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LETTER TO THE EDITOR

Finite-size effects in the ideal Fermi gas

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Abstract. The ideal Fermi gas in a finite volume is studied in the low-temperature regime where the thermal correlation length is comparable to the size L of the system. Physical quantities such as the density of fermions and the appropriate ordering susceptibility show oscillatory fluctuations around a smooth background as L is varied. These are investigated numerically and analytically. The amplitude of the fluctuations depends on the observable in question and on the container shape. Finite-size scaling does not hold directly for thermodynamic quantities but is recoverable by averaging the mean-squared fluctuations over an appropriate range in L.

Physical properties are known to be affected strongly when the size of a system is reduced sufficiently. Such finite-size effects have been the subject of much interest (Hill 1963, 1964, Fisher 1972, Baltes and Hilf 1976, Barber 1983) and have been studied extensively in the ideal Bose gas (Pathria 1983). The size-dependent properties of the ideal Fermi gas in a finite volume are also of interest from several points of view. First, the model caricatures certain important features of physical systems such as atomic nuclei (Bohr and Mottelson 1975) and small metal particles (Perenboom *et al* 1981, Kubo *et al* 1984, Halperin 1986). Second, a knowledge of finite-size effects is required to extrapolate to the bulk (infinite-volume) limit from Monte Carlo results on finite systems of interacting fermions (Ceperley 1978), with the ideal gas corresponding to the high-density limit. Finally, the study of finite-size effects close to a critical point is of intrinsic theoretical interest (Fisher 1972, Barber 1983); as explained below, the ideal Fermi gas in the bulk is critical at zero temperature, so that interesting effects occur at low temperatures in the finite system when the size is comparable to the thermal correlation length.

We consider a system of non-interacting spinless fermions of mass m at temperature T and chemical potential μ in a bounded three-dimensional region Ω of volume V. The Hamiltonian is

$$\mathscr{H}=\sum_i \varepsilon_i a_i^\dagger a_i \tag{1}$$

where ε_i is the energy of the single-particle state i, and $a_i^\dagger$ and a_i are the corresponding fermion creation and annihilation operators. Both ε_i and the single-particle wavefunction $\phi_i(\boldsymbol{r})\equiv\langle \boldsymbol{r}|a_i^\dagger|0\rangle$ depend on the region Ω and the boundary conditions. We deal mainly with two geometries: a cubic box with periodiic boundary conditions, and a sphere with an impenetrable surface (Dirichlet boundary conditions). We denote the characteristic length of Ω by L; e.g. the edge length of the cube is $2\pi L$, whereas the radius of the equal volume sphere is $(6\pi^2)^{1/3}L$.

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In the bulk limit $L \to \infty$, the system exhibits critical behaviour at low temperatures in the sense that the correlation length and an appropriate susceptibility diverge as $T \to 0$. For $T \ll \mu$, the two-point correlation function $\Gamma_{\mu,T}(\boldsymbol{r})$ defined as $\langle a_0^\dagger a_r \rangle$ is given by

$$\Gamma_{\mu,T}(\boldsymbol{r}) \simeq \frac{1}{2\pi^2 r\xi} \frac{\partial}{\partial r}\left(\frac{\sin k_F r}{\sinh r/\xi}\right). \tag{2}$$

Here $k_F \equiv \sqrt{2m\mu/\hbar^2}$ is the Fermi wavevector and $\xi \equiv 2\mu/(\pi T k_F)$ is the correlation length. ξ governs the exponential decay of the amplitude of $\Gamma_{\mu,T}(\boldsymbol{r})$ for large r, and diverges as $T \to 0$. Further, consider the response to adding the term

$$-h\psi_{\boldsymbol{q}} \equiv -h \int \mathrm{d}^3 r (\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} a_r^\dagger + \mathrm{HC}) \tag{3}$$

to $\mathscr{H}$. (A similar term with $q = 0$ is added on in the study of the ideal Bose gas (Bogoliubov 1970).) The corresponding susceptibility

$$\chi_{\boldsymbol{q}} \equiv \frac{1}{V} \frac{\partial}{\partial h} \langle \psi_{\boldsymbol{q}} \rangle |_{h \to 0} \tag{4}$$

is found by direct calculation to be

$$\chi_{\boldsymbol{q}} = \frac{2 \tanh((\varepsilon_{\boldsymbol{q}} - \mu)/2T)}{(\varepsilon_{\boldsymbol{q}} - \mu)}. \tag{5}$$

We see for $|\boldsymbol{q}| = k_F$ that $\chi_{\boldsymbol{q}} \to \infty$ as $T \to 0$. This divergence, along with the non-trivial dependence on q, again indicates that the bulk Fermi gas is critical at $T = 0$.

