TFY4210, Quantum theory of many-particle systems, 2016: Solution to tutorial 8

1. The sublattice magnetization correction for the Heisenberg antiferromagnet at nonzero temperature.

(a) We have

$$\gamma_{\boldsymbol{k}} = \frac{2}{z}\sum_{\boldsymbol{\delta}} \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}) = \frac{1}{d}\sum_{\boldsymbol{\delta}} \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}). \tag{1}$$

Using $\cos x \approx 1 - x^2/2$ for $x \to 0$ we get, for small $\boldsymbol{k}$,

$$\gamma_{\boldsymbol{k}} \approx \frac{1}{d}\sum_{\boldsymbol{\delta}}\left[1 - \frac{1}{2}(\boldsymbol{k}\cdot\boldsymbol{\delta})^2\right] = \frac{1}{d}\left[d - \frac{1}{2}\boldsymbol{k}^2\right] = 1 - \frac{k^2}{2d} \tag{2}$$

where $k = |\boldsymbol{k}|$. Here we used that $\boldsymbol{\delta}$ runs over the d orthogonal unit vectors in d dimensions (e.g. in 3 dimensions, $\boldsymbol{\delta}$ runs over $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$). This gives, for small $\boldsymbol{k}$,

$$\omega_{\boldsymbol{k}} = JSz\sqrt{1-\gamma_{\boldsymbol{k}}^2} \approx 2JSd\sqrt{1 - \left(1 - \frac{k^2}{2d}\right)^2} = 2JSd\sqrt{\frac{k^2}{d} - \frac{k^4}{4d^2}} \approx 2JS\sqrt{d}\,k. \tag{3}$$

(b) Converting the $\boldsymbol{k}$-sum to an integral and using that $n_{\boldsymbol{k}}$ is given by the Bose-Einstein distribution function, the temperature-dependent part of the sublattice magnetization correction can be written

$$\frac{2}{N}\sum_{\boldsymbol{k}\in\text{MBZ}} n_{\boldsymbol{k}} \frac{1}{\sqrt{1-\gamma_{\boldsymbol{k}}^2}} \propto \int_{\text{MBZ}} d^d k\, \frac{1}{e^{\beta\omega_{\boldsymbol{k}}}-1}\frac{1}{\sqrt{1-\gamma_{\boldsymbol{k}}^2}} \tag{4}$$

where MBZ denotes the magnetic Brillouin zone. Since we here want to look at the contribution from the vicinity of $k=0$ we use the results in (a) and also (since $\omega_{\boldsymbol{k}} \to 0$ as $k \to 0$) $e^{\beta\omega_{\boldsymbol{k}}} \approx 1 + \beta\omega_{\boldsymbol{k}}$ to get

$$\frac{1}{e^{\beta\omega_k}-1}\frac{1}{\sqrt{1-\gamma_{\boldsymbol{k}}^2}} \propto \frac{1}{k^2} \quad \text{for } k \to 0. \tag{5}$$

Also taking into account the factor k^{d-1} from the integration measure, the k-dependence of the radial part of the $\boldsymbol{k}$-integral then becomes proportional to $k^{d-1}\frac{1}{k^2} = k^{d-3}$ at small k. Therefore the contribution from the lower limit $k=0$ to the radial integral becomes

$$\int_0 dk\; k^{d-3} = \begin{cases} \int_0 dk\; k^{-2} = -\frac{1}{k}|_0 = +\infty & d=1, \\ \int_0 dk\; k^{-1} = \ln k|_0 = +\infty & d=2. \end{cases} \tag{6}$$

Thus both in $d=1$ and $d=2$ there is a divergence coming from the lower integration limit.

(c) By putting $d = 3$ in the integral on the lhs of (6) one sees that there is no divergence from the $k = 0$ limit in this case. To find the leading T-dependence of the finite-temperature correction ($T \to 0$) to the sublattice magnetization, we note that due to the factor $e^{\beta\omega_{\boldsymbol{k}}}$ the contributions to the integral will decrease very rapidly with $\boldsymbol{k}$ when $\beta \to \infty$. We therefore approximate the integral by using the small-$\boldsymbol{k}$ approximations derived in (a) for all $\boldsymbol{k}$ and also replacing the integral over the MBZ by an integral over all $\boldsymbol{k}$. Thus (4) becomes

$$\begin{aligned} \int_{\text{all k}} d^3k \, \frac{1}{e^{2\beta JS\sqrt{3}\,k} - 1} \frac{\sqrt{3}}{k} &= \sqrt{3} \cdot 4\pi \int_0^\infty dk \frac{k}{e^{2\beta JS\sqrt{3}\,k} - 1} \\ &\overset{x=2\sqrt{3}\beta JSk}{=} \frac{4\pi\sqrt{3}}{(2\sqrt{3}\beta JS)^2} \int_0^\infty dx \frac{x}{e^x - 1} \end{aligned} \tag{7}$$

where a change of integration variable led to the last expression in which the remaining integral is a dimensionless number. The T^2 temperature dependence is now evident from the factor β^{-2}.

