

## Exam solution, spring 2013

### TFY4210 Quantum theory of many-particle systems

#### Problem 1

(a) Let us e.g. express the anticommutator  $\{a_1, a_1^\dagger\} = 1$  in terms of the  $c$ -operators:

$$1 = \{a_1, a_1^\dagger\} = \{uc_1 - vc_2^\dagger, uc_1^\dagger - vc_2\} = u^2\{c_1, c_1^\dagger\} - uv\{c_1, c_2\} - uv\{c_1^\dagger, c_2^\dagger\} + (-v)^2\{c_2, c_2^\dagger\} \quad (1)$$

where we also used  $\{A, B\} = \{B, A\}$  for any  $A, B$ . Now using the standard fermionic anti-commutation relations  $\{c_1, c_1^\dagger\} = \{c_2, c_2^\dagger\} = 1$  and  $\{c_1, c_2\} = \{c_1^\dagger, c_2^\dagger\} = 0$  gives  $1 = u^2 + v^2$ .

(b) Expressing the  $a$ -operators in terms of the  $c$ -operators gives

$$a_1^\dagger a_1 = (uc_1^\dagger - vc_2)(uc_1 - vc_2^\dagger) = u^2 c_1^\dagger c_1 - uv(c_1^\dagger c_2^\dagger + \text{h.c.}) - v^2 c_2^\dagger c_2 + v^2, \quad (2)$$

$$a_2^\dagger a_2 = (vc_1 + uc_2^\dagger)(vc_1^\dagger + uc_2) = -v^2 c_1^\dagger c_1 - uv(c_1^\dagger c_2^\dagger + \text{h.c.}) + u^2 c_2^\dagger c_2 + v^2, \quad (3)$$

$$a_1^\dagger a_2^\dagger = (uc_1^\dagger - vc_2)(vc_1 + uc_2^\dagger) = uv c_1^\dagger c_1 + u^2 c_1^\dagger c_2^\dagger - v^2 c_2 c_1 + uv c_2^\dagger c_2 - uv, \quad (4)$$

where we also used  $c_i c_i^\dagger = 1 - c_i^\dagger c_i$ . Thus

$$\begin{aligned} H &= [\varepsilon(u^2 - v^2) + \Delta \cdot 2uv](c_1^\dagger c_1 + c_2^\dagger c_2) \\ &+ [\Delta(u^2 - v^2) - \varepsilon \cdot 2uv](c_1^\dagger c_2^\dagger + \text{h.c.}) \\ &+ [\varepsilon \cdot 2v^2 - \Delta \cdot 2uv]. \end{aligned} \quad (5)$$

Now we pick  $u$  and  $v$  such that the coefficient of  $(c_1^\dagger c_2^\dagger + \text{h.c.})$  vanishes. Expressing  $u$  and  $v$  in terms of  $\theta$  and using the given formulas for the cosine and sine of a double angle, we find:

$$\begin{aligned} \varepsilon \cdot 2uv - \Delta(u^2 - v^2) &= 0 \\ \Rightarrow \varepsilon \sin 2\theta &= \Delta \cos 2\theta \\ \Rightarrow \tan 2\theta &= \frac{\Delta}{\varepsilon}. \end{aligned} \quad (6)$$

(c)  $H$  now takes the form

$$H = F(c_1^\dagger c_1 + c_2^\dagger c_2) + G \quad (7)$$

with

$$F = \varepsilon(u^2 - v^2) + \Delta \cdot 2uv, \quad (8)$$

$$G = \varepsilon \cdot 2v^2 - \Delta \cdot 2uv. \quad (9)$$

Using the double-angle formulas and (6) gives

$$\begin{aligned} F &= \varepsilon \cos 2\theta + \Delta \sin 2\theta = \cos 2\theta(\varepsilon + \Delta \tan 2\theta) = \cos 2\theta \left( \varepsilon + \Delta \cdot \frac{\Delta}{\varepsilon} \right) \\ &= \frac{\cos 2\theta}{\varepsilon}(\varepsilon^2 + \Delta^2). \end{aligned} \quad (10)$$

