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Current correlation functions of ideal Fermi gas at finite temperature

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Abstract. Expressions for transverse and longitudinal current–current correlation functions of an ideal Fermi gas describing the current fluctuations induced in the electron system by external probe perpendicular and parallel to the propagation of electron wave, have been obtained at finite temperature. The results obtained for transverse and longitudinal functions are presented for different values of wavelength and frequency at different temperatures. The diamagnetic susceptibility as a function of temperature has also been obtained from transverse current correlation function as its long wavelength and static limit, which smoothly cross over from known quantum values to the classical limit with increase in temperature.

Keywords. Fermi gas; diamagnetic susceptibility; current correlations.

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1. Introduction

The transverse and longitudinal current–current correlation functions describing the current fluctuations induced in the electron system by a weak external probe perpendicular and parallel to the propagation of electron wave, respectively, are two basic quantities in the theory of Fermi liquid. The longitudinal current correlation function $\chi_{\mathrm{L}}(\mathbf{q}, \omega)$ [1–4] has sought more attention in the past than the transverse current correlation function, $\chi_{\mathrm{T}}(\mathbf{q}, \omega)$. Recently the knowledge of $\chi_{\mathrm{T}}(\mathbf{q}, \omega)$ have become essential in order to make advancement in the study of time dependent density functional theory [5] due to the work of Vignale and Kohn [6,7]. They obtained explicitly an expression for the exchange vector potential in the linear response regime in terms of correlations of longitudinal and transverse currents. In the absence of the knowledge of $\chi_{\mathrm{T}}(\mathbf{q}, \omega)$ which includes the effect of temperature and interactions, Vignale and Kohn have used only some of the aspects of this function. Tosi and co-workers [8,9] have subsequently made some calculations of transverse exchange kernel but only at zero temperature. In fact the dynamics of $\chi_{\mathrm{T}}(\mathbf{q}, \omega)$ is not known yet which include the effect of correlations and finite temperature. Moreover, the transverse part has relevance to the study of viscous effects [10] in the electron gas and to the diamagnetic susceptibility [11–13] of the system. Therefore in the present work, as a first step, we make theoretical calculations at finite temperature, but neglect the effect of interactions. We will also be presenting the result for longitudinal current–current correlation function at finite temperature for the sake of completeness and to make the comparison of its behavior with its transverse counterpart. Expressions for both longitudinal and transverse current correlation functions in the long wavelength and static limit are obtained. It is found that the diamagnetic susceptibility, related to the transverse part, smoothly cross over from quantum values to classical limit with increase in temperature.

The lay out of this paper is as follows: In §2, we present expressions for real and imaginary parts of longitudinal and transverse current correlation functions. The limiting cases along with expression of diamagnetic susceptibility are also given there. Numerical results obtained at different temperatures of $\chi_{\rm L}(\mathbf{q}, \omega)$, $\chi_{\rm T}(\mathbf{q}, \omega)$ and diamagnetic susceptibility are presented and discussed in §3. In §4 we present the conclusion.

2. Theory

In a homogeneous and isotropic system the current–current correlation function has only two independent components, namely, longitudinal $(\chi_{\rm L})$ and transverse $(\chi_{\rm T})$. The Gauge invariance and the continuity equation allow to relate the density–density response function (χ_ρ) to the longitudinal component of the current correlation function [1] through the following equation

$$\chi_{\rm L}(\mathbf{q},\omega) = -\frac{n}{m} + \frac{\omega^2}{q^2}\chi_\rho(\mathbf{q},\omega), \tag{1}$$

where the density–density response function for the non-interacting electron gas is defined as

$$\chi_\rho(\mathbf{q},\omega) = \sum_{\mathbf{k}} \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega - \omega(\mathbf{k},\mathbf{q})}\ , \qquad \hbar = 1. \tag{2}$$

Here $\omega(\mathbf{k},\mathbf{q}) = \omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}}$ with $\omega_{\mathbf{k}} = \mathbf{k}\cdot\mathbf{k}/2m$ is the energy of free particles having the wave vector $\mathbf{k}$. ω and $\mathbf{q}$ are the transferred energy and momentum in scattering, respectively, and $n_{\mathbf{k}} = 1/(1+\mathrm{e}^{(\omega_{\mathbf{k}}-\mu)/k_{\rm B}T})$ is the Fermi function with μ and $k_{\rm B}$ as the chemical potential and the Boltzmann constant, respectively.

