulomb interaction, we can write the interaction part as

$$H_{\text{int}} = \frac{1}{2} \sum_{i\sigma\sigma'} \sum_{\mu\mu'\nu\nu'} V(\mu\nu;\mu'\nu') c^\dagger_{i\mu\sigma} c^\dagger_{i\nu\sigma'} c_{i\nu'\sigma'} c_{i\mu'\sigma}, \tag{3}$$

with the site index i and the band indices μ, ν, μ', and ν'. A further restriction is applied on the scattering which is taken only between two bands and considering only *direct terms* ($U_{\mu\nu} := V(\mu\nu;\mu\nu)$) and *exchange terms* ($J_{\mu\nu} := V(\mu\nu;\nu\mu)$), leaving us with

$$\tilde{H}_{\text{int}} = \frac{1}{2} \sum_{i\sigma\sigma'} \sum_{\mu\nu} ((1 - \delta_{\mu\nu}\delta_{\sigma\sigma'}) U_{\mu\nu} n_{i\mu\sigma} n_{i\nu\sigma'} + (1 - \delta_{\mu\nu}) J_{\mu\nu} c^\dagger_{i\mu\sigma} c^\dagger_{i\nu\sigma'} c_{i\mu\sigma'} c_{i\nu\sigma}). \tag{4}$$

Show that $\tilde{H}_{\text{int}}$ can be split into $\tilde{H}_{\text{int}} = H_U + H_{\text{dir}} + H_{\text{ex}}$ with

$$H_U = \frac{1}{2} \sum_{i\sigma} \sum_{\mu} U_{\mu\mu} n_{i\mu\sigma} n_{i\mu(-\sigma)}, \tag{5}$$

$$H_{\text{dir}} = \frac{1}{2} \sum_{i\mu\nu}^{\mu\neq\nu} \left(U_{\mu\nu} - \frac{1}{2} J_{\mu\nu} \right) n_{i\mu} n_{i\nu} \quad \text{with} \quad n_{i\mu} = \sum_\sigma n_{i\mu\sigma}, \tag{6}$$

$$H_{\text{ex}} = -\frac{1}{\hbar^2} \sum_{i\mu\nu}^{\mu\neq\nu} J_{\mu\nu} \mathbf{s}_{i\mu} \cdot \mathbf{s}_{i\nu} \quad \text{with} \quad \mathbf{s} = \frac{\hbar}{2}\boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}. \tag{7}$$

3. Hubbard Model ..... [10P]

One of the simplest models which allows a study of an interplay between the kinetic energy, the Coulomb interaction, and Fermionic statistics is the Hubbard model.[1] The corresponding Hamiltonian $H = H_t + H_U$ consisting of a hopping term

$$H_t = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} \tag{8}$$

and the interaction term (see Eq. 5, here for one band)

$$H_U = \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i(-\sigma)}, \tag{9}$$

with the operator $c^\dagger_{i\sigma}$ creating an electron on site i with spin $\sigma = \{1 \equiv \uparrow\}, \{-1 \equiv \downarrow\}$ and $n_{i\sigma}$ the corresponding particle number operator.

and

a)(3P) Show that H possesses spin-rotational invariance by rewriting H_U in the form

$$H_U = \frac{UN}{2} - \frac{2U}{3} \sum_i \mathbf{S}_i^2, \quad \text{with } N \text{ the number of spins.} \tag{10}$$

Explain the statement "*H_U wants as many uncompensated spins as possible*".

b)(3P) In the following, we analyze a system of two quantum dots A and B. This system is filled with two electrons (half-filling due to the spin degree of freedom). Represent H in the basis of states given by all possible electron configurations $\{\{\cancel{\uparrow\downarrow} —\}, \{\uparrow \downarrow\}, \ldots\}$ for both electrons and the two sites $\{A, B\}$.

c)(3P) Show that $S_z = (1/2) \sum_j (n_{j\uparrow} - n_{j\downarrow})$ is a conserved quantity and use this finding to explain the block-diagonal structure of the represented Hamiltonian. To simplify the representation, check the parity of the basis states using the orbital parity operator $\hat{P}$ (Majorana operator), which is given by $\hat{P} c^\dagger_{x,\sigma} c^\dagger_{x',\sigma'} |0\rangle = c^\dagger_{f(x),\sigma} c^\dagger_{f(x'),\sigma'} |0\rangle$ with $f(A) = B, f(B) = A$. Not all basis states defined in a) are eigenstates of $\hat{P}$. Find a basis with elements of well defined parity P.

d)(3P) Diagonalize H. What is the ground state (singlet/triplet) and how large is the energy gap to the first excited state?

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[1] J. Hubbard, Proc. R. Soc. London **A276**, 238 (1963), J. Kanamori, Progr. Theor. Phys. **A30**, 275 (1963), M. C. Gutzwiller, Phys. Rev. Lett. **A10**, 59 (1963)