Next we use the given formula relating  $\cos^2 x$  and  $\tan^2 x$  to find

$$\cos^2 2\theta = \frac{1}{1 + \tan^2 2\theta} = \frac{1}{1 + (\Delta/\varepsilon)^2} \Rightarrow \cos 2\theta = \frac{1}{\sqrt{1 + (\Delta/\varepsilon)^2}} \quad (11)$$

where we picked the positive solution. Inserting this in (10) gives

$$F = \sqrt{\varepsilon^2 + \Delta^2}. \quad (12)$$

Next, to find  $G$  we use that

$$2v^2 = v^2 + v^2 = v^2 + (1 - u^2) = 1 - (u^2 - v^2) = 1 - \cos 2\theta. \quad (13)$$

This gives

$$\begin{aligned} G &= \varepsilon(1 - \cos 2\theta) - \Delta \sin 2\theta = \varepsilon - (\varepsilon \cos 2\theta + \Delta \sin 2\theta) \\ &= \varepsilon - F = \varepsilon - \sqrt{\varepsilon^2 + \Delta^2}. \end{aligned} \quad (14)$$

(d) We have

$$H = F(\hat{n}_1 + \hat{n}_2) + G \quad (15)$$

where  $\hat{n}_1 \equiv c_1^\dagger c_1$  and  $\hat{n}_2 \equiv c_2^\dagger c_2$  are number operators. As they commute with each other, the eigenstates of  $H$  can be labeled by  $(n_1, n_2)$  where  $n_1$  and  $n_2$  are the eigenvalues of  $\hat{n}_1$  and  $\hat{n}_2$ , respectively. As the particles are fermions these eigenvalues are limited to 0 and 1. Therefore  $H$  has 4 eigenstates, labeled as  $(n_1, n_2) = (0, 0), (1, 0), (0, 1),$  or  $(1, 1)$ .<sup>1</sup> The corresponding eigenvalue is the energy

$$E(n_1, n_2) = F(n_1 + n_2) + G, \quad (16)$$

giving

$$E(0, 0) = G, \quad (17)$$

$$E(1, 0) = F + G, \quad (18)$$

$$E(0, 1) = F + G, \quad (19)$$

$$E(1, 1) = 2F + G. \quad (20)$$

Thus there are 3 energy levels, with energies  $G$ ,  $F + G$ , and  $2F + G$ . The first and last of these are nondegenerate (i.e. degeneracy 1), while the middle one is doubly degenerate (i.e. degeneracy 2).

## **Problem 2**

(a) We have

$$H = - \sum_{\langle i, j \rangle} [J_\perp (S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z] = - \sum_{\langle i, j \rangle} \left[ \frac{J_\perp}{2} (S_i^+ S_j^- + S_i^- S_j^+) + J_z S_i^z S_j^z \right]. \quad (21)$$

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<sup>1</sup>Using Fock space notation we would write these states as  $|n_1, n_2\rangle$ , i.e.  $|0, 0\rangle, |1, 0\rangle, |0, 1\rangle,$  and  $|1, 1\rangle$ .

As only nearest-neighbour spins interact we can set  $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}$  where  $\boldsymbol{\delta}$  runs over the two unit vectors  $+\hat{\mathbf{x}}$  and  $+\hat{\mathbf{y}}$  on the square lattice ( $-\hat{\mathbf{x}}$  and  $-\hat{\mathbf{y}}$  are excluded to avoid double counting). For short we write this relation as  $j = i + \boldsymbol{\delta}$  when it appears as a subscript. This gives

$$H = - \sum_{i, \boldsymbol{\delta}} \left[ \frac{J_{\perp}}{2} (S_i^+ S_{i+\boldsymbol{\delta}}^- + S_i^- S_{i+\boldsymbol{\delta}}^+) + J_z S_i^z S_{i+\boldsymbol{\delta}}^z \right]. \quad (22)$$