On the other hand, using Green's function theory [14] the transverse current correlation function of the non-interacting homogeneous electron gas is defined [11] as

$$\chi^0_{\rm T}(\mathbf{q},\omega) = \frac{1}{m^2}\sum_{\mathbf{k}} k_y^2 \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega - \omega(\mathbf{k},\mathbf{q})}\ . \tag{3}$$

In the above equation, k_y is y component of the wave vector when the transferred momentum $\mathbf{q}$ is taken along the x-axis, i.e. $(q, 0, 0)$.

2.1 *Expressions for $\chi^0_{\rm T}(\mathbf{q}, \omega)$ and diamagnetic susceptibility*

In order to have useful expression for transverse current correlation function we follow a method similar to that of Khanna and Glyde [2] and apply the adiabatic boundary conditions to the response function to ensure that the system response follows the probe linearly.

This is equivalent to replacing the real frequency ω by a complex frequency $(\omega + \mathrm{i}\eta)$, where η is positive and infinitesimally small, which is taken to be zero at the end of the calculations. It is convenient to write eq. (3) as

$$\chi_{\mathrm{T}}^{0}(\mathbf{q},\omega) = \frac{1}{m^2}\sum_{\mathbf{k}} k_y^2 n_{\mathbf{k}} \left(\frac{1}{\omega + \mathrm{i}\eta - \omega_{\mathbf{k-q}} + \omega_{\mathbf{k}}} - \frac{1}{\omega + \mathrm{i}\eta - \omega_{\mathbf{k}} + \omega_{\mathbf{k-q}}} \right) . \tag{4}$$

This equation can be evaluated using the dispersion relation to separate the real and imaginary part and then perform angular integration. Quite lengthy calculations leads to the expression for real and imaginary parts of transverse current–current correlation function, respectively, given as

$$\begin{aligned} \mathrm{Re}\,\chi_{\mathrm{T}}^{0}(q,\omega,z) = &-\frac{k_{\mathrm{F}}^3}{m\pi^2}\int_0^{\infty} \mathrm{d}k k^2 n_k + \frac{k_{\mathrm{F}}^3}{4m\pi^2 q}\left(\frac{q^3}{3} + \frac{\omega^2}{q}\right)\int_0^{\infty}\mathrm{d}k n_k \\ &+ \frac{k_{\mathrm{F}}^3 z}{4m\pi q}\sum_j \Bigg[\left(\frac{q^3}{3}+\frac{\omega^2}{q}\right)\frac{k_j''}{|k_j|^2} + 2qk_j'' + \left(\alpha_2^2 - \gamma\right) \\ &\times \tan^{-1}\left(\frac{2\alpha_2 k_j''}{\alpha_2^2 - |k_j|^2}\right) - \left({\alpha_1}^2 - \gamma\right)\tan^{-1}\left(\frac{2\alpha_1 k_j''}{{\alpha_1}^2 - |k_j|^2}\right) \\ &- k_j' k_j'' \ln\left(\frac{[(\alpha_1 - k_j')^2 + k_j''^2][(\alpha_2 + k_j')^2 + k_j''^2]}{[(\alpha_1 + k_j')^2 + k_j''^2][(\alpha_2 - k_j')^2 + k_j''^2]}\right)\Bigg] , \end{aligned} \tag{5}$$

and

$$\mathrm{Im}\,\chi_{\mathrm{T}}^{0}(q,\omega,z) = -\frac{k_{\mathrm{F}}^3 z}{4m\pi q}\int_{-\alpha_2}^{\alpha_1} \mathrm{d}k\, k \ln(1 + \mathrm{e}^{-(k^2-\gamma)/z}) , \tag{6}$$

where

$$\alpha_1 = \frac{\omega}{2q} - \frac{q}{2}, \qquad \alpha_2 = \frac{\omega}{2q} + \frac{q}{2},$$

and $k_j = k_j' + \imath k_j''$ with

$$k_j' = \frac{1}{\sqrt{2}}\left[\gamma + \{\gamma^2 + (\pi z(2j+1))^2\}^{1/2}\right]^{1/2},$$

$$k_j'' = \frac{1}{\sqrt{2}}\left[-\gamma + \{\gamma^2 + (\pi z(2j+1))^2\}^{1/2}\right]^{1/2}.$$