2. 0th and 1st order perturbation theory for the interacting electron gas.

(a) We have

$$\frac{1}{n} = \frac{\Omega}{N} = \frac{4\pi}{3} r_0^3 = \frac{4\pi}{3}(r_s a_B)^3. \tag{8}$$

Using $n = k_F^3/(3\pi^2)$ (derived in the lectures) then gives

$$k_F a_B = (3\pi^2 n)^{1/3} a_B = \left(3\pi^2 \cdot \frac{3}{4\pi(r_s a_B)^3}\right)^{1/3} a_B = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s}. \tag{9}$$

In the lectures we also showed that $E^{(0)}/N = (3/5)\varepsilon_F$, where the Fermi energy $\varepsilon_F = \hbar^2 k_F^2/(2m)$. Thus

$$\frac{E^{(0)}}{N} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}(k_F a_B)^2 \text{ Ry} = \frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3} \frac{1}{r_s^2} \text{ Ry} \approx \frac{2.210}{r_s^2} \text{ Ry}. \tag{10}$$

(b) From 1st order perturbation theory, $E^{(1)} = \langle \text{FS}|H_I|\text{FS}\rangle$, where H_I is the Coulomb interaction term in H. Thus

$$\frac{E^{(1)}}{N} = \frac{1}{2\Omega N} \sum_{\boldsymbol{q}\neq 0} \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{\sigma,\sigma'} \frac{e^2}{\varepsilon_0 q^2} \langle \text{FS}| c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} c_{\boldsymbol{k}',\sigma'} c_{\boldsymbol{k},\sigma} |\text{FS}\rangle. \tag{11}$$

Let us consider the matrix element in this expression. The annihilation operators acting on $|\text{FS}\rangle$ will give zero unless their wavevectors $\boldsymbol{k}$ and $\boldsymbol{k}'$ are occupied in $|\text{FS}\rangle$, giving the requirement $|\boldsymbol{k}| \leq k_F$ and $|\boldsymbol{k}'| \leq k_F$. To get a nonzero matrix element, the two creation

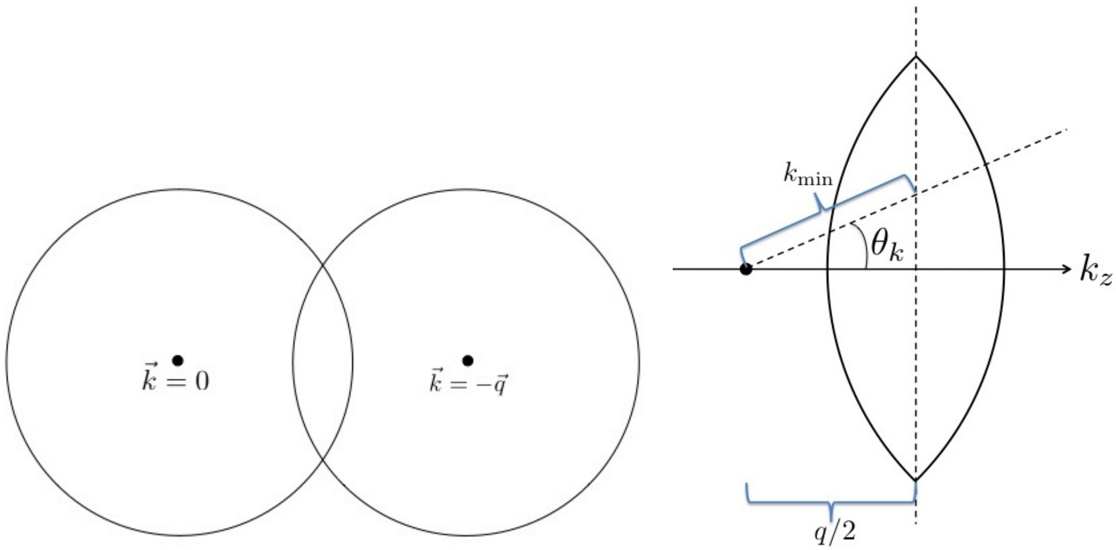

Figure 1: Left: For a given $\boldsymbol{q}$, the $\boldsymbol{k}$-integral is the volume of the intersection of two spheres of radius k_F centered at $\boldsymbol{k}=0$ and $\boldsymbol{k}=-\boldsymbol{q}$ respectively. Right: Blowup of the intersection.

