In condensed matter theory one often considers the simplest interacting lattice model, namely the Hubbard model [1, 2]

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \tag{1}$$

where $c^\dagger_{i,\sigma}$ creates a particle in a Wannier state [3][1] $\phi_i(\mathbf{r})$ at site i with spin $\sigma \in \{\uparrow,\downarrow\}$, $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$ is the particle number operator at site i and $\langle i,j\rangle$ denotes the sum over nearest neighbors. t and U are parameters describing hopping and on-site interaction, respectively.

Task 8.1 Towards the Hubbard Hamiltonian

a) Derive the Hubbard Hamiltonian (1) from

$$\begin{aligned} H &= \sum_\sigma \left[\int d^3\mathbf{r}\, \psi^\dagger_\sigma(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) \right) \psi_\sigma(\mathbf{r}) \right] + \\ &\quad \sum_{\sigma,\sigma'} \left[\iint d^3\mathbf{r} d^3\mathbf{r}' \psi^\dagger_\sigma(\mathbf{r}) \psi^\dagger_{\sigma'}(\mathbf{r}') U_{\sigma,\sigma'}(\mathbf{r}-\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_\sigma(\mathbf{r}) \right], \end{aligned} \tag{2}$$

where $V(\mathbf{r})$ is a periodic potential and $U_{\sigma,\sigma'}(\mathbf{r}-\mathbf{r}')$ describes a two-body interaction. What assumptions are required?

b) Diagonalize the Hamiltonian (1) for $U = 0$.

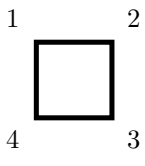
c) What is the effect of longer range hopping on the free dispersion?

Task 8.2 Low-energy effective Hamiltonian at half filling

The Hubbard model is not exactly solvable. But for dominating $U \gg t$ and half filling ($\mu = U/2$) one can start from $t = 0$. Find an effective Hamiltonian for low lying excitations and write it as a spin Hamiltonian.

Task 8.3 Four-site problem: Heisenberg

This task is motivated by the rich physics of benzene [4, 5]. Having six atoms in a ring structure this molecule is too complicated to be treated in a QMII exercise. The same basic features, however, are observed in a four-site model. For small t/U the effective Hamiltonian from Task 8.2 should capture the essential low energy physics.



a) Solve

$$H = J \sum_{i=1}^{4} \mathbf{S}_i \cdot \mathbf{S}_{(i+1) \bmod 4} - J = J\, \mathbf{T}_\diagdown \cdot \mathbf{T}_\diagup - J, \tag{3}$$

where $\mathbf{T}_\diagdown = \mathbf{S}_1 + \mathbf{S}_3$ and $\mathbf{T}_\diagup = \mathbf{S}_2 + \mathbf{S}_4$.

b) Compare the energies of two singlets on $1-2$ and $3-4$ with the ground state. Why is the ground state called resonating valence bond (RVB)? The RVB state is not only relevant for benzene but is also an actively discussed phenomenon in various lattice models [6, 7, 8]

[1] References that are of particular technical interest for solving the exercise are marked with a star.

Task 8.4 Four-site problem: Hubbard

The four-site Hubbard model is considerably harder to solve then the Heisenberg model of Task 8.3. The Hilbert space is $4^4 = 256$-dimensional. A careful discussion of the model's symmetries is needed in order to find the Eigenenergies and Eigenstates analytically.

a) Read the paper by Noce and Cuoco [9] and find the lowest 3 energies corresponding to the states that should be described by Task 8.3.

b) Plot the lowest three energies versus t/U and and compare with Task 8.3.

References

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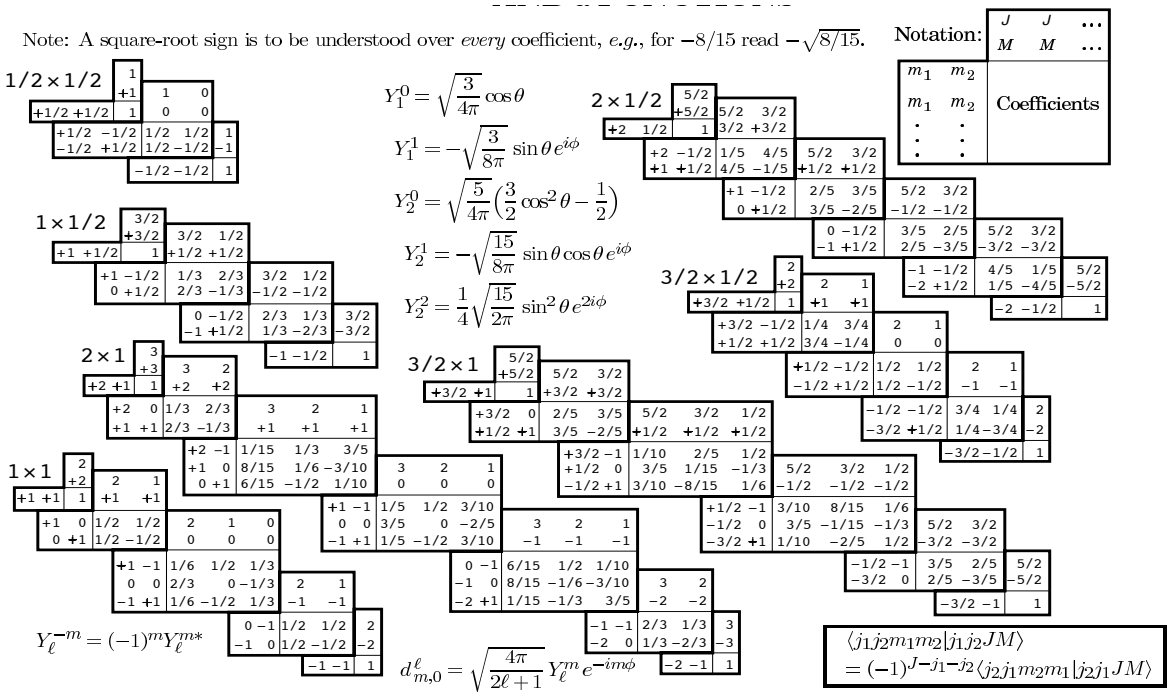

Figure 1: Clebsch-Gordon coefficient for Task 8.3.

S.H.