To derive the above expressions we have used reduced variables, namely

$$k = \frac{\mathbf{k}}{k_{\mathrm{F}}},\ \ q = \frac{\mathbf{q}}{k_{\mathrm{F}}},\ \ \omega = \frac{\omega}{\varepsilon_{\mathrm{F}}},\ \ \gamma = \frac{\mu}{\varepsilon_{\mathrm{F}}},\ \ z = \frac{k_{\mathrm{B}}T}{\varepsilon_{\mathrm{F}}} \text{ and } n_k = \frac{1}{1 + \mathrm{e}^{(k^2-\gamma)/z}} . \tag{7}$$

On taking the long wavelength limit in expression (5) we get the following expression for the transverse current correlation function

$$\mathrm{Re}\,\chi_{\mathrm{T}}^{0}(q\to 0,\omega,z) = -\frac{n}{m} + \frac{k_{\mathrm{F}}^{3}}{4m\pi^{2}}\left(\frac{q^{2}}{3}+\frac{\omega^{2}}{q^{2}}\right)\int_{0}^{\infty}\mathrm{d}kn_{k} + \frac{k_{\mathrm{F}}^{3}z}{4m\pi}\sum_{j}\left[\frac{k_{j}''}{|k_{j}|^{2}}\right.$$
$$\times\left(\frac{q^{2}}{3}+\frac{\omega^{2}}{q^{2}}\right) + 4k_{j}'' + \frac{16k_{j}''^{3}q^{2}(q^{4}-12q^{2}|k_{j}|^{2}-9\omega^{2})}{3(\omega^{2}-4q^{2}|k_{j}|^{2})^{2}}$$
$$-\frac{16k_{j}'^{2}k_{j}''q^{2}(q^{4}+4q^{2}|k_{j}|^{2}-\omega^{2})}{(\omega^{2}+4q^{2}|k_{j}|^{2})^{2}} - \frac{256k_{j}''q^{4}(q^{4}+3\omega^{2})}{3}$$
$$\left.\times\left(\frac{k_{j}''^{4}}{(\omega^{2}-4q^{2}|k_{j}|^{2})^{3}}+\frac{k_{j}'^{4}}{(\omega^{2}+4q^{2}|k_{j}|^{2})^{3}}\right)\right]. \tag{8}$$

From the above expressions, it appears that terms of the order of q^{8} are included in the expression. However, when j is large these terms reduce to the order of q^{2} only. Now if we take $\omega = 0$, we get

$$\mathrm{Re}\,\chi_{\mathrm{T}}{}^{0}(q\to 0^{\mathrm{I}},\omega=0^{\mathrm{II}},z) = -\frac{n}{m} + \frac{k_{\mathrm{F}}^{3}q^{2}}{12m\pi^{2}}\int_{0}^{\infty}\mathrm{d}kn_{k} - \frac{k_{\mathrm{F}}^{3}\gamma zq^{2}}{2m\pi}\sum_{j}\frac{k_{j}''}{|k_{j}|^{4}}. \tag{9}$$