As  $J_z > J_{\perp}$  in general, we expect that in the ordered state of the system, the spins will order ferromagnetically in the  $+\hat{z}$  or  $-\hat{z}$  direction. Among these two possibilities let us assume the standard one of ordering in the  $+\hat{z}$  direction, as then we can use the given Holstein-Primakoff (HP) expressions without any modifications. In the expansion of the square roots it is sufficient to only keep the leading term, because the first subleading term in the Hamiltonian (of order  $\sqrt{S}\sqrt{S}S^{-1} = S^0$ ) involves 4 boson operators and thus represents magnon-magnon interactions which should be neglected. Thus effectively the HP expressions for  $S^+$  and  $S^-$  are simplified to

$$S_i^+ \approx \sqrt{2S} a_i, \quad S_i^- \approx \sqrt{2S} a_i^{\dagger}. \quad (23)$$

This gives

$$\begin{aligned} H &= - \sum_{i, \boldsymbol{\delta}} \left[ \frac{J_{\perp}}{2} (\sqrt{2S})^2 (a_i a_{i+\boldsymbol{\delta}}^{\dagger} + a_i^{\dagger} a_{i+\boldsymbol{\delta}}) + J_z (S - n_i)(S - n_{i+\boldsymbol{\delta}}) \right] \\ &= - \sum_{i, \boldsymbol{\delta}} [J_{\perp} S (a_{i+\boldsymbol{\delta}}^{\dagger} a_i + \text{h.c.}) + J_z (S^2 - 2S n_i)]. \end{aligned} \quad (24)$$

Here we neglected the  $O(S^0)$  terms with factors  $n_i n_{i+\boldsymbol{\delta}}$  in the second line as these also represent interactions between magnons. We also used the simplification  $\sum_i n_{i+\boldsymbol{\delta}} = \sum_i n_i$  which follows from the periodic boundary conditions. The constant term in  $H$  is  $-J_z S^2 \sum_{i, \boldsymbol{\delta}} = -2N J_z S^2$  since  $\boldsymbol{\delta}$  runs over two vectors (here  $N$  is the number of lattice sites). Thus

$$H = -2J_z N S^2 - S \sum_{i, \boldsymbol{\delta}} [J_{\perp} (a_{i+\boldsymbol{\delta}}^{\dagger} a_i + \text{h.c.}) - 2J_z a_i^{\dagger} a_i]. \quad (25)$$

Now we do a Fourier transformation, writing

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} a_{\mathbf{k}} \quad (26)$$

where the  $\mathbf{k}$ -sum goes over the 1st Brillouin zone. This gives (with  $\mathbf{r}_{i+\boldsymbol{\delta}} = \mathbf{r}_i + \boldsymbol{\delta}$ )

$$\begin{aligned} \sum_i a_{i+\boldsymbol{\delta}}^{\dagger} a_i &= \sum_i \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} e^{-i\mathbf{k} \cdot (\mathbf{r}_i + \boldsymbol{\delta})} e^{i\mathbf{k}' \cdot \mathbf{r}_i} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} = \sum_{\mathbf{k}, \mathbf{k}'} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} e^{-i\mathbf{k} \cdot \boldsymbol{\delta}} \underbrace{\frac{1}{N} \sum_i e^{-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_i}}_{\delta_{\mathbf{k}, \mathbf{k}'}} \\ &= \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} e^{-i\mathbf{k} \cdot \boldsymbol{\delta}}, \end{aligned} \quad (27)$$

$$\sum_i a_i^{\dagger} a_i = \sum_i \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} e^{-i\mathbf{k} \cdot \mathbf{r}_i} e^{i\mathbf{k}' \cdot \mathbf{r}_i} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} = \sum_{\mathbf{k}, \mathbf{k}'} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} \underbrace{\frac{1}{N} \sum_i e^{-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_i}}_{\delta_{\mathbf{k}, \mathbf{k}'}} = \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}. \quad (28)$$

