Physics 503, Problem Set 2 Solutions

1a) By Taylor expanding the exponent to second order and using:

$$\int d\psi_1 d\psi_2 d\psi_3 d\psi_4 \psi_4 \psi_3 \psi_2 \psi_1 = 1 \tag{1}$$

and the anti-commutation property of Grassmann variables we see that:

$$P(M) \equiv \int d\psi_1 d\psi_2 d\psi_3 d\psi_4 \psi_4 \exp\left[\frac{1}{2}\sum_{i,j=1}^{4} \psi_i M_{ij} \psi_j\right] = M_{12}M_{34} + M_{14}M_{23} - M_{13}M_{24} \tag{2}$$

The plus or minus sign in each term is determined by the parity of permutation of the indices, i.e. by whether an even or odd number of permutations is needed to get them in the order 1234 which is equivalent to 4321.
b) The full matrix M can be written:

$$M = \begin{pmatrix} 0 & M_{12} & M_{13} & M_{14} \\ -M_{12} & 0 & M_{23} & M_{24} \\ -M_{13} & -M_{23} & 0 & M_{34} \\ -M_{14} & -M_{24} & -M_{34} & 0 \end{pmatrix}. \tag{3}$$

The determinant can be written:

$$\begin{aligned}
\mathrm{Det}M &= -M_{12}\cdot \mathrm{Det}\begin{pmatrix} -M_{12} & M_{23} & M_{24} \\ -M_{13} & 0 & M_{34} \\ -M_{14} & -M_{34} & 0 \end{pmatrix} + M_{13}\cdot \mathrm{Det}\begin{pmatrix} -M_{12} & 0 & M_{24} \\ -M_{13} & -M_{23} & M_{34} \\ -M_{14} & -M_{24} & 0 \end{pmatrix} - M_{14}\cdot \mathrm{Det}\begin{pmatrix} -M_{12} & 0 & M_{23} \\ -M_{13} & -M_{23} & 0 \\ -M_{14} & -M_{24} & -M_{34} \end{pmatrix} \\
&= M_{12}(M_{12}M_{34}^2 + M_{23}M_{34}M_{14} - M_{24}M_{13}M_{34}) + M_{13}(-M_{12}M_{34}M_{24} + M_{24}^2 M_{13} - M_{24}M_{23}M_{14}) \\
&\quad + M_{14}(M_{12}M_{23}M_{34} - M_{23}M_{13}M_{24} + M_{23}^2 M_{14}) \\
&= (M_{12}M_{34})^2 + (M_{13}M_{24})^2 + (M_{14}M_{23})^2 + 2(M_{12}M_{34})(M_{23}M_{14}) - 2(M_{12}M_{34})(M_{13}M_{24}) - 2(M_{23}M_{14})(M_{13}M_{24}) \\
&= (M_{12}M_{34} + M_{14}M_{23} - M_{13}M_{24})^2.
\end{aligned} \tag{4}$$

In the case of an integral over $2n$ Grassmann variables with a general $2n \times 2n$ anti-symmetric matrix M, it can be seen that:

$$\int \prod_{i=1}^{2n} d\psi_i \exp\left[\frac{1}{2}\sum_{i,j=1}^{2n} \psi_i M_{ij} \psi_j\right] = \sum_{\{i_1,i_2,\dots i_{2n}\}} \mathrm{sgn}(\{i_1, i_2, \dots i_{2n}\})(M_{i_1 i_2} M_{i_3 i_4} \dots M_{1_{2n-1} i_{2n}} \tag{5}$$

where $\{i_1, i_2, \dots i_{2n}\}$ denotes an arbitrary permutation of the indices $1, 2, 3, \dots 2n$ and $\mathrm{sgn}(\{i_1, i_2, \dots i_{2n}\})$ denotes the sign of the permutation. A sum over all permutations is taken. The function of M on the right hand side of Eq. (5) is known as the Pfaffian of the matrix M, Pf (M). It can be proven in general that:

$$(\mathrm{Pf}\ M)^2 = \mathrm{Det}\ M. \tag{6}$$

2a) First Method: The imaginary part of the green function is

$$\mathrm{Im}G^a_{ret}(\omega, \vec{q}) = -e^{\beta\Omega}\pi \sum_{n,m}(1 + e^{\beta\omega})e^{-\beta E_m}| < n|S^a_{\vec{q}}|m > |^2 \tag{7}$$