In finite systems we investigate the behaviour of two thermodynamic quantities: the density of fermions (which in the bulk is a regular function of T for $T \ll \mu$), and the ordering susceptibility $\chi_{q=k_F}$ (which is singular in the bulk as $T \to 0$). The density of fermions is given by

$$\rho(L, \mu, T) = \frac{1}{V} \sum_i \frac{1}{\exp[(\varepsilon_i - \mu)/T] + 1} \tag{6a}$$

$$= \frac{1}{4T} \int \mathrm{d}E\, \mathcal{N}_\Omega(E) \operatorname{sech}^2 \frac{E - \mu}{2T} \tag{6b}$$

where

$$\mathcal{N}_\Omega(E) \equiv \frac{1}{V} \sum_i \Theta(E - \varepsilon_i) \tag{7}$$

is the integrated density of states. The susceptibility $\chi_{\boldsymbol{q}}$ depends on the single-particle wavefunctions $\phi_i(\boldsymbol{r})$ also, and is found to be

$$\chi_{\boldsymbol{q}} = \frac{1}{V} \sum_i \frac{2 \tanh((\varepsilon_i - \mu)/2T)}{(\varepsilon_i - \mu)} |\hat{\phi}_i(\boldsymbol{q})|^2 \tag{8}$$

where $\hat{\phi}_i(\boldsymbol{q})$ is the Fourier transform of $\phi_i(\boldsymbol{r})$.

Since ε_i and $\phi_i(\boldsymbol{r})$ are determined by solving the free-particle Schrödinger equation with periodic or Dirichlet boundary conditions, the combinations $\varepsilon_i L^2$ and $|\hat{\phi}_i(\boldsymbol{q})|^2/L^3$ are left invariant if the size, but not the shape or boundary conditions, of Ω is changed. Consequently, under a dilatation by a factor λ, we have the manifest scaling forms

$$\rho(L, \mu, T) = \lambda^3 \rho(\lambda L, \lambda^{-2}\mu, \lambda^{-2}T) \tag{9a}$$

$$\chi_{\boldsymbol{q}}(L, \mu, T) = \lambda^{-2} \chi_{\boldsymbol{q}/\lambda}(\lambda L, \lambda^{-2}\mu, \lambda^{-2}T). \tag{9b}$$

Manifest scaling holds in all ranges of parameter values. In the critical regime $T \to 0$, $L \to \infty$, additional scaling properties would be expected to emerge; below we will see to what extent this expectation is borne out.

Let us recall some facts about the structure of the integrated density of states. Figure 1 shows the variation of $\mathcal{N}_\Omega$ with E for the periodic box and the hard-walled sphere. In both cases, $\mathcal{N}_\Omega$ is the sum of a smooth background $\mathcal{N}_{\text{smooth}}$ (shown dotted in figure 1) and a fluctuating part. For the periodic box, $\mathcal{N}_{\text{smooth}}$ has contributions from the bulk alone, whereas surface and curvature terms also contribute in the case of the sphere:

$$\mathcal{N}_{\text{smooth}} = g_{\text{bulk}} k^3 + g_{\text{surf}} \frac{k^2}{L} + g_{\text{curv}} \frac{k}{L^2} \tag{10}$$

where $\hbar k = \sqrt{2mE}$. The constant $g_{\text{bulk}} = 1/6\pi^2$ is independent of the geometry, while g_{surf} and g_{curv} (which vanish for the periodic box) depend, in general, on the shape of Ω and are known analytically (Balian and Bloch 1970, Baltes and Hilf 1976). If Ω has sharp edges or corners, as in the hard-walled box, there are more terms in (10). Figure 1 illustrates an important point, well established for the quantum mechanical counterparts of classically integrable systems (Berry 1983, 1987), namely $\mathcal{N}_\Omega(E)$ displays fluctuations on two distinct energy scales. On the finest scale, $\mathcal{N}_\Omega$ has the character of a staircase with steps at distinct values of the eigenenergies ε_i and step heights equal to the degeneracies of the states. The typical step length is denoted by $\delta_L(E)$ (see figure 1). But also apparent in figure 1 are larger-scale fluctuations associated with excursions of $\mathcal{N}_\Omega$ on either side of the smooth curve. These oscillations correspond to shell effects in nuclear physics (Ramamurthy and Kapoor 1972, Bohr and Mottelson