(An alternative and quicker way to get (28) would be to replace  $\boldsymbol{\delta}$  by 0 in (27).) Also using that  $a_{\mathbf{k}}^\dagger a_{\mathbf{k}} e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} + \text{h.c.} = a_{\mathbf{k}}^\dagger a_{\mathbf{k}} (e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} + e^{i\mathbf{k}\cdot\boldsymbol{\delta}}) = a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \cdot 2 \cos(\mathbf{k} \cdot \boldsymbol{\delta})$ , we find that

$$H = E_0 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \quad (29)$$

with

$$E_0 = -2J_z N S^2, \quad (30)$$

$$\omega_{\mathbf{k}} = 2S \sum_{\boldsymbol{\delta}} [J_z - J_{\perp} \cos(\mathbf{k} \cdot \boldsymbol{\delta})] \quad (= 2S[2J_z - J_{\perp}(\cos k_x + \cos k_y)]) \quad (31)$$

(b) For small  $|\mathbf{k}| = k$  we can approximate  $\cos(\mathbf{k} \cdot \boldsymbol{\delta}) \approx 1 - \frac{1}{2}(\mathbf{k} \cdot \boldsymbol{\delta})^2$ . Using also  $\sum_{\boldsymbol{\delta}} (\mathbf{k} \cdot \boldsymbol{\delta})^2 = (\mathbf{k} \cdot \hat{\mathbf{x}})^2 + (\mathbf{k} \cdot \hat{\mathbf{y}})^2 = k_x^2 + k_y^2 = k^2$ , we get

$$\omega_{\mathbf{k}} \approx 4S(J_z - J_{\perp}) + SJ_{\perp}k^2. \quad (32)$$

Comparing this with the form given in the problem text we can identify

$$\Delta = 4S(J_z - J_{\perp}), \quad (33)$$

$$m = \frac{1}{2SJ_{\perp}}. \quad (34)$$

(c) We see from (33) that  $\Delta \rightarrow 0$  in the limit  $J_{\perp} \rightarrow J_z$ . Note also that  $\Delta$  is the minimum value of  $\omega_{\mathbf{k}}$  considered as a function of  $\mathbf{k}$ . This means that in the limit  $J_{\perp} \rightarrow J_z$  the system becomes gapless. On the other hand, Goldstone's theorem says that if the ground state breaks a continuous symmetry of the Hamiltonian, the system has gapless excitations. When  $J_{\perp} = J_z$  the Hamiltonian reduces to the Heisenberg model  $H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ , which has a continuous symmetry corresponding to global spin rotations by any angle around an arbitrary axis, and this symmetry is broken by the ferromagnetic ground state. Hence, by Goldstone's theorem, gapless excitations are expected in this limit, and thus the value  $\Delta = 0$  in this limit is expected.

### **Problem 3**

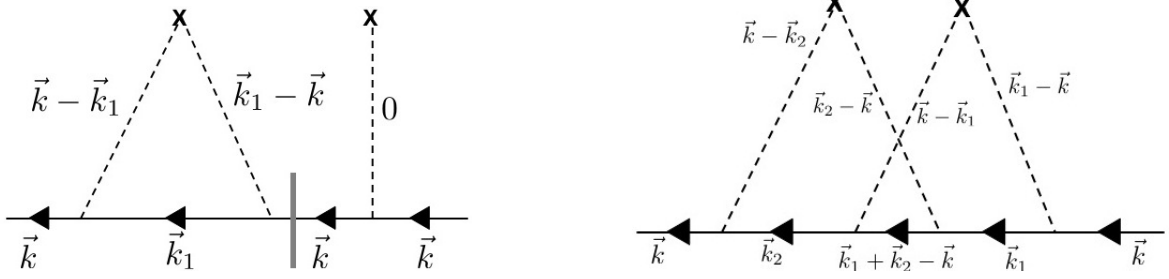
In the diagrams we have (as in the problem text) for simplicity not drawn the downward-pointing arrows on the dashed interaction lines.

(a) 1. The order  $n$  is the number of (dashed) interaction lines, equivalently one less than the number of (full) electron lines.