In order to see whether two limits commute, we now first take the static limit and then long wavelength limit. The limit $\omega = 0$ in eq. (5) leads to the static transverse current response function given by

$$\mathrm{Re}\,\chi_{\mathrm{T}}{}^{0}(q,\omega=0,z) = -\frac{k_{\mathrm{F}}^{3}}{m\pi^{2}}\int_{0}^{\infty}\mathrm{d}kk^{2}n_{k} + \frac{k_{\mathrm{F}}^{3}q^{2}}{12m\pi^{2}}\int_{0}^{\infty}\mathrm{d}kn_{k} + \frac{k_{\mathrm{F}}^{3}z}{4m\pi q}$$
$$\times\sum_{j}\left[\frac{q^{3}k_{j}''}{3|k_{j}|^{2}} + 2qk_{j}'' + \left(\frac{q^{2}}{2}-2\gamma\right)\tan^{-1}\left(\frac{qk_{j}''}{\frac{q^{2}}{4}-|k_{j}|^{2}}\right)\right.$$
$$\left.+2k_{j}'k_{j}''\ln\left(\frac{(\frac{q}{2}-k_{j}')^{2}+k_{j}''^{2}}{(\frac{q}{2}+k_{j}')^{2}}\right)\right]. \tag{10}$$

In the long wavelength limit, the above expression for static current response function becomes

$$\mathrm{Re}\,\chi_{\mathrm{T}}^{0}(q\to 0^{\mathrm{II}},\omega=0^{\mathrm{I}},z) = -\frac{n}{m} + \frac{k_{\mathrm{F}}^{3}q^{2}}{12m\pi^{2}}\int_{0}^{\infty}\mathrm{d}kn_{k}, \tag{11}$$

where use of $\int_{0}^{\infty}\mathrm{d}kk^{2}n_{k} = \frac{1}{3}$ and $k_{\mathrm{F}}^{3} = 3n\pi^{2}$ have been made. It is interesting to note that the first two terms in eqs (9) and (11) are the same as that obtained for zero temperature except its dependence on z through n_{k}. Now if z is made equal to zero, the last term in eq. (9) becomes identically zero. Thus $q\to 0$ and $\omega = 0$ limits commute when z is made equal to zero. Here it may be noted that these limits (i.e. $q\to 0$ and $\omega = 0$ limits) do not commute [8] when z is taken to be zero in the beginning of the calculations.

The diamagnetic susceptibility of the system is related [11,12] to the static and long wavelength limit of the transverse current correlation function through the relation

$$\chi_{\rm dia}(q\to 0,\omega=0,z) = -\frac{e^2}{c^2q^2k_{\rm F}^2}\left[\chi_{\rm T}^0(q\to 0,\omega=0,z)+\frac{n}{m}\right], \tag{12}$$

which leads to the expression

$$\frac{\chi_{\rm dia}(q\to 0,\omega=0,z)}{\chi_{\rm Landau}} = \int_0^\infty {\rm d}k n_k, \tag{13}$$

where $\chi_{\rm Landau} = -(e^2k_{\rm F}/12\pi^2mc^2)$ is the Landau diamagnetism.

2.2 *Expression for* $\chi_{\rm L}^0(q,\omega,z)$

Following the same procedure as followed above, in this subsection we evaluate the density response function χ_ρ, and hence longitudinal current correlation function, using eq. (1). Expressions obtained for its real and imaginary parts are, respectively, given as

$$\begin{aligned}{\rm Re}\ \chi_{\rm L}^0(q,\omega,z) = &-\frac{n}{m}-\frac{k_{\rm F}^3\omega^2}{4m\pi^2q^2}\int_0^\infty {\rm d}k n_k + \frac{k_{\rm F}^3\omega^2 z}{8m\pi q^3}\sum_j\left[\frac{2qk_j''}{|k_j|^2}\right.\\ &\left.+\tan^{-1}\left(\frac{2\alpha_2 k_j''}{\alpha_2^2-|k_j|^2}\right)-\tan^{-1}\left(\frac{2\alpha_1 k_j''}{\alpha_1^2-|k_j|^2}\right)\right]\end{aligned} \tag{14}$$

and

$${\rm Im}\ \chi_{\rm L}^0(q,\omega,z) = -\frac{k_{\rm F}^3\omega^2 z}{16m\pi q^3}\ln\left(\frac{1+{\rm e}^{-(\alpha_1^2-\gamma)/z}}{1+{\rm e}^{-(\alpha_2^2-\gamma)/z}}\right). \tag{15}$$

The real part contains a term $2qk_j''/|k_j|^2$, which is not present in the expression obtained by Khanna and Glyde [2].