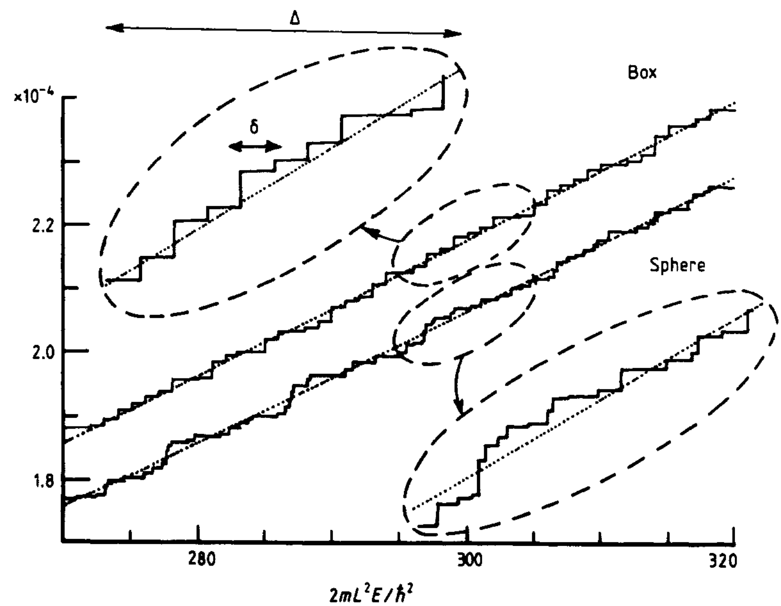

Figure 1. The exact integrated density of states (full line) for a particle in a box with periodic boundary conditions and a sphere with Dirichlet boundary conditions. The dotted curves represent analytically calculated smooth contributions. There are two scales for fluctuations: δ is a typical step size, while Δ is the size of a fluctuation around the smooth curve.

1975, Brack and Bartel 1985) and their energy scale is denoted by $\Delta_L(E)$. The two scales are governed by different powers of L. The inter-energy separation $\delta_L(E)$ scales as $L^{-p}E^{1-p/2}$, where the value of the exponent $p(>1)$ depends on Ω; it is equal to dimensionality 3 for irregularity shaped bodies (Kubo *et al* 1984, Berry 1987), while it is between 1 and 3 for more regular bodies like the cube and the sphere. By contrast, $\Delta_L(E)$ scales as $L^{-1}E^{1/2}$; the number of discrete steps in each large-scale fluctuation diverges as $L\to\infty$.

The existence of two energy scales in $\mathcal{N}_\Omega(E)$ implies two temperature regimes for the finite Fermi gas. In the very low-temperature region $T<\delta_L(\mu)$, thermodynamic behaviour is exponentially activated, and deviations of thermodynamic variables from their $T=0$ values are described by $\exp[-C\delta_L(\mu)/T]$ with C an order unity constant which depends on the precise locations of energy states *vis à vis* μ. This is the temperature regime addressed by conventional theories of fine particles (Perenboom *et al* 1981, Kubo *et al* 1984, Halperin 1986). But more interesting, from the point of view of finite-size scaling, is the intermediate-temperature regime $\delta_L(\mu)\ll T\sim\Delta_L(\mu)$, as the correlation length ξ is then comparable to the size L.

We investigated the density of fermions numerically by evaluating the sum in 6(a) for the periodic cube and the sphere, noting that the energy eigenvalues in the two cases are determined by the sums of three squared integers and by the zeros of spherical Bessel functions respectively. The density $\rho(L,\mu,T)$ has a smooth background part $\rho_{\text{smooth}}(L,\mu,T)$ defined by writing $\mathcal{N}_{\text{smooth}}$ in place of $\mathcal{N}_\Omega$ in (6b). ρ_{smooth} can be evaluated using the low-temperature (Sommerfeld) expansion for the Fermi gas (Landau and Lifshitz 1958), in conjunction with (10). The fluctuation in density

$$\rho_{\text{fluc}}(L,\mu,T)\equiv\rho(L,\mu,T)-\rho_{\text{smooth}}(L,\mu,T) \tag{11}$$

is shown in figure 2 for a particular value of the temperature between $\delta_L(\mu)$ and $\Delta_L(\mu)$. At such intermediate temperatures, the fine-scale fluctuations corresponding to staircase steps are averaged out, but pronounced fluctuations on the scale of $\Delta_L(\mu)$ remain.