operators must then bring the state back to $|\mathrm{FS}\rangle$, which requires $\boldsymbol{q}=0$ or $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{q}$, $\sigma'=\sigma$. But $\boldsymbol{q}=0$ is excluded from the $\boldsymbol{q}$-sum in H_I. Therefore

$$\begin{aligned}
\langle \mathrm{FS}|c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}c_{\boldsymbol{k}',\sigma'}c_{\boldsymbol{k},\sigma}|\mathrm{FS}\rangle &= \delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}}\delta_{\sigma',\sigma}\langle \mathrm{FS}|c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k}+\boldsymbol{q},\sigma}c_{\boldsymbol{k},\sigma}|\mathrm{FS}\rangle \\
&= -\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}}\delta_{\sigma',\sigma}\langle \mathrm{FS}|\hat{n}_{\boldsymbol{k}+\boldsymbol{q},\sigma}\hat{n}_{\boldsymbol{k},\sigma}|\mathrm{FS}\rangle \\
&= -\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}}\delta_{\sigma',\sigma}\theta(k_F-|\boldsymbol{k}+\boldsymbol{q}|)\theta(k_F-|\boldsymbol{k}|), \qquad (12)
\end{aligned}$$

where we again used that $\boldsymbol{q}\neq 0$ when anticommuting the two middle operators. Inserting this in (11) and doing the spin summations (which give a factor of 2) and the summation over $\boldsymbol{k}'$ gives

$$\frac{E^{(1)}}{N} = -\frac{e^2}{\Omega N\varepsilon_0}\sum_{\boldsymbol{q}\neq 0}\frac{1}{q^2}\sum_{\boldsymbol{k}}\theta(k_F-|\boldsymbol{k}+\boldsymbol{q}|)\theta(k_F-|\boldsymbol{k}|). \qquad (13)$$

Converting the two sums to integrals ($\sum_{\boldsymbol{k}} \to \frac{\Omega}{(2\pi)^3}\int d^3k$) and using spherical coordinates (ϕ_q,θ_q,q) and (ϕ_k,θ_k,k) gives

$$\begin{aligned}
\frac{E^{(1)}}{N} &= -\frac{e^2}{N\varepsilon_0}\frac{\Omega}{(2\pi)^6}\int_0^{2\pi}d\phi_q\int_{-1}^{1}d(\cos\theta_q)\int_0^\infty dq\, q^2\frac{1}{q^2} \\
&\times \int_0^{2\pi}d\phi_k\int_{-1}^{1}d(\cos\theta_k)\int_0^\infty dk\, k^2\theta(k_F-|\boldsymbol{k}+\boldsymbol{q}|)\theta(k_F-|\boldsymbol{k}|). \qquad (14)
\end{aligned}$$

Consider the $\boldsymbol{k}$-integral (second line here) for a fixed $\boldsymbol{q}$. The two step functions are equivalent to the requirements $|\boldsymbol{k}|<k_F$ and $|\boldsymbol{k}-(-\boldsymbol{q})|<k_F$. Thus the $\boldsymbol{k}$-integral is the volume of the intersection of two spheres of radius k_F, one centered at $\boldsymbol{k}=0$ and the other centered at $\boldsymbol{k}=-\boldsymbol{q}$ (see Fig. 1). Although the latter sphere moves as the direction of $\boldsymbol{q}$ is changed, the volume of the intersection of the two spheres is independent of the direction of $\boldsymbol{q}$. Thus the angular part of the $\boldsymbol{q}$-integral can be done trivially, giving $\int_0^{2\pi}d\phi_q\int_{-1}^{1}d(\cos\theta_q)=4\pi$.

