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Oscillatory structure of the harmonic oscillator Wigner function

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Abstract. Some simple closed-form approximations are derived for the oscillatory part of the Wigner function F for a system of degenerate fermions completely filling the first M shells of an oscillator potential in N dimensions. The formalism for a general dimensionality is retained since various properties of the physical case ($N = 3$) may be related to similar systems in one dimension higher or lower. In particular the magnitude of the oscillations increases with N , but it is shown that if the last shell is only half filled the structure is decreased to that obtained for a closed-shell system in one dimension lower. The structure is shown to decrease slowly in the 'classical' or 'macroscopic' limit of large particle number, when the density is shown to tend to its Thomas–Fermi value. The formula for the full-shell case is sufficiently simple to generalise to the problem of almost degenerate fermions at a finite temperature T , where it is seen that substantial damping of the oscillations may be obtained for any particle number. An explicit expression for the damping is derived and this implies that for deep-inelastic nuclear reactions at a temperature of around 2 to 3 MeV, considerable structure may still be present in F . A simple expression relating the Fermi energy and the particle number of the system at finite temperature is given.

1. Introduction

The Wigner function (Wigner 1932) for an N -dimensional system of fermions is defined as

$$F(\mathbf{q}, \mathbf{p}) = \frac{1}{(2\pi\hbar)^N} \int d^N \mathbf{s} \exp(i\mathbf{p} \cdot \mathbf{s}/\hbar) \rho(\mathbf{q} + \frac{1}{2}\mathbf{s}, \mathbf{q} - \frac{1}{2}\mathbf{s}) \quad (1.1)$$

where $\mathbf{s} = (s_1, s_2, \dots, s_N)$ and ρ is the single-particle density matrix. In a mean-field approximation, ρ may be written as

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_i n_i \phi_i(\mathbf{r}) \phi_i^*(\mathbf{r}') \quad (1.2)$$

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where n_i are the occupation numbers of the single-particle states $\phi_i(\mathbf{r})$ generated by the average potential $V(\mathbf{r})$. (We shall, of course, be principally concerned with three dimensions but shall retain a general N since various relations exist between the Wigner functions for different dimensionalities.)

The interest in this function lies in the fact that F is strongly analogous to a classical phase-space probability distribution in that expectation values of operators depending on \mathbf{p} and \mathbf{q} may be written as integrals of F with an appropriate weight function e.g. the density of the system may be simply written

$$\rho(\mathbf{q}) \equiv \rho(\mathbf{q}, \mathbf{q}) = \int F(\mathbf{q}, \mathbf{p}) d^N \mathbf{p}. \quad (1.3)$$

Unlike its classical counterpart, however, the Wigner function, which is real, may display strong quantal oscillations (to the extent that it may even become negative) and thus F loses some of its intuitive appeal as a probability distribution. It is interesting, therefore, to examine the conditions under which these quantal oscillations may be ignored and a smooth approximation to the function taken. The oscillations in F also clearly lead to structure in quantities such as the density (1.3) and if we find conditions under which F is smooth, then we may also take similarly smooth approximations to many other functions e.g. the Thomas-Fermi approximation for $\rho(\mathbf{q})$ (Durand *et al* 1978). Such smooth approximations to the Wigner function can also be used as input for dynamical calculations which involve solving the Vlasov equation with collision integrals (Schuck and Winter 1982). Extensive studies of both static and dynamic properties of nuclei using exact and approximate Wigner functions have been made (Bertsch 1975, 1978, Ring and Schuck 1980, Kolomietz and Tang 1981, Brink and di Toro 1981).

In order to obtain some insight into this problem it is instructive to consider the case where V is a harmonic oscillator potential giving the Hamiltonian

$$H = \sum_{j=1}^A ((\mathbf{p}_j^2/2m) + \frac{1}{2}m\omega^2 \mathbf{q}_j^2) \quad (1.4)$$

where the sum on j runs over all A particles in the system. In this case if we consider a degenerate system of fermions completely filling a certain number of oscillator shells, then $F(\mathbf{q}, \mathbf{p})$ depends only on the 'energy'

$$\varepsilon = (\mathbf{p}^2/2m) + \frac{1}{2}m\omega^2 \mathbf{q}^2 \quad (1.5)$$

and for the N -dimensional case we may write F in terms of the associated Laguerre functions L_K^{N-1} (Magnus *et al* 1966) as (Shlomo and Prakash 1981)

$$F_M^N(\varepsilon) = \sum_{K=0}^M f_K^N(\varepsilon) = \frac{e^{-2\tilde{\varepsilon}}}{(\hbar\pi)^N} \sum_{K=0}^M (-1)^K L_K^{N-1}(4\tilde{\varepsilon}) \quad (1.6)$$