Turning to an analytical theory of the fluctuations, we first derive an exact relationship between density fluctuations in the periodic box and the two-point correlation function in the bulk. Eigenstates are labelled by points $\boldsymbol{p}$ on a cubic lattice in momentum space, and the energy of each state is proportional to p^2. On using the Poisson summation formula (Lighthill 1958) the sum over $\boldsymbol{p}$ in (6) can be eliminated in favour of a sum over three integers (τ_x,τ_y,τ_z), collectively denoted by $\boldsymbol{\tau}$, with the result

$$\rho_{\text{fluc}}(L,\mu,T)=\sum_{\boldsymbol{\tau}\neq 0}\Gamma_{\mu,T}(2\pi L\boldsymbol{\tau}) \tag{12}$$

where $\Gamma_{\mu,T}(\boldsymbol{r})$ is the bulk correlation function. The sum is over integer triplets (τ_x,τ_y,τ_z), excluding $(0,0,0)$ which gives the smooth bulk contribution. As we can see from (2), $\Gamma(\boldsymbol{r})$ decays exponentially for $r\gg\xi$. Thus (12) provides an efficient way of computing ρ_{fluc}. The result of keeping only terms up to $|\boldsymbol{r}|=6$ is shown in figure 2. The resulting approximation displays the main features of the oscillations; by retaining a few more terms, the detailed structure in this range can be reproduced as well. For the cube with hard walls the calculation for ρ_{fluc} parallels that for the periodic box, with the difference that the points $\boldsymbol{p}$ in momentum space are confined to the strictly positive octant, and are closer together than for the periodic box. The result for ρ_{fluc} now has several terms. The leading term (in powers of L^{-1}) is given by (12), except that L is replaced by $2L$ on the right-hand side.

For non-cuboidal geometries it does not seem possible to obtain an exact correspondence to bulk correlation functions as in (12). But one can use the classical path

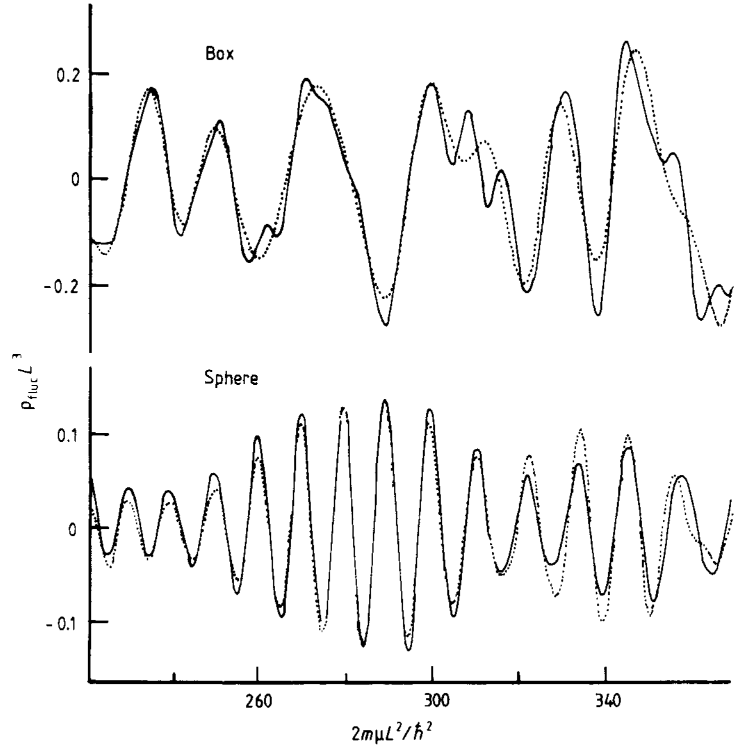

Figure 2. Fluctuations in the density of fermions witth $T = 1.475\hbar^2/2mL^2$ for the box and the sphere. The continuous curves are obtained by performing the sum in (6) numerically and subtracting the smooth contribution. The dotted curves represent approximations obtained by keeping only a few terms in (12) and (13). For the box only terms up to $|\tau| = 6$ are kept, while for the sphere terms up to $t = 5$ (with five values of p for each) are retained.