In the static and long wavelength limit, the density response function which is related to longitudinal response function through eq. (1) is given by

$${\rm Re}\ \chi_\rho^0(q\to 0,\omega=0,z) = -\frac{k_{\rm F}m}{\pi^2}\int_0^\infty {\rm d}k n_k\,. \tag{16}$$

On the other hand, if we reverse the order of limits, i.e., on taking first the long wavelength limit and then taking the static limit we obtain

$${\rm Re}\ \chi_\rho^0(q\to 0,\omega=0,z) = -\frac{k_{\rm F}m}{\pi^2}\int_0^\infty {\rm d}k n_k - \frac{k_{\rm F}mq^2z}{\pi}\sum_j\frac{k_j''}{|k_j|^4}\,. \tag{17}$$

The above expression differ from eq. (16) in respect of the last term which is proportional to z. And at zero temperature, both equations (eqs (16) and (17)) reduce to

$${\rm Re}\ \chi_\rho^0(q\to 0,\omega=0,z=0) = -\frac{k_{\rm F}m}{\pi^2}. \tag{18}$$

Thus we see that if we take $T=0$ after taking the static and long wavelength limits then two limits commute. However, when $T=0$ is taken at the beginning, the two limits do not commute [1].

3. Results and discussion

The numerical calculations of the real and imaginary part of the current–current correlation function require the knowledge of chemical potential, μ, at different values of temperature. To calculate μ we have numerically solved the following equation for different values of z and μ

$$\int_0^\infty \mathrm{d}k k^2 \frac{1}{1+\mathrm{e}^{(k^2-\gamma)/z}} = \frac{1}{3}\,, \qquad \text{with } \gamma = \frac{\mu}{\varepsilon_\mathrm{F}}\,. \tag{19}$$

The validity of this method has also been checked by using its low-temperature expansion

$$\gamma = \frac{\mu}{\varepsilon_\mathrm{F}} = 1 - \frac{1}{12}(\pi z)^2 - \frac{7}{960}(\pi z)^4\,. \tag{20}$$

However, at large values of temperature, eq. (19) reduces to $\gamma = z\ \ln\left(4/3\sqrt{\pi}(z)^{3/2}\right)$, and for convenience we used this expression for large values of z to calculate diamagnetic susceptibility numerically as a function of z.

The imaginary parts of $\chi_\mathrm{L}^0(q,\omega,z)$ and $\chi_\mathrm{T}^0(q,\omega,z)$ are directly evaluated from the expressions (6) and (15). However, to evaluate the real parts numerically we have used Kramers–Kronig relation. The direct expression of real part are slightly more complicated to be evaluated numerically due to the presence of multi-valued functions.

The numerical results obtained for real and imaginary parts of $(-m/n)\chi_\mathrm{T}^0(q,\omega,z)$ and $(-m/n)\chi_\mathrm{L}^0(q,\omega,z)$ are shown in figures 1 and 2, respectively, as a function of reduced