Thus we have

$$\int \frac{d\omega}{2\pi}\omega \mathrm{Im}G^a_{ret}(\omega, \vec{q}) = -\frac{e^{\beta\Omega}}{2}\sum_{m,n}(e^{-\beta E_m} + e^{-\beta E_n})(E_m - E_n) < n|S^a_{\vec{q}}|m >< m|S^a_{-\vec{q}}|n > \tag{8}$$

By using the identity

$$(E_m - E_n) < n|S^a_{\vec{q}}|m >< m|S^a_{-\vec{q}}|n > = < n|S^a_{\vec{q}}H|m >< m|S^a_{-\vec{q}}|n > - < n|HS^q_{\vec{q}}|m >< m|S^a_{-\vec{q}}|n > \tag{9}$$

We have

$$\begin{aligned}
\int \frac{d\omega}{2\pi}\omega \mathrm{Im}G^a_{ret}(\omega, \vec{q}) &= -\frac{1}{2}\left[(< S^a_{\vec{q}}HS^a_{-\vec{q}} > + < S^a_{-\vec{q}}S^a_{\vec{q}}H >) - (< HS^a_{\vec{q}}S^a_{-\vec{q}} > + < S^a_{-\vec{q}}HS^a_{\vec{q}} >)\right] \\
&= \frac{1}{2}\langle [[H, S^a_{\vec{q}}], S^a_{-\vec{q}}] \rangle
\end{aligned} \tag{10}$$

Thus $c = 1/2$.

Second Method:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\omega, \vec{q}) = -i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega \int_0^{\infty} dt e^{i\omega t} \langle [S^a_{\vec{q}}(t), S^a_{-\vec{q}}] \rangle = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_0^{\infty} dt \left(\frac{d}{dt} e^{i\omega t} \right) \langle [S^a_{\vec{q}}(t), S^a_{-\vec{q}}] \rangle. \tag{11}$$

Now we integrate by parts inside the t-integral:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\omega, \vec{q}) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_0^{\infty} dt e^{i\omega t} \langle \left[\frac{d}{dt} S^a_{\vec{q}}(t), S^a_{-\vec{q}} \right] \rangle. \tag{12}$$

Using $S^a_{\vec{q}}(t) = e^{iHt} S^a_{\vec{q}} e^{-iHt}$, we can write:

$$\frac{d}{dt} S^a_{\vec{q}}(t) = i e^{iHt} [H, S^a_{\vec{q}}] e^{-iHt}. \tag{13}$$

We also change the order of the ω and t integral to write:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\omega, \vec{q}) = i \int_0^{\infty} dt \langle \left[e^{iHt} [H, S^a_{\vec{q}}] e^{-iHt}, S^a_{-\vec{q}} \right] \rangle \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega t} \tag{14}$$

The ω integral gives a Dirac δ-function, $\delta(t)$. Assuming that:

$$\int_0^{\infty} dt f(t) \delta(t) = (1/2) f(0) \tag{15}$$

we obtain:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\omega, \vec{q}) = (i/2) \langle \left[[H, S^a_{\vec{q}}], S^a_{-\vec{q}} \right] \rangle \tag{16}$$

the desired result with $c = 1/2$ since Eq. 5 of PS2 is the sum rule for ImG. Note that we have also obtained a sum rule for the real part.