analysis of Balian and Bloch (1972) to study spectral oscillations, and thus ρ_{fluc}, asymptotically as $L \to \infty$. However, explicit answers can be obtained only for relatively simple geometries. For the Sinai billiard (a periodic square with a circle cut out from the centre) (Berry 1981), density oscillations are proportional to ρ_{fluc} for a periodic square in the temperature range $T \sim \Delta_L(\mu)$, though very different for $T \sim \delta_L(\mu)$. For the sphere with Dirichlet boundary conditions, the result for $k_F L \gg 1$, $T \ll \mu$ is

$$\rho_{fluc}(L, \mu, T) = \frac{k_F^{3/2}}{L^{1/2}\xi} \sum_{\substack{t \geq 1 \\ p \geq 2t+1}} \frac{A(t,p)}{\sinh(L\psi/\xi)} \left[\cos\left(k_F L\psi + \frac{\pi p}{2} - \frac{\pi}{4}\right) - \frac{3}{2k_F\xi}\coth(L\psi/\xi)\sin\left(k_F L\psi + \frac{\pi p}{2} - \frac{\pi}{4}\right)\right] \tag{13a}$$

where

$$A(t,p) = \tfrac{3}{2}(6\pi^8)^{-1/6}(-1)^t \sin(2\pi t/p)\sqrt{\frac{\sin(\pi t/p)}{\pi p}} \tag{13b}$$

and

$$\psi = 2(6\pi^2)^{1/3} p \sin(\pi t/p). \tag{13c}$$

Terms with large values of t and p are damped, and an approximation which keeps only a few terms works quite well as evidenced by figure 2. The beat structure apparent in the figure can be traced to interference between the $t=1, p=3$ and $t=1, p=4$ terms in (13a).

The susceptibility χ_q shows even stronger oscillations than the density for both the periodic box and the sphere. In the box, χ_q depends both on the magnitude and the direction of $\boldsymbol{q}$. The result for $\boldsymbol{q} \equiv \boldsymbol{Q} = (k_F, 0, 0)$ obtained by explicitly performing the sum in (8) is displayed in figure 3. Relatively small changes in $k_F L$ are seen to lead to very strong variations of χ_Q once ξ exceeds L. As in the case of fermion density (equation (12)), for the periodic box the Poisson sum formula leads to a rapidly convergent series representation for χ_q for general $\boldsymbol{q}$:

$$\mu\chi_q(L, \xi) = k_F L \sum_{\tau} \exp(\mathrm{i}2\pi L\boldsymbol{q}\cdot\boldsymbol{\tau}) F_{\tau}(L/\xi). \tag{14}$$

For $k_F\xi \gg 1$, and $\boldsymbol{q} = k_F\hat{q}$ (with $\hat{q}$ a unit vector), we have

$$F_{\tau}(x) = \frac{16}{\pi^2}\int \mathrm{d}^3u \cos(\boldsymbol{\tau}\cdot\boldsymbol{u})\frac{\tanh(\boldsymbol{u}\cdot\hat{\boldsymbol{q}}/4x)}{\boldsymbol{u}\cdot\hat{\boldsymbol{q}}}\prod_{i=1}^{3}\frac{\sin^2(u_i/2)}{u_i^2} \tag{15}$$

The $\boldsymbol{\tau}=0$ term in the summation in (14) gives the smooth (in L) contribution χ_{smooth}, while the rest of the terms define the fluctuating part χ_{fluc}. Notice that χ_{smooth} and the amplitude of χ_{fluc} are both proportional to L, a property which persists for the sphere as well.

In the critical region $T\to 0$, $L\to\infty$, it is natural to first express all lengths in units of the interparticle spacing, which is proportional to k_F^{-1} at low temperature. This accomplished by choosing the factor λ in (9) to be k_F. Then $k_F^{-3}\rho$ and $k_F^2\chi_q$ (with $|\boldsymbol{q}| = k_F$) are functions only of the reduced variables $l \equiv 2\pi k_f L$ and $\zeta \equiv k_F\xi$, and we can ask whether they assume the finite-size scaling form (Fisher 1972, Barber 1983)