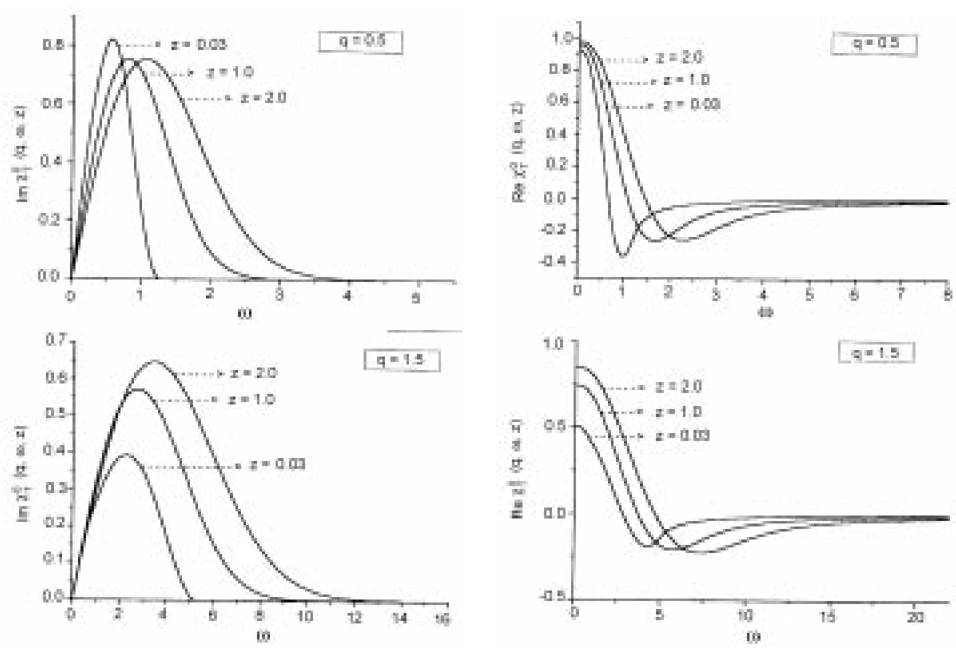

Figure 1. Real and imaginary parts of $\chi_\mathrm{T}(q,\omega,z)$ for reduced wave vector $\mathbf{q} = 0, 5$ and 1.5 and for reduced temperatures $z = 0.03$, 1.0 and 2.0 versus reduced energy transfer, ω.

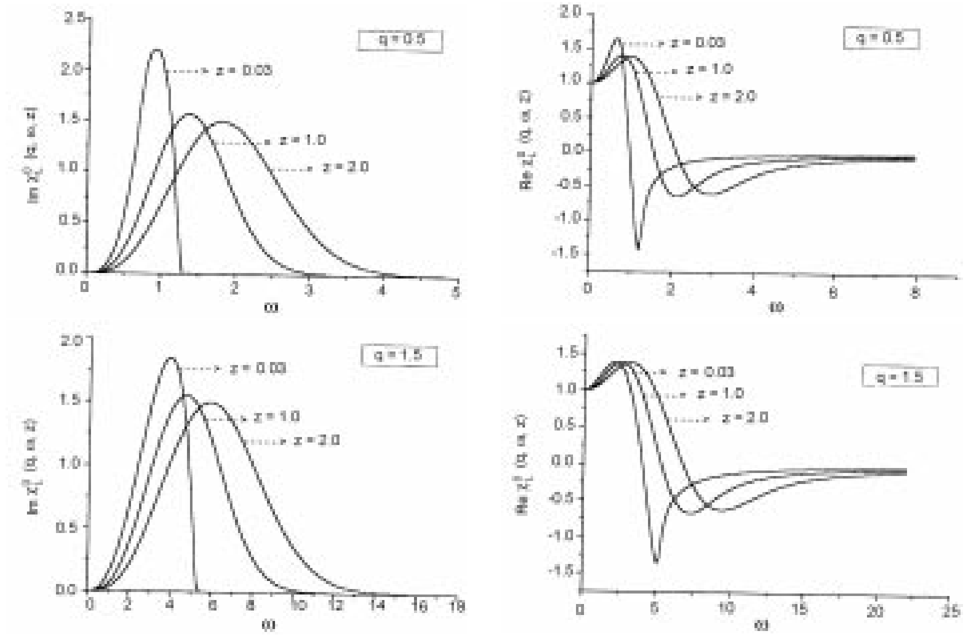

Figure 2. Same as that of figure 1 but for $\chi_{\mathrm{L}}(q,\omega,z)$.

