University of California at San Diego – Department of Physics – TA: Shauna Kravec

# Quantum Mechanics B (Physics 212B) Winter 2019
# Worksheet 6 – Solutions

## Problems

This shows the origin of effective Hamiltonians for magnetism from perturbation theory.

1. **A Pair of Spinful Fermions**

   Consider a pair of fermions with "spin", a label on the electron creation operators $\sigma = \{\uparrow, \downarrow\}$. Let $i = \{1, 2\}$ be the site label.

   The fermionic algebra in this case is $\{c_{i\sigma}, c^\dagger_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$

   (a) Compute the dimension of the Hilbert space and write explicitly a representation for the different states such as $|\uparrow\downarrow, 0\rangle = c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}|0, 0\rangle$

   There are $2^4 = 16$ states written, in order of total fermion number, as:
   $|0, 0\rangle$
   $|\uparrow, 0\rangle, |0, \uparrow\rangle, |\downarrow, 0\rangle, |0, \downarrow\rangle$
   $|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle, |\uparrow, \uparrow\rangle, |\downarrow, \downarrow\rangle$
   $|\uparrow\downarrow, \uparrow\rangle, |\uparrow\downarrow, \downarrow\rangle, |\uparrow, \uparrow\downarrow\rangle, |\downarrow, \uparrow\downarrow\rangle$
   $|\uparrow\downarrow, \uparrow\downarrow\rangle$

   (b) Give operator expressions for the different fermion number operators.

   $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$ which then by summing over $i$, $\sigma$, or both you compute the total fermion number of the associated type.

   (c) The operator $c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}$ has the interpretation of allowing "hopping" of a spin between sites. Justify this interpretation.

   The individual terms create a particle of spin $\sigma$ on a site while simultaneously removing a particle of the same spin from the neighbor site.

   (d) The operator $c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{i\sigma'}c_{j\sigma}$ has the interpretation of an "interaction". Justify this interpretation. What symmetry does it respect?

   It involves a complicated process by which particles are moved between sites and allowed to switch spin label. It is also not quadratic in the fermion operators, meaning that a generic Hamiltonian involving terms like this won't necessarily be solvable. This operator still conserves particle number.

   (e) Define the operator $\vec{S}_i = \frac{1}{2}\sum_{\sigma\sigma'} c^\dagger_{i\sigma}\vec{\sigma}_{\sigma\sigma'}c_{i\sigma'}$ as the "spin operator" at a site $i$. Suppose we're in the sector of the Hilbert space with a single fermion at site $i$. Show that the $su(2)$ algebra is satisfied.

We must show $[S_i^\alpha, S_i^\beta] = \mathbf{i}\epsilon^{\alpha\beta\gamma} S_i^\gamma$ where the greek letters refer to different components. For simplicity, let's suppress the site label $i$.

As a matrix multiplication, we can write $S^\alpha = \begin{pmatrix} c_\uparrow^\dagger, c_\downarrow^\dagger \end{pmatrix} \frac{1}{2}\sigma^\alpha \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$

Then $S^\alpha S^\beta = \begin{pmatrix} c_\uparrow^\dagger, c_\downarrow^\dagger \end{pmatrix} \frac{1}{2}\sigma^\alpha \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} \begin{pmatrix} c_\uparrow^\dagger, c_\downarrow^\dagger \end{pmatrix} \frac{1}{2}\sigma^\beta \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \begin{pmatrix} c_\uparrow^\dagger, c_\downarrow^\dagger \end{pmatrix} \frac{1}{2}\sigma^\alpha (2-n_i) \frac{1}{2}\sigma^\beta \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$

where $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$

By assumption $n_i = 1$ so $(2 - n_i) = 1$. This lets us write the commutator as:

$[S^\alpha, S^\beta] = \begin{pmatrix} c_\uparrow^\dagger, c_\downarrow^\dagger \end{pmatrix} [\frac{1}{2}\sigma^\alpha, \frac{1}{2}\sigma^\beta] \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \mathbf{i}\epsilon^{\alpha\beta\gamma} \begin{pmatrix} c_\uparrow^\dagger, c_\downarrow^\dagger \end{pmatrix} \frac{1}{2}\sigma^\gamma \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \mathbf{i}\epsilon^{\alpha\beta\gamma} S^\gamma$

2. **Direct Exchange**

   Consider the Hamiltonian for the two electrons:

$$H = -t \sum_\sigma (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + V \sum_{\sigma\sigma'} c_{1\sigma}^\dagger c_{2\sigma'}^\dagger c_{1\sigma'} c_{2\sigma} \tag{1}$$

   where $t \gg V$ such that the interaction can be treated as a perturbation.

   Consider the space of states with a single electron per site. Show that to first order in perturbation theory, the effective interaction Hamiltonian is given by:

$$H_{eff} = -2V \vec{S}_1 \cdot \vec{S}_2 + \text{const} \tag{2}$$

   The unperturbed degenerate states are $\{|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$

   First order perturbation theory dictates that $H_{eff}$ is just determined by $\langle H_{int}\rangle$ in these states. Since they satisfy that $n_i = 1$ for each $i$, we can use facts about the spin vector $\vec{S}_i$ defined above.

