Physics 503 Problem Set 1 Solutions

The Hamiltonian could be written in the following form

$$H = \sum_\sigma (c^\dagger_{1\sigma}\ c^\dagger_{2\sigma}) \begin{pmatrix} \epsilon_1 & -t \\ -t & \epsilon_2 \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \end{pmatrix} \tag{1}$$

We could simply diagonalized this Hamiltonian. In terms of transformed operators the Hamiltonian will be

$$H = \sum_\sigma E_+ e^\dagger_{+\sigma} e_{+\sigma} + E_- e^\dagger_{-\sigma} e_{-\sigma} \tag{2}$$

Where, by assuming that $\epsilon_1 = \epsilon - \Delta$ and $\epsilon_2 = \epsilon + \Delta$ we have

$$E_\pm = \epsilon \pm \sqrt{\Delta^2 + t^2} \tag{3}$$

and $e_{\pm,\sigma} = \alpha_1^\pm c_{1,\sigma} + \alpha_2^\pm c_{2,\sigma}$ with $\alpha_i^\pm$ is given by

$$\begin{aligned} \alpha_1^- &= \frac{\sqrt{1 + \frac{\Delta}{\sqrt{\Delta^2+t^2}}}}{\sqrt{2}} & \alpha_2^- &= \frac{\sqrt{1 - \frac{\Delta}{\sqrt{\Delta^2+t^2}}}}{\sqrt{2}} \\ \alpha_1^+ &= -\frac{\sqrt{1 - \frac{\Delta}{\sqrt{\Delta^2+t^2}}}}{\sqrt{2}} & \alpha_2^+ &= \frac{\sqrt{1 + \frac{\Delta}{\sqrt{\Delta^2+t^2}}}}{\sqrt{2}} \end{aligned} \tag{4}$$

In terms of the transformed operators the two-particle eigenstates are given by

$$\begin{aligned} |-,-,\uparrow,\downarrow> = |\text{Ground}> &= e^\dagger_{-,\uparrow} e^\dagger_{-,\downarrow}|0> & E_G &= 2E_- = 2(\epsilon - \sqrt{\Delta^2+t^2}) \\ |-,+,\sigma,\sigma'> &= e^\dagger_{-,\sigma} e^\dagger_{+,\sigma'}|0> & E_{-+} &= E_- + E_+ = 2\epsilon \\ |+,+,\uparrow,\downarrow> &= e^\dagger_{-,\uparrow} e^\dagger_{-,\downarrow}|0> & E_{++} &= 2E_- = 2(\epsilon + \sqrt{\Delta^2+t^2}) \end{aligned} \tag{5}$$

these are all the six eigenstates and eigenvalues of the Hamiltonian, for two electron system. The ground state is given by $|\text{Ground}>$ and its energy is $E_G = 2(\epsilon - \sqrt{\Delta^2+t^2})$.

1a) For $\Delta = 0$ we have $E_G = 2(\epsilon - t)$, and the eigenstate is given by $|G>= \frac{1}{2}(c_{1,\uparrow} + c_{2,\uparrow})^\dagger (c_{1,\downarrow} + c_{2,\downarrow})^\dagger |0>$.
1b) The Hamiltonian is symmetric under parity. Thus $H \to H$ as if $c_1 \longleftrightarrow c_2$, thus it means for any eigenstate of the Hamiltonian we have $< n_1 >=< n_2 >$, we also have $< n_1 > + < n_2 >= 2$, thus we have

$$< n_1 >=< n_2 >= 1 \tag{6}$$

this symmetry argument holds also at finite temperature and we have

$$< n_1 >_T =< n_2 >_T = 1 \tag{7}$$

1c) For the ground state we have $< G|H|G >= E_G$ by using the equation for Hamiltonian we have

$$\begin{aligned} < G|H|G > &= \epsilon_1 < G|n_1|G > +\epsilon_2 < G|n_2|G > -t \sum_\sigma < G|c^\dagger_{1,\sigma} c_{2,\sigma} + h.c|G > \\ &= 2\epsilon - t \sum_\sigma < G|c^\dagger_{1,\sigma} c_{2,\sigma} + h.c|G >= E_G = 2(\epsilon - t) \end{aligned} \tag{8}$$

Thus we have $\sum_\sigma < G|c^\dagger_{1,\sigma} c_{2,\sigma} + h.c|G >= 2$.

