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Theoretical Solid-State Physics, Herbstsemester 2012

Blatt 10

Abgabe: 20. December, 12:00H (Treppenhaus 4. Stock)
Tutor: Dr. Rakesh Tiwari

(1) **Hubbard sectors** (4 Points)
As discussed in the lecture, the analysis of the Hubbard model becomes easier to carry out if we organize the electronic Hilbert space in Hubbard sectors, where each sector contains configurations with the same number of doubly-occupied sites (e.g., those within the lowest Hubbard sector do not contain any doubly-occupied site).

(a) Assume that we have N_e electrons and N sites. Express the total number of electronic configurations (the total size of the Hilbert space), as well as the dimension of the lowest Hubbard sector, in terms of N_e and N. Then find these numbers explicitly for $N_e = 10$ and $N = 20$.

(b) Now consider $N_e = 2$ electrons on a "Hubbard triangle" (three sites). Group all possible electronic configurations into Hubbard sectors. By making use of the conservation of the z component of the total electron spin, solve the problem (i.e., find the eigenstates and eigenvalues of the Hubbard Hamiltonian) in the limit $U/t \to \infty$.

(2) **Derivation of an effective antiferromagnetic Heisenberg model from the Hubbard model at half-filling** (3 Points)
As shown in the lecture, in the lowest Hubbard sector (no doubly-occupied sites) the Hubbard Hamiltonian reduces to that of the extended $t - J$ model, and in the special case of half-filling (one particle per site) the latter simplifies to

$$H_{\text{eff}}^{(2)} = -\frac{J}{2} \sum_{i,\delta,\sigma,\sigma'} c^{\dagger}_{i+\delta,\sigma'} c_{i,\sigma'} n_{i,\bar{\sigma}'} n_{i,\bar{\sigma}} c^{\dagger}_{i,\sigma} c_{i+\delta,\sigma} \, . \tag{1}$$

Here $n_{i,\sigma} \equiv c^{\dagger}_{i,\sigma} c_{i,\sigma}$, $\bar{\sigma}$ is the opposite spin projection from σ (i.e., if $\sigma = \uparrow$, then $\bar{\sigma} = \downarrow$ and vice versa), $i + \delta$ denotes the nearest neighbors of the site i, while $J \equiv 2t^2/U$ is the energy scale characterizing the virtual hopping fluctuations between Hubbard sectors – the "superexchange interaction."
By making use of the $su(2)$ algebra for spin 1/2 , expressed in terms of fermion operators $[\, S_i^z = (c^{\dagger}_{i\uparrow} c_{i\uparrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow})/2 \;,\; S_i^+ = c^{\dagger}_{i\uparrow} c_{i\downarrow} \;,\; S_i^- = c^{\dagger}_{i\downarrow} c_{i\uparrow} \,]$, demonstrate that the Hamiltonian in Eq. (1) can be rewritten as an (spin-only) antiferromagnetic Heisenberg Hamiltonian

$$H_{\text{eff}}^{(2)} = J \sum_{i,\delta} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+\delta} - \frac{1}{4} \right) , \tag{2}$$

where $\mathbf{S}_i \equiv (S_i^x, S_i^y, S_i^z)$ and $S_i^{\pm} = S_i^x \pm i S_i^y$.

Hint: Beware that at half-filling $n_{i,\uparrow} + n_{i,\downarrow}$ yields 1 when acting on an arbitrary state in the lowest Hubbard sector; similarly, $n_{i,\uparrow} n_{i,\downarrow}$ yields 0.

(3) **Holstein-Primakoff transformation** (3 Points)

As we have seen in the lecture, the Holstein-Primakoff transformation for spin-S particles is introduced as

$$S_i^z = S - b_i^\dagger b_i \,, \tag{3}$$

$$S_i^+ = (2S)^{1/2} \sqrt{1 - \frac{b_i^\dagger b_i}{2S}}\, b_i \,, \tag{4}$$

$$S_i^- = (2S)^{1/2} b_i^\dagger \sqrt{1 - \frac{b_i^\dagger b_i}{2S}} \,. \tag{5}$$

(a) Demonstrate explicitly that the operators S_i^z, S_i^+, and S_i^- defined above form an $su(2)$ algebra for an arbitrary value of S. In other words, show that they satisfy the commutation relations

$$[S_i^z, S_i^\pm] = \pm\, S_i^\pm \quad , \quad [S_i^+, S_i^-] = 2\, S_i^z \,.$$

(b) The square root in the above transformation can be expanded as

$$\sqrt{1 - \frac{b_i^\dagger b_i}{2S}} = \alpha + \beta\, b_i^\dagger b_i + \gamma\, (b_i^\dagger b_i)^2 + \ldots \,. \tag{6}$$

Determine the coefficients in this expansion for both $S = 1/2$ and $S = 1$.

(c) For $S = 1/2$, express the Heisenberg Hamiltonian in terms of Holstein-Primakoff bosons, up to and including the (quartic) boson interaction terms.