b)

$$[H, S^z_{\vec{R}}] = 2J \sum_{\vec{\delta}} [\vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}+\vec{\delta}}, S^z_{\vec{R}}]. \tag{17}$$

Here we have used the fact that the only terms in H which don't commute with $S^z_{\vec{R}}$ are the ones on nearest neighbour links with one end at $\vec{R}$. The way we have written the Hamiltonian, each link appears twice, giving the factor of 2. Considering separately the two terms $S^x_{\vec{R}} S^x_{\vec{R}+\vec{\delta}}$ and $S^y_{\vec{R}} S^y_{\vec{R}+\vec{\delta}}$ in Eq. (17) we find:

$$[H, S^z_{\vec{R}}] = -2Ji \sum_{\vec{\delta}} (S^x_{\vec{R}} S^y_{\vec{R}+\vec{\delta}} - S^y_{\vec{R}} S^x_{\vec{R}+\vec{\delta}}) \tag{18}$$

Now consider the double commutator $\left[[H, S^z_{\vec{R}}], S^z_{\vec{0}} \right]$. From Eq. (18), we see that this vanishes unless either $\vec{R} = \vec{0}$ or $\vec{R} + \vec{\delta} = \vec{0}$. Thus we may write:

$$\left[[H, S^z_{\vec{R}}], S^z_{\vec{0}} \right] = \delta_{\vec{R},\vec{0}} \cdot 2iJ \sum_{\vec{\delta}} [S^x_{\vec{0}} S^y_{\vec{\delta}} - S^y_{\vec{0}} S^x_{\vec{\delta}}, S^z_{\vec{0}}] + 2iJ \sum_{\vec{\delta}} \delta_{\vec{R}+\vec{\delta},\vec{0}} [S^x_{-\vec{\delta}} S^y_{\vec{0}} - S^y_{-\vec{\delta}} S^x_{\vec{0}}, S^z_{\vec{0}}] \tag{19}$$

Calculating the commutators gives:

$$\left[[H, S^z_{\vec{R}}], S^z_{\vec{0}} \right] = 2\delta_{\vec{R},\vec{0}} J \sum_{\vec{\delta}} (S^x_{\vec{0}} S^x_{\vec{\delta}} + S^y_{\vec{0}} S^y_{\vec{\delta}}) - 2J \sum_{\vec{\delta}} \delta_{\vec{R}+\vec{\delta},\vec{0}} (S^x_{\vec{0}} S^x_{-\vec{\delta}} + S^y_{\vec{0}} S^y_{-\vec{\delta}}) \tag{20}$$

We may invert the dummy summation vector $\vec{\delta} \to -\vec{\delta}$ in the second term to write more compactly:

$$\left[[H, S^z_{\vec{R}}], S^z_{\vec{0}} \right] = 2J \sum_{\vec{\delta}} (\delta_{\vec{R},\vec{0}} - \delta_{\vec{R},\vec{\delta}}) (S^x_{\vec{0}} S^x_{\vec{\delta}} + S^y_{\vec{0}} S^y_{\vec{\delta}}). \tag{21}$$

c) First, let us prove that $\int \omega \mathrm{Re} G^a_{ret}(\omega, q) d\omega = 0$. We have

$$\int \frac{\omega}{2\pi} \mathrm{Re} G^a_{ret}(\omega, q) d\omega = e^{\beta\Omega} \sum |<n|S^a_{\vec{q}}|m>|^2 (e^{-\beta E_n} - e^{-\beta E_m}) \int \frac{\omega}{2\pi} \mathrm{Re} \frac{d\omega}{\omega + \Delta E_{nm} + i\eta}$$
$$= e^{\beta\Omega} \sum |<n|S^a_{\vec{q}}|m>|^2 (e^{-\beta E_n} - e^{-\beta E_m}) \int \frac{\omega}{2\pi} \frac{\omega + \Delta E_{nm}}{(\omega + \Delta E_{nm})^2 + \eta^2} d\omega$$
$$= e^{\beta\Omega} \sum |<n|S^a_{\vec{q}}|m>|^2 (e^{-\beta E_n} - e^{-\beta E_m}) \int \frac{\omega}{2\pi} \frac{\omega - \Delta E_{nm}}{\omega^2 + \eta^2} d\omega$$