1d) By using equations (4) and (5) we have

$$\begin{aligned} <\downarrow,\uparrow,-,-|n_1|-,-,\uparrow,\downarrow> &= 2|\alpha_1^-|^2 \\ < \sigma',\sigma,-,+|n_1|-,+,\sigma,\sigma' > &= |\alpha_1^-|^2 + |\alpha_1^+|^2 = 1 \\ <\downarrow,\uparrow,+,+|n_1|+,+,\uparrow,\downarrow> &= 2|\alpha_1^+|^2 \end{aligned} \tag{9}$$

For the average number of particles at site 2, we need just to change subscript $1 \to 2$. For the Ground state we have

$$< n_1 > = 1 + \frac{\Delta}{\sqrt{\Delta^2 + t^2}}$$
$$< n_2 > = 1 - \frac{\Delta}{\sqrt{\Delta^2 + t^2}} \tag{10}$$

For very large Δ we have $< n_1 > \approx 2$ and $< n_1 > \approx 0$, which is very sensible result.
At very very large temperatures compared to ϵ and Δ, we expect that all states be equally probable and we should have $< n_1 >=< n_2 >= 1$. Let us check this result for finite temperature we have

$$< n_1 >= \frac{1}{Z} \sum < m|n_1|m > e^{-\beta E_m}$$

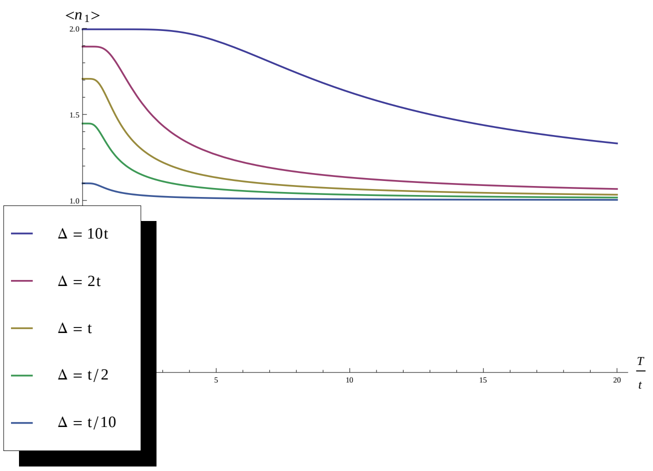
By use of (9) we have

$$\begin{aligned} < n_1 > &= \frac{1}{4 + 2\cosh 2\beta\sqrt{\Delta^2 + t^2}} \left(2|\alpha_1^-|^2 e^{2\beta\sqrt{\Delta^2+t^2}} + 2|\alpha_1^+|^2 e^{-2\beta\sqrt{\Delta^2+t^2}} + 4(|\alpha_1^-|^2 + |\alpha_1^+|^2)\right) \\ &= 1 + \frac{\Delta}{\sqrt{\Delta^2 + t^2}} \times \frac{\sinh 2\beta\sqrt{\Delta^2 + t^2}}{2 + \cosh 2\beta\sqrt{\Delta^2 + t^2}} \end{aligned} \tag{11}$$

For very large T we have , $\beta \approx 0$ and

$$< n_1 > \approx 1 \tag{12}$$

The average number $< n_1 >$ as function of temperature is depicted in following graph for different values of Δ/t



2a) The number of particles, N, parity $P = \pm$ and energies E, are given in Table 1. The energy of the vacuum state is clearly zero since it is annihilated by the hopping term ($\propto t$) and also the interaction term. The energy of the only possible 2-particle state, with one particle on each site, is simply V since no hopping is possible from this state. A basis of single particle states is $c_1^\dagger|0\rangle$ and $c_2^\dagger|0\rangle$. These are unaffected by the interaction term since $\hat{n}_2$ is zero in the first and $\hat{n}_1$ in the second. The hopping term just introduces an off-diagonal mixing of these 2 states corresponding to the matrix:

$$H = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix}. \tag{13}$$

The eigenvalues, corresponding to symmetric and anti-symmetric combinations of the basis states (i.e. wave-vector 0 or π) are $\mp t$ respectively.