2. The diagram is proportional to  $n_{\text{imp}}^m$  where  $m$  is the number of impurity crosses.

(b) The two diagrams are redrawn below with wavevectors assigned. The expression for the left diagram can be written

$$N^2 U(0) (\mathcal{G}^{(0)}(\mathbf{k}))^3 \sum_{\mathbf{k}_1} U(\mathbf{k} - \mathbf{k}_1) U(\mathbf{k}_1 - \mathbf{k}) \mathcal{G}^{(0)}(\mathbf{k}_1). \quad (35)$$

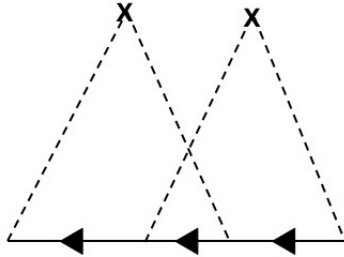


This diagram is reducible, as it falls apart by cutting the right internal electron line as shown in the figure (the thick grey line indicates the cut).

The expression for the right diagram can be written

$$N^2(\mathcal{G}^{(0)}(\mathbf{k}))^2 \sum_{\mathbf{k}_1, \mathbf{k}_2} U(\mathbf{k} - \mathbf{k}_2)U(\mathbf{k}_2 - \mathbf{k})U(\mathbf{k} - \mathbf{k}_1)U(\mathbf{k}_1 - \mathbf{k})\mathcal{G}^{(0)}(\mathbf{k}_1)\mathcal{G}^{(0)}(\mathbf{k}_2)\mathcal{G}^{(0)}(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}). \quad (36)$$

This diagram is irreducible, as cutting any one of the three internal electron lines will not make it fall apart. The corresponding self-energy diagram is obtained by removing the two external electron lines and is shown below. Its mathematical expression is obtained from (36) by removing the factor  $(\mathcal{G}^{(0)}(\mathbf{k}))^2$  associated with the two external electron lines.



Finally, we note that alternative assignments of the internal wavevectors being summed over are possible. For example, the expression for the first diagram could be written

$$N^2U(0)(\mathcal{G}^{(0)}(\mathbf{k}))^3 \sum_{\mathbf{k}_1} U(-\mathbf{k}_1)U(\mathbf{k}_1)\mathcal{G}^{(0)}(\mathbf{k} + \mathbf{k}_1). \quad (37)$$

(c) 1. In  $\Sigma_{1B}$  each diagram has one impurity cross, so  $\Sigma_{1B} \propto n_{\text{imp}}$ . We therefore expect it to be good for low impurity densities. Furthermore, the diagrams in  $\Sigma_{1B}$  are of low order (respectively of 1st and 2nd order) in the scattering potential  $U$ . We therefore expect  $\Sigma_{1B}$  to be good for weak scattering.

In  $\Sigma_{FB}$  each diagram has one impurity cross, so  $\Sigma_{FB} \propto n_{\text{imp}}$ . We therefore expect it to be good for low impurity densities (note that the reasoning here is the same as for  $\Sigma_{1B}$ ). Furthermore,  $\Sigma_{FB}$  contains diagrams of arbitrarily high order in the scattering potential. It can therefore be expected to be good also for stronger scattering, i.e. it is not limited to

weak scattering as  $\Sigma_{1B}$  is.

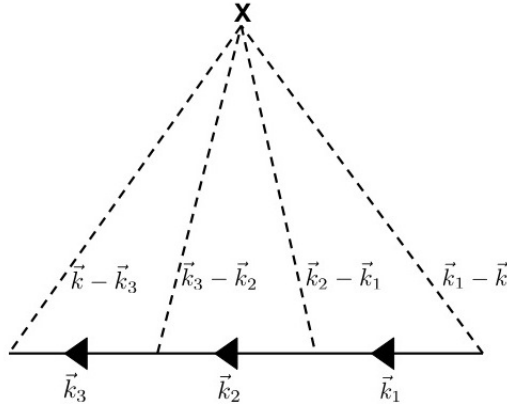
2. The  $n$ 'th diagram has  $n$  factors of the scattering potential and  $n - 1$  Green functions, with  $n - 1$  internal wavenectors that are summed over. The expression for this diagram can be written

$$N \sum_{\mathbf{k}_1, \dots, \mathbf{k}_{n-1}} U(\mathbf{k}_1 - \mathbf{k}) U(\mathbf{k}_2 - \mathbf{k}_1) \cdots U(\mathbf{k} - \mathbf{k}_{n-1}) \mathcal{G}^{(0)}(\mathbf{k}_1) \mathcal{G}^{(0)}(\mathbf{k}_2) \cdots \mathcal{G}^{(0)}(\mathbf{k}_{n-1}). \quad (38)$$