$$Q(l, \zeta) = l^{\Theta} Y(l/\zeta) \tag{16}$$

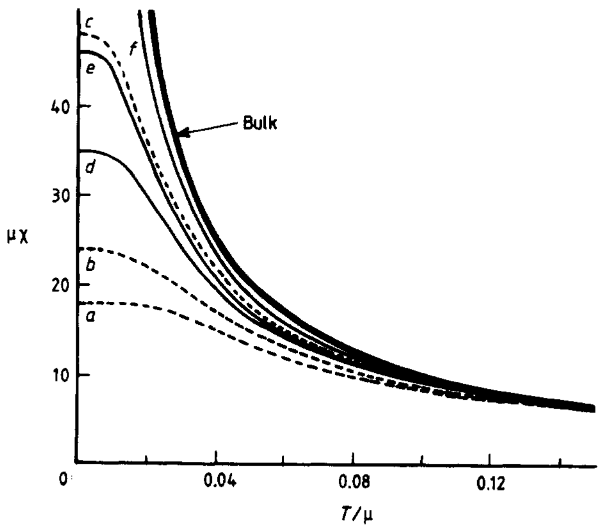

Figure 3. The ordering susceptibility χ_Q, with $Q=(k_F, 0, 0)$, for various values of $k_F L$. The bold curve is the bulk value $\chi = 1/T$. The curves marked a to f are obtained from (8) for $k_F L = (a)$ 10.5, (b) 10.65, (c) 10.8, (d) 20.5, (e) 20.65, (f) 20.8.

in the limit $l \to \infty$, $\zeta \to \infty$ with the ratio l/ζ held fixed. From (12), (13) and (14), it is easy to verify that $2\pi^2 k_F^{-3} \rho_{fluc} \equiv n_{fluc}$ and $k_F^2 \chi_{fluc} \equiv S_{fluc}$ do *not* obey finite-size scaling. For instance, for the density fluctuations in the box we obtain to leading order

$$n_{fluc}(l, \zeta) = l^{-1} \zeta^{-1} \sum_{\tau \neq 0} \frac{D(\tau) \cos \tau l}{\tau \sinh(\tau l/\zeta)} \tag{17}$$

where $\mathscr{D}(\tau)$ is the number of combinations of the set of integers (τ_x, τ_y, τ_z) such that $\tau_x^2 + \tau_y^2 + \tau_z^2 = \tau^2$ holds. n_{fluc} is not of the form required by (16) because of the oscillatory terms in (17). Similarly, from (14) we see that S_{fluc} has oscillatory terms which spoil scaling.

However, it proves possible to recover the finite-size scaling form by averaging physical quantities over a range in l. For instance, consider the root-mean-squared fluctuation function $\sigma(l, \zeta)$ defined by

$$\sigma^2(l, \zeta) = \frac{1}{2\Delta l} \int_{l-\Delta l}^{l+\Delta l} n_{fluc}^2(l', \zeta)\, dl' \tag{18}$$

where the interval Δl is small compared with l, but large enough to contain many oscillations of n_{fluc}. Since scaling involves consideration of the limit $l \to \infty$, $\zeta \to \infty$ with l/ζ fixed, we may take the window width Δl to grow as l^x with $x < 1$, so that $\Delta l / l \to 0$. The right-hand side of (18) is then independent of Δl, and $\sigma(l, \zeta)$ is seen to conform with the scaling form (16). For the box, we have $\Theta = -2$ and the scaling function is given by

$$Y_{box}^2(y) = \sum_{\tau \neq 0} \frac{y^2 \mathscr{D}^2(\tau)}{2\tau^2 \sinh^2 \tau y}. \tag{19}$$

For the sphere, $\Theta = -\frac{3}{2}$ and the scaling function is similar to (19), except that τ and $\mathscr{D}(\tau)$ are replaced by appropriate functions involving ψ and $A(t, p)$.

In contrast to the decreasing amplitude of density fluctuations, the amplitude of fluctuations of the scaled susceptibility S_{fluc} grows with l as rapidly as the smooth part. Window-averaging yields scaling forms with $\Theta = 1$ for both the box and the sphere though the scaling functions are different.

In conclusion, finite-size effects in the ideal Fermi gas at low temperatures are characterised by pronounced oscillations whose amplitude depends both on the shape of the container and on the thermodynamic quantity in question. It would be interesting to see if these results are altered by interactions between fermions, particularly in view of the fact that weak interactions which preserve the normal character of Fermi liquid do not affect singularities in single-particle properties significantly in the bulk.

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