Furthermore, one sees from the figure that a nonzero intersection requires the magnitude of $\boldsymbol{q}$ to satisfy $q < 2k_F$. Taking these things into account gives

$$\frac{E^{(1)}}{N} = -\frac{e^2}{N\varepsilon_0}\frac{\Omega}{16\pi^5}\int_0^{2k_F} dq\,\mathrm{Vol}(q) \tag{15}$$

where $\mathrm{Vol}(q)$ is the intersection volume, which by symmetry is twice the volume of the right half of the intersection. To calculate this half-volume, we take the k_z axis to point in the direction of $-\boldsymbol{q}$. Then the angle θ_k is as shown in Fig. 1. For a given θ_k, k is integrated from $k_{\min}$ to $k_{\max}$. While $k_{\max} = k_F$ independently of θ_k, $k_{\min}$ is given by (see Fig. 1):

$$\cos\theta_k = \frac{q/2}{k_{\min}} \quad \Rightarrow \quad k_{\min} = \frac{q}{2\cos\theta_k}. \tag{16}$$

As θ_k is increased, $k_{\min}$ grows. The maximum value of θ_k corresponds to $k_{\min} = k_{\max}$, giving

$$(\cos\theta_k)_{\min} = \frac{q}{2k_F}. \tag{17}$$

There are no constraints on the variable ϕ_k, so the ϕ_k-integral just gives 2π. Thus

$$\begin{aligned}
\mathrm{Vol}(q) &= 2\cdot 2\pi\int_{q/(2k_F)}^{1} d(\cos\theta_k)\int_{q/(2\cos\theta_k)}^{k_F} dk\,k^2 \\
&= 4\pi\int_{q/(2k_F)}^{1} d(\cos\theta_k)\cdot\frac{1}{3}\left[k_F^3 - \left(\frac{q}{2\cos\theta_k}\right)^3\right] \\
&= \frac{4\pi}{3}\left\{k_F^3\left(1-\frac{q}{2k_F}\right) - \left(\frac{q}{2}\right)^3\cdot\left(\frac{1}{-2}\right)\left[1^{-2} - \left(\frac{q}{2k_F}\right)^{-2}\right]\right\} \\
&= \frac{4\pi}{3}\left(k_F^3 - \frac{3}{4}k_F^2 q + \frac{1}{16}q^3\right).
\end{aligned} \tag{18}$$

(As a check of the correctness of this result, note that for $q = 0$ it becomes $4\pi k_F^3/3$ (i.e. the volume of a sphere of radius k_F) and for $q = 2k_F$ it becomes 0; both cases are as expected.) Thus

$$\begin{aligned}
\frac{E^{(1)}}{N} &= -\frac{e^2}{N\varepsilon_0}\frac{\Omega}{16\pi^5}\cdot\frac{4\pi}{3}\int_0^{2k_F} dq\,\left(k_F^3 - \frac{3}{4}k_F^2 q + \frac{1}{16}q^3\right) \\
&= -\frac{e^2}{N\varepsilon_0}\frac{\Omega}{12\pi^4}\left(k_F^3\cdot 2k_F - \frac{3}{4}k_F^2\cdot\frac{1}{2}(2k_F)^2 + \frac{1}{16}\cdot\frac{1}{4}(2k_F)^4\right) \\
&= -\frac{e^2}{N\varepsilon_0}\frac{\Omega}{16\pi^4}k_F^4.
\end{aligned} \tag{19}$$

Using $\Omega/N = 1/n$ and $k_F^3 = 3\pi^2 n$ gives $E^{(1)}/N = -\frac{e^2}{\varepsilon_0}\frac{3}{16\pi^2}k_F$. Expressing this in Rydberg units, it can be rewritten as follows:

$$\frac{E^{(1)}}{N} = -\frac{e^2}{\varepsilon_0}\frac{3}{16\pi^2}k_F\frac{2ma_B^2}{\hbar^2}\ \mathrm{Ry}$$

$$
\begin{aligned}
&= -\frac{e^2}{\varepsilon_0}\frac{3}{16\pi^2}k_F\frac{2m}{\hbar^2}\cdot\frac{4\pi\varepsilon_0\hbar^2}{me^2}\cdot a_B \text{ Ry} \\
&= -\frac{3}{2\pi}(k_F a_B) \text{ Ry} \\
&= -\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s} \text{ Ry} \approx -\frac{0.916}{r_s} \text{ Ry}.
\end{aligned} \tag{20}
$$