Alternatively, a more explicit way of writing it is

$$N \sum_{\mathbf{k}_1, \dots, \mathbf{k}_{n-1}} U(\mathbf{k}_1 - \mathbf{k}) \mathcal{G}^{(0)}(\mathbf{k}_1) \left[ \prod_{i=2}^{n-1} U(\mathbf{k}_i - \mathbf{k}_{i-1}) \mathcal{G}^{(0)}(\mathbf{k}_i) \right] U(\mathbf{k} - \mathbf{k}_{n-1}). \quad (39)$$

As a concrete example, the  $n = 4$  diagram is shown below.



3. Again consider the  $n$ 'th diagram. If the  $\mathbf{k}$ -dependence of the scattering potential can be neglected, the dependence on the scattering potential simplifies to a constant  $U$ . The wavevector summations then simplify to  $n - 1$  identical summations over a single wavevector. To get  $\Sigma_{FB}$  we sum over all diagrams, i.e. over  $n$  from  $n = 1$  to  $\infty$ :

$$\Sigma_{FB} = N \sum_{n=1}^{\infty} U^n \left( \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1) \right)^{n-1} = NU \sum_{n=0}^{\infty} \left( U \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1) \right)^n. \quad (40)$$

This is a geometric series. It can be evaluated either by using the (given) result for the sum of such a series, or by noting that it can be written in terms of itself as  $NU + \Sigma_{FB} U \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1)$  and solving for  $\Sigma_{FB}$ . This gives (we do not address questions about convergence here)

$$\Sigma_{FB} = \frac{NU}{1 - U \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1)}. \quad (41)$$

4. Using the Feynman rules, the second diagram in  $\Sigma_{FB}$  is given by

$$NU^2 \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1) = n_{\text{imp}u} \cdot U \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1). \quad (42)$$

Thus, using the information given in the text about the expression for this diagram, we get (reinstating the Matsubara frequency dependence of  $\mathcal{G}^{(0)}$ , which we have suppressed in the notation so far)

$$U \sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}_1, ip_m) = \frac{1}{n_{\text{imp}} u} \left( -\frac{i}{2\tau_{1\text{B}}} \text{sgn}(p_m) \right) = -i\pi u D(0) \text{sgn}(p_m). \quad (43)$$

Inserting this into the expression for  $\Sigma_{\text{FB}}$  gives

$$\Sigma_{\text{FB}}(ip_m) = \frac{n_{\text{imp}} u}{1 + i\pi u D(0) \text{sgn}(p_m)} = n_{\text{imp}} u \frac{1 - i\pi u D(0) \text{sgn}(p_m)}{1 + (\pi u D(0))^2}. \quad (44)$$

The imaginary part is

$$\text{Im } \Sigma_{\text{FB}}(ip_m) = -\frac{\pi n_{\text{imp}} u^2 D(0)}{1 + (\pi u D(0))^2} \text{sgn}(p_m) \equiv -\frac{1}{2\tau_{\text{FB}}} \text{sgn}(p_m). \quad (45)$$

Therefore

$$\tau_{\text{FB}} = \frac{1 + (\pi u D(0))^2}{2\pi n_{\text{imp}} u^2 D(0)}. \quad (46)$$

This result can alternatively be written in the form  $\tau_{\text{FB}} = \tau_{1\text{B}} \left( 1 + \frac{1}{(2\tau_{1\text{B}} N U)^2} \right)$ , which also could have been found without invoking the explicit result  $1/\tau_{1\text{B}} = 2\pi n_{\text{imp}} u^2 D(0)$ .