   $c_{1\sigma}^\dagger c_{2\sigma'}^\dagger c_{1\sigma'} c_{2\sigma} = -c_{1\sigma}^\dagger c_{1\sigma'} c_{2\sigma'}^\dagger c_{2\sigma}$ by anti-commutator

   The significant piece of algebra is the following:

   $\sum_{\sigma\sigma'} a_{i\sigma}^\dagger a_{i\sigma'} a_{j\sigma'}^\dagger a_{j\sigma} = \frac{1}{2} n_i n_j + 2S_i^z S_j^z + S_i^+ S_j^- + S_i^- S_j^+ = \frac{1}{2} n_i n_j + 2\vec{S}_i \cdot \vec{S}_j$

   Since $\langle n_i n_j\rangle = 1$ in the degenerate manifold, this completes the argument.

3. **Super-Exchange**

   Consider the following Hamiltonian:

$$H = -t \sum_\sigma (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \equiv T + V \tag{3}$$

   (a) Write the 4 basis states with $N = 2$ total electrons and $S_{tot}^z = 0$

   $\{|\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle\}$

(b) Write down $H$ as a matrix in this subspace. Be careful with the minus signs!

Consider $|\uparrow\downarrow, 0\rangle = c^\dagger_{1\uparrow} c^\dagger_{1\downarrow}|0,0\rangle$. We expand the action of $T$ on this state and use the fermionic algebra, keeping track of the signs:

$T|\uparrow\downarrow, 0\rangle = -t(\sum_\sigma c^\dagger_{2\sigma} c_{1\sigma}) c^\dagger_{1\uparrow} c^\dagger_{1\downarrow}|0,0\rangle = -t(-|\downarrow,\uparrow\rangle + |\uparrow,\downarrow\rangle)$

Therefore: $H = \begin{pmatrix} U & 0 & t & -t \\ 0 & U & -t & t \\ t & -t & 0 & 0 \\ -t & t & 0 & 0 \end{pmatrix}$

(c) Consider the limit of $U \gg t$ such that the kinetic piece can be treated as a perturbation. Show that the effective Hamiltonian is given by:

$$H = 4\frac{t^2}{U}\vec{S}_1 \cdot \vec{S}_2 + \text{const} \tag{4}$$

The degenerate ground-states are $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$

First order perturbation theory is trivial as $\langle T\rangle$ will always vanish as it takes you out of the degenerate manifold.

Second order degenerate perturbation theory gives the following expression for the effective Hamiltonian:

$H_{eff} = P\sum_k \frac{T|k\rangle\langle k|T}{E_0 - E_k} P$ where $k$ runs over states outside the degenerate manifold and $P$ is the projector into the degenerate manifold.

$E_0 = 0$ as there are no double occupancies in the degenerate manifold: e.g. $n_{i\uparrow} n_{i\downarrow}|\uparrow,\downarrow\rangle = 0$ . Similarly $E_k = U$. This is what gives the $H_{eff} \sim \frac{t^2}{U}$

As we saw above, there's an overlap $\langle\uparrow\downarrow, 0|T|\uparrow,\downarrow\rangle = -t$ and similar, determined by the matrix above.

From here one could proceed to count and compute matrix elements to build up $H_{eff}$. Alternatively we can compute the effective Hamiltonian by "integrating out" the high energy states.

Looking at the $4 \times 4$ model above it is block diagonal as $H = \begin{pmatrix} H_{high} & T \\ T & H_{low} \end{pmatrix}$ where $H_{low}$ describes the degenerate states of interest.

One can define the "resolvent" $G(\epsilon) = (\epsilon - H)^{-1} = [\epsilon - (H_{low} + T(\epsilon - H_{high})^{-1}T)]^{-1}$

Where in the last step we've formally computed the inverse of the "2 x 2" Hamiltonian with matrix elements.

Notice this looks like the resolvent of a 2x2 Hamiltonian on the low-energy Hilbert space with $H_{eff}(\epsilon) = T(\epsilon - H_{high})^{-1}T$ where we should set $\epsilon$ at the energies typical of these states.

In our case $\epsilon = 0$ and we can compute:

$H_{eff} = \begin{pmatrix} t & -t \\ -t & t \end{pmatrix} \cdot \begin{pmatrix} -\frac{1}{U} & 0 \\ 0 & -\frac{1}{U} \end{pmatrix} \cdot \begin{pmatrix} t & -t \\ -t & t \end{pmatrix} = -\frac{2t^2}{U}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$

This is exactly the middle block of $\vec{S}_1 \cdot \vec{S}_2$ ; recall we dropped the states $|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$

It's eigenvalues are $E_0 = -\frac{4t^2}{U}$ corresponding to the singlet state and $E_1 = 0$ corresponding to the $m = 0$ triplet state.