N	P	E	$Eigenstate$
0	+	0	$\|0,0\rangle$
1	+	-t	$(c_1^\dagger\|0\rangle + c_2^\dagger\|0\rangle)/\sqrt{2}$
1	-	t	$(c_1^\dagger\|0\rangle - c_2^\dagger\|0\rangle)/\sqrt{2}$
2	-	V	$\|1,1\rangle$

(14)

3) We can readily solve this problem by going to momentum space for the c and d particles. This gives:

$$H = -\sum_{\vec{k}} \left[\epsilon_0(\vec{k}) c^\dagger_{\vec{k}} c_{\vec{k}} + tV(c^\dagger_{\vec{k}} d_{\vec{k}} + h.c.) \right]. \tag{15}$$

Here:

$$\epsilon_0(\vec{k}) \equiv -2t \sum_{i=1}^{3} \cos(k_i a) \tag{16}$$

the usual tight-binding dispersion relation. $h.c.$ stands for the Hermitean conjugate of the previous term. We now get a 2×2 matrix each for eacah value of $\vec{k}$:

$$H_{\vec{k}} = \begin{pmatrix} \epsilon_0(\vec{k}) & tV \\ tV & 0 \end{pmatrix}. \tag{17}$$

with the 2 energy bands:

$$\epsilon_\pm(\vec{k}) \equiv \epsilon_0(\vec{k})/2 \pm \sqrt{\epsilon_0(\vec{k})^2/4 + t^2V^2}. \tag{18}$$

Spin was not mentioned in the statement of this problem. If we include it we simply get identical bands for spins up and down.

4) We may write a spectral decomposition for the electron Green's function:

$$\mathrm{Im}G_{\mathrm{ret}}(\vec{p}, \omega) = -e^{\beta\Omega} \left(1 + e^{\beta\omega}\right) \pi \sum_{n,m} |\langle n|c_{\vec{p}}|m\rangle|^2 e^{-\beta E_m} \delta(\omega + E_n - E_m). \tag{19}$$

(This actually differs from the decomposition that I derived in class in which the factor of $e^{\beta\omega}$ was replaced by $e^{-\beta\omega}$ and the factor of $e^{-\beta E_m}$ by $e^{-\beta E_n}$. These are easily seen to be the same using $E_m = E_n + \omega$ which follows from the δ-function.) Using the δ-function again, and cancelling the $n_F(\omega)$ factors, we obtain:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} n_F(\omega) \omega^2 G_{\mathrm{ret}}(\vec{p}, \omega) = -\frac{1}{2} e^{\beta\Omega} \sum_{n,m} (E_n - E_m)^2 |\langle n|c_{\vec{p}}|m\rangle|^2 e^{-\beta E_m}. \tag{20}$$

Now observing that:

$$(E_n - E_m)\langle n|c_{\vec{p}}|m\rangle = \langle n|[H, c_{\vec{p}}]|m\rangle \tag{21}$$

we may rewrite this as:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} n_F(\omega) \omega^2 G_{\mathrm{ret}}(\vec{p}, \omega) = \frac{1}{2} e^{\beta\Omega} \sum_{n,m} \langle m|[H, c^\dagger_{\vec{p}}]|n\rangle \langle n|[H, c_{\vec{p}}]|m\rangle e^{-\beta E_m}. \tag{22}$$

Note that I switched the order of the two matrix elements in order to make it clear that there is a sum over a complete set of states here:

$$\sum_n |n\rangle\langle n| = I \tag{23}$$

which may be dropped, leaving:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} n_F(\omega) \omega^2 G_{\mathrm{ret}}(\vec{p}, \omega) = \frac{1}{2} e^{\beta\Omega} \sum_m \langle m|[H, c^\dagger_{\vec{p}}][H, c_{\vec{p}}]|m\rangle e^{-\beta E_m}. \tag{24}$$

Finally we recognize this as the Boltzmann average of the product of commutators:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} n_F(\omega) \omega^2 G_{\mathrm{ret}}(\vec{p}, \omega) = \frac{1}{2} \langle |[H, c^\dagger_{\vec{p}}][H, c_{\vec{p}}]| \rangle. \tag{25}$$