energy transfer, ω for $q = 0.5$ and 1.5 at different values of reduced temperature z (0.3, 1.0 and 2.0). From figures 1 and 2, we see that the main effect of increasing temperature for particular q is to spread both Im $\chi^0_{\mathrm{L,T}}(q,\omega,z)$ and Re $\chi^0_{\mathrm{L,T}}(q,\omega,z)$ over larger values of energy transfer. This may be due to broadening of free particle spectrum with increase in temperature. In fact, at high temperature the width is proportional to $\sqrt{z}$. We note that the peak height got depressed at $q = 0.5$ for both Im $\chi^0_{\mathrm{L,T}}(q,\omega,z)$ with increase in temperature. But at $q = 1.5$ the peak height of Im $\chi^0_{\mathrm{T}}(q,\omega,z)$ increases with increase in temperature. Here it can also be noted from figures 1 and 2 that Re $\chi_{\mathrm{L}}(q,\omega,z)$ starts from the same value (i.e. 1.0) whereas $\chi_{\mathrm{T}}(q,\omega,z)$ does not. This is due to the fact that $\chi_{\mathrm{L,T}}(q,\omega,z)$ are calculated in terms of $(-n/m)$ which is the normalization constant for χ_{L} but not for χ_{T}.

Finally in figure 3, we have plotted diamagnetic susceptibility calculated from eq. (13) as a function of temperature. At very low temperature χ_{dia} becomes the Landau diamagnetism. This is due to the fact that for $T \to 0$, Fermi function appearing in eq. (13) becomes a unit step function. But as the temperature increases the diamagnetic susceptibility decreases from χ_{Landau} value. On the other hand, at high temperature, in the classical limit, γ which is a function of z becomes negative and Fermi function reduces to Boltzmann–Maxwell function. This provides

$$\begin{aligned}\frac{\chi_{\mathrm{dia}}}{\chi_{\mathrm{Landau}}} &= \mathrm{e}^{\gamma/z}\int_0^\infty \mathrm{d}k\mathrm{e}^{-k^2/z} \\ &= \frac{\mathrm{e}^{\gamma/z}\sqrt{z}}{2}\Gamma\left(\frac{1}{2}\right) = \frac{2}{3z} \qquad (21)\end{aligned}$$

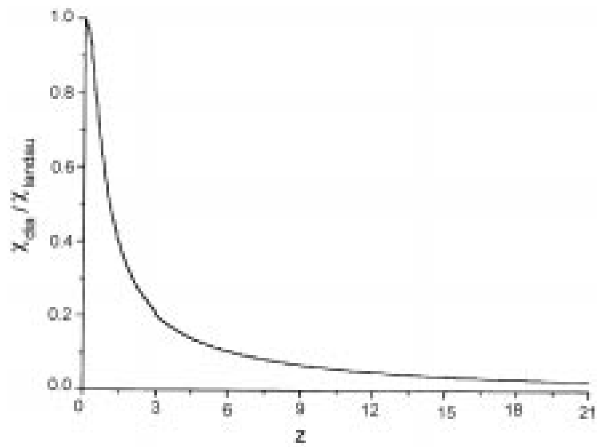

Figure 3. Variation of diamagnetic susceptibility $\chi_{\rm dia}$ with reduced temperature z.

with $\gamma/z = \ln(4/3\sqrt{\pi}(z)^{3/2})$ and $\Gamma(1/2) = \sqrt{\pi}$. Thus for large values of temperature, $\chi_{\rm dia}$ varies as inverse of temperature, which is also evident from figure 3. Thus diamagnetic susceptibility smoothly cross over from quantum values to classical limit on increasing temperature.

4. Conclusion

Expressions for the real and imaginary parts of the transverse and longitudinal current–current correlation function at finite temperature have been obtained. For the purpose of numerical calculations, the imaginary parts of $\chi^0_{\rm L,T}(q,\omega,z)$ have been evaluated from their direct expressions whereas real parts are calculated using Kramers–Kronig relation. Results are presented as a function of energy transfer at different temperature and different wave vectors. It is shown that the long wavelength and static limits do not commute for longitudinal as well as transverse part of current–current correlation function at finite temperature as in the zero temperature limit [1,8]. However, if the temperature is taken to be zero after these limits, then these two limits commute.

The diamagnetic susceptibility has also been studied as a function of temperature and it is shown that this reproduces $T = 0$ result as well as high temperature results known in the classical limit.

The present expressions for current–current correlation functions will be useful in any Fermi system in which temperature dependence of excitation energy and viscous effects are of interest and for the advancement of time dependent density functional theory.

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