In going from the second line to third line we use the change of variables in integral $\omega \to \omega - \Delta E_{nm}$. From above equation we have

$$\int \frac{\omega}{2\pi} \mathrm{Re} G^a_{ret}(\omega, q) d\omega = \frac{e^{\beta\Omega}}{2\pi} \sum |<n|S^a_{\vec{q}}|m>|^2 (e^{-\beta E_n} - e^{-\beta E_m}) \int_{-\infty}^{\infty} \left[1 - \frac{\omega\, \Delta E_{n,m}}{\omega^2 + \eta^2} - \frac{\eta^2}{\omega^2 + \eta^2}\right] d\omega \tag{22}$$

In this equation, the second term is zero because its an integration of odd function. The third term is zero in the limit of $\eta \to 0$, because it is equal to $\eta\, \pi$. Finally it remains to prove that the first term is zero too, this is not the consequence of the integration but is the result of summation over m, n, it is easy to see that

$$e^{\beta\Omega} \sum |<n|S^a_{\vec{q}}|m>|^2 (e^{-\beta E_n} - e^{-\beta E_m}) = \langle [S^a_{\vec{q}}, S^a_{-q}] \rangle = 0$$

To proceed with proving the sum rule it is convenient to undo the Fourier transform and rewrite the result in part a) as:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\vec{R}, \omega) = (i/2) \langle \Big[[H, S^a_{\vec{R}}], S^a_{\vec{0}} \Big] \rangle. \tag{23}$$

We now Fourier transform back and use the result of part b) to write:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\vec{q}, \omega) = J \sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\vec{R}, \omega) = iJ \sum_{\vec{\delta}} \left[1 - e^{i\vec{q}\cdot\vec{\delta}}\right] \langle S^x_{\vec{0}} S^x_{\vec{\delta}} + S^y_{\vec{0}} S^y_{\vec{\delta}} \rangle. \tag{24}$$

(Here the Kroenecker δ-functions in Eq. (21) were used to do the sum over $\vec{R}$, leaving only the sum over $\vec{\delta}$.) Now let's compare $J\langle S^x_{\vec{0}} S^x_{\vec{\delta}} + S^y_{\vec{0}} S^y_{\vec{\delta}} \rangle$ to $\langle H \rangle$. Due to the various symmetries of the equilibrium state, $\langle H \rangle$ actually consists of $3 \cdot 4 \cdot N$ equal terms, taking into account the 3 terms in the scalar product $\vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{R}+\vec{\delta}}$, the 4 terms in the sum over $\vec{\delta}$ and the N terms in the sum over $\vec{R}$. On the other hand, only 2 of these equal terms occur in Eq. (24). Thus we may write:

$$J\langle S^x_{\vec{0}} S^x_{\vec{\delta}} + S^y_{\vec{0}} S^y_{\vec{\delta}} \rangle = \langle H \rangle / (6N). \tag{25}$$

Thus:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\vec{q}, \omega) = i \sum_{\vec{\delta}} \left[1 - e^{i\vec{q}\cdot\vec{\delta}}\right] \langle H \rangle / (6N). \tag{26}$$

The sum over $\vec{\delta}$ is now straightforward and gives, for a square lattice of spacing a:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega G^a_{ret}(\vec{q}, \omega) = i[2 - \cos(q_x a) - \cos(q_y a)] \langle H \rangle / (3N). \tag{27}$$

Thus the function $f(\vec{q})$ is:

$$f(\vec{q}) = [2 - \cos(q_x a) - \cos(q_y a)] / (3N). \tag{28}$$

(The sum rule for the real part vanishes.) Also note that $\langle H \rangle < 0$ for the Heisenberg model so this integral is generally < 0, as expected. This sum rule provides a very useful check on approximate numerical calculations of the spectral function and also on neutron scattering measurements which will not cover the full range of frequencies.