3. Single-particle retarded Green function for noninteracting bosons.

Given the Hamiltonian for noninteracting bosons,

$$H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu, \tag{21}$$

we consider the single-particle retarded Green function

$$G_0^R(\nu, t) = -i\theta(t)\langle[c_\nu(t), c_\nu^\dagger(0)]\rangle. \tag{22}$$

Here

$$c_\nu(t) = e^{iH_0t}c_\nu e^{-iH_0t} = e^{-i\xi_\nu t}c_\nu, \tag{23}$$

where the last expression follows in exactly the same way as for the fermionic case discussed in the lecture notes (Sec. 2.4). Thus

$$G_0^R(\nu, t) = -i\theta(t)e^{-i\xi_\nu t}\langle[c_\nu, c_\nu^\dagger]\rangle = -i\theta(t)e^{-i\xi_\nu t} \tag{24}$$

where we used the equal-time commutation relation $[c_\nu, c_\nu^\dagger] = 1$. The result (24) takes exactly the same form as for fermions. It follows that the Fourier transform also takes exactly the same form as for fermions:

$$G_0^R(\nu, \omega) = \frac{1}{\omega - \xi_\nu + i\eta}. \tag{25}$$

Note however that if we had wished to find the Green functions $G^>$ or $G^<$, the expressions would have contained the expectation value $\langle c_\nu^\dagger c_\nu\rangle$, which for noninteracting bosons is given by the Bose-Einstein distribution function $(e^{\beta\xi_\nu} - 1)^{-1}$ and not the Fermi-Dirac distribution function $(e^{\beta\xi_\nu} + 1)^{-1}$ appearing in the fermionic case.

4. The basis invariance of the trace.

Let us consider two arbitrary basis sets, denoted $\{|\alpha\rangle\}$ and $\{|\tilde{\alpha}\rangle\}$. Let us define Tr O as the sum of the diagonal matrix elements of O in the basis $\{|\alpha\rangle\}$:

$$\text{Tr } O \equiv \sum_\alpha \langle\alpha|O|\alpha\rangle. \tag{26}$$

Using the resolution of the identity operator I in terms of the basis $\{|\tilde{\alpha}\rangle\}$, i.e. $I = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|$, the two basis sets can be related as

$$|\alpha\rangle = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|\alpha\rangle = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle|\tilde{\alpha}\rangle. \tag{27}$$

Thus

$$\begin{aligned}
\mathrm{Tr}\ O &= \sum_{\alpha} \langle\alpha|O|\alpha\rangle = \sum_{\alpha}\sum_{\tilde{\alpha}}\sum_{\tilde{\beta}} \langle\tilde{\alpha}|O|\tilde{\beta}\rangle\langle\tilde{\alpha}|\alpha\rangle^{*}\langle\tilde{\beta}|\alpha\rangle \\
&= \sum_{\tilde{\alpha}}\sum_{\tilde{\beta}} \langle\tilde{\alpha}|O|\tilde{\beta}\rangle\langle\tilde{\beta}|\,\underbrace{(\sum_{\alpha} |\alpha\rangle\langle\alpha|)}_{I}\,|\tilde{\alpha}\rangle = \sum_{\tilde{\alpha}}\sum_{\tilde{\beta}} \langle\tilde{\alpha}|O|\tilde{\beta}\rangle\,\underbrace{\langle\tilde{\beta}|\tilde{\alpha}\rangle}_{\delta_{\tilde{\alpha}\tilde{\beta}}} \\
&= \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|O|\tilde{\alpha}\rangle,
\end{aligned} \tag{28}$$

which shows that Tr O is also equal to the sum of the diagonal elements of O in the basis $\{|\tilde{\alpha}\rangle\}$. As the basis sets used here are arbitrary we conclude that the sum of the diagonal elements is independent of the basis.

In the above proof we expressed both the ket $|\alpha\rangle$ and the bra $\langle\alpha|$ in terms of the new basis, thus using the resolution of the identity twice. Actually, a simpler proof can be given by just using it once, e.g. for the ket only, as follows:

$$\mathrm{Tr}\ O = \sum_{\alpha} \langle\alpha|O|\alpha\rangle = \sum_{\alpha,\tilde{\alpha}} \langle\alpha|O|\tilde{\alpha}\rangle\langle\tilde{\alpha}|\alpha\rangle = \sum_{\alpha,\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle\langle\alpha|O|\tilde{\alpha}\rangle = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|O|\tilde{\alpha}\rangle. \tag{29}$$