3a) For $S_I[\theta_{cl}+\theta_{qu}]$ we have

$$S_I[\theta_{cl}+\theta_{qu}] = S_I[\theta_{cl}] + S_I[\theta_{qu}] - I\int_0^\beta d\tau \frac{d\theta_{cl}}{d\tau}\frac{d\theta_{qu}}{d\tau}$$

We only need to show that the last term is zero, by using integration by parts we have

$$\int_0^\beta d\tau \frac{d\theta_{cl}}{d\tau}\frac{d\theta_{qu}}{d\tau} = \left[\frac{d\theta_{cl}}{d\tau}\theta_{qu}\right]_0^\beta - \int_0^\beta d\tau \frac{d^2\theta_{cl}}{d\tau^2}\theta_{qu}$$

In above equation, the first term is zero because of boundary conditions on quantum fluctuation θ_{qu}. The second term is zero, because θ_{cl} by definition satisfies classical equation of motion.
3b) By using boundary conditions Eq. (12), we see that for any integer n we have a classical solution $\theta_{cl}^{(n)}$, which satisfies the boundary conditions $\theta_{cl}^{(n)}(0)=\theta_i$ and $\theta_{cl}^{(n)}(\beta)=\theta_f+2\pi n$ thus we have

$$\begin{aligned}\int d[\theta]e^{S_I[\theta]} &= \sum_n \int d[\theta_{qu}]e^{S_I[\theta_{cl}^{(n)}+\theta_{qu}]} = \sum_n \int d[\theta_{qu}]e^{S_I[\theta_{cl}^{(n)}]+S_I[\theta_{qu}]} \\ &= \sum_n e^{S_I[\theta_{cl}^{(n)}]}\int d[\theta_{qu}]e^{S_I[\theta_{qu}]} = C\sum_n e^{S_I[\theta_{cl}^{(n)}]}\end{aligned} \tag{29}$$

Where $C=\int d[\theta_{qu}]e^{S_I[\theta_{qu}]}$, and it is independent of $\theta_{i,f}$.
3c) By using classical equation of motion we have $d^2\theta_{cl}/d\tau^2=0$, by solving this equation we get

$$\theta_{cl}^{(n)}(\tau) = A_n\tau + B_n \tag{30}$$

And by imposing the boundary conditions we get $B_n=\theta_i$, $A_n=(2\pi n+\theta_f-\theta_i)/\beta$. Thus for classical action we have

$$S_I[\theta_{cl}^{(n)}] = \frac{-I}{2}\int_0^\beta d\tau (A_n)^2 = \frac{-I}{2\beta}(2\pi n+\theta_f-\theta_i)^2 \tag{31}$$

And for the correlation we have

$$<\theta_f|e^{-\beta H}|\theta_i> = C\sum_n e^{\frac{-I}{2\beta}(2\pi n+\theta_f-\theta_i)^2} \tag{32}$$

By using Poisson sum formula we have

$$\sum_n e^{\frac{-I}{2\beta}(2\pi n+\theta_f-\theta_i)^2} = \sum_m \int_{-\infty}^{\infty} e^{\frac{-I}{2\beta}(2\pi x+\theta_f-\theta_i)^2} e^{-2i\pi m x}dx \tag{33}$$

The integral is a straightforward integration and we have

$$\int_{-\infty}^{\infty} e^{\frac{-I}{2\beta}(2\pi x+\theta_f-\theta_i)^2} e^{-2i\pi m x}dx = \sqrt{\frac{4\pi\beta}{I}}e^{-\beta\frac{m^2}{2I}+im(\theta_f-\theta_i)}$$

For the correlation we get

$$<\theta_f|e^{-\beta H}|\theta_i> = C\sum_n e^{\frac{-I}{2\beta}(2\pi n+\theta_f-\theta_i)^2} = \sqrt{\frac{4\pi\beta}{I}}C\sum_m e^{-\beta\frac{m^2}{2I}+im(\theta_f-\theta_i)} \tag{34}$$

the last term is exactly $\sum_m \psi_m^*(\theta_f)\psi_m(\theta_i)e^{-\beta E_m}$.

4a) Consider the sum over S_{2i+1} for some arbitrary site in the chain (not at the edge). This gives:

$$\sum_{S_{2i+1}=\pm 1} \exp[(2J/T)S_{2i+1}(S_{2i}+S_{2i+2})] = 2\cosh[(2J/T)(S_{2i}+S_{2i+2})]. \tag{35}$$

We would like to write this in the form:

$$2\cosh[(2J/T)(S_{2i}+S_{2i+2})] = c\exp[(2J_{eff}/T)S_{2i}S_{2i+2}] \tag{36}$$

for some effective coupling J_{eff}. Noting that the left hand side equals 2 when S_{2i} and S_{2i+2} are anti-parallel and $2\cosh(4J/T)$ when they are parallel, we see that:

$$J_{eff} = (T/4)\ln[\cosh(4J/T)]. \tag{37}$$

b) For the square lattice case, summing over the spin at site $\vec{0}$ gives

$$2\cosh[(2J/T)(S_1+S_2+S_3+S_4)] \tag{38}$$

where the S_i are the 4 nearest neighbour spins at δ. (The factor of 2 occurs here because each link appears twice in the sum defining the Hamiltonian.) Noting that this as the values 2 when 2 spins are up and 2 are down, $2\cosh(4J/T)$ when one points oppositely to the other 3 and $2\cosh(8J/T)$ when they all point the same direction we can write the effective Hamiltonian in the desired form. Noting that this function is completely symmetric under interchanging the 4 spins we should be able to write:

$$2\cosh[(2J/T)(S_1+S_2+S_3+S_4)] = C\exp[\alpha(S_1+S_2+S_3+S_4)^2 + \delta S_1S_2S_3S_4] \tag{39}$$

for 3 constants, C, α and δ. The 3 cases give the 3 equations in 3 unknowns:

$$2 = ce^{\delta} \tag{40}$$
$$2\cosh(4J/T) = ce^{4\alpha-\delta} \tag{41}$$
$$2\cosh(8J/T) = ce^{16\alpha+\delta}. \tag{42}$$

These give:

$$\alpha = \frac{1}{16}\ln[\cosh(8J/T)] \tag{43}$$
$$\delta = \frac{1}{8}\ln[\cosh(8J/T)/\cosh^4(4J/T)]. \tag{44}$$

Thus from summing over the spin at $\vec{0}$ we generate first neighbour and second neighbour couplings:

$$J_1/T = J_2/T = 2\alpha \quad ?? \tag{45}$$

and a plaquette coupling:

$$J_P/T = \delta. \tag{46}$$

However, we must take into account that each first neighbour coupling gets an equal contribution from summing over the spins at 2 different sites. For instance, we develop a coupling $S_{a\hat{x}}S_{a\hat{y}}$ from summing over $S_{\vec{0}}$ and also $S_{a\hat{x}+a\hat{y}}$. On the other hand, the second neighbour and plaquette couplings arise from summing over the spin on a unique site. We must also take into account that, the way the Hamiltonian was written in the statement of the problem, each first and second neighbour link occurs twice while each plaquette occurs only once. Thus, the final answers are:

$$J_1 = \frac{T}{8}\ln[\cosh(8J/T)] \tag{47}$$
$$J_2 = \frac{T}{16}\ln[\cosh(8J/T)] \tag{48}$$
$$J_P = \frac{T}{8}\ln[\cosh(8J/T)/\cosh^4(4J/T)]. \tag{49}$$