where $\tilde{\varepsilon} = \varepsilon/\hbar\omega$ is the energy in units of the oscillator level spacing and $f_K^N(\varepsilon)$ is the Wigner function of the K th shell. The last full shell is the M th and the system contains, therefore, a total number of particles

$$A(N, M) = \sum_{K=0}^M g_K^N = \sum_{K=0}^M \binom{K+N-1}{K} = \binom{M+N}{M} \quad (1.7)$$

where g_K^N is the degeneracy of the K th shell in N dimensions. The above values of A and of F_M^N correspond to one particle in each oscillator state and both should be

multiplied by the appropriate spin (s) and isospin (t) degeneracies (i.e. by $(2s + 1)$ and $(2t + 1)$) appropriate to the physical system in question.

The above problem of the oscillatory structure in $F_M^N(\epsilon)$ has to some extent been studied numerically by Prakash *et al* (1981) and our aim in the present paper is to derive some simple closed-form approximations to these oscillations which will permit a general discussion of the conditions under which they may be neglected. Since the above expression (1.6) corresponds to the last full oscillator shell having energy $\epsilon_M = (M + \frac{1}{2}N)\hbar\omega$ and the first empty shell having energy $\epsilon_{M+1} = (M + 1 + \frac{1}{2}N)\hbar\omega$ we take the Fermi energy of the system to be half-way between these levels i.e.

$$\epsilon_F = [M + \frac{1}{2}(N + 1)]\hbar\omega = \gamma\hbar\omega. \tag{1.8}$$

It will then often be convenient to work in terms of ϵ_F as our energy unit (this is rather natural if one is interested in the ‘macroscopic’ properties of the system) and we define

$$z = \epsilon/\epsilon_F = \tilde{\epsilon}/\gamma \tag{1.9}$$

as our new variable in this case. (Note that this gives $\partial/\partial\epsilon = \epsilon_F^{-1}\partial/\partial z$.) In terms of this quantity equation (1.6) then becomes

$$F_M^N(\epsilon) = \sum_{K=0}^M f_K^N(\epsilon) = \frac{\exp(-2\gamma z)}{(\hbar\pi)^N} \sum_{K=0}^M (-1)^K L_K^{N-1}(4\gamma z). \tag{1.10}$$

We shall see later that in the limit of large $\gamma = M + \frac{1}{2}(N + 1)$ (i.e. a ‘macroscopic’ number of particles) we find the result

$$(2\pi\hbar)^N \lim_{\gamma \rightarrow \infty} F_M^N(\epsilon) = 1 \tag{1.11}$$

for any fixed ϵ in the range $0 < \epsilon < \epsilon_F$ (i.e. for $0 < z < 1$). Anticipating this result we work, henceforth, in terms of a dimensionless ‘normalised’ Wigner function defined by $\bar{F}_M^N(\epsilon) = (2\pi\hbar)^N F_M^N(\epsilon)$ and write equation (1.10) in the form

$$\bar{F}_M^N(\epsilon) = \sum_{K=0}^M \bar{f}_K^N(\epsilon) \tag{1.12}$$

with

$$\bar{f}_K^N(\epsilon) = (-1)^K 2^N \exp(-2\gamma z) L_K^{N-1}(4\gamma z). \tag{1.13}$$

This will facilitate the comparison of our results for different dimensionalities. Note also that for large M equation (1.7) becomes

$$A(N, M) \sim (1/N!)\gamma^N. \tag{1.14}$$

The above equation (1.13) now contains no reference to the level spacing $\hbar\omega$ and the limit $\gamma \rightarrow \infty$ may be taken for any value of this quantity. However, if we take this limit at a fixed Fermi energy $\epsilon_F = \gamma\hbar\omega$ (physically of course we do not want $\epsilon_F \rightarrow \infty$) then this corresponds to taking $\gamma \rightarrow \infty$ with $\hbar\omega \rightarrow 0$ and may then be thought of as a sort of semiclassical limit (Berry 1977) though it is very different from the case $\hbar\omega \rightarrow 0$ at fixed particle number. (We shall see though that our approximations are good, even for relatively small particle numbers.)

Note that the case of increasing particle number and decreasing oscillator frequency at fixed Fermi energy is similar to the nuclear structure problem for which $\hbar\omega \approx 41A^{-1/3}$ MeV. Since in three dimensions equation (1.14) gives $A \sim \frac{2}{3}\gamma^3$ (accounting

for a factor 4 from spin and isospin degeneracy) the above relation is equivalent to $\hbar\omega \approx 47/\gamma$ MeV as in equation (1.8).

In addition to the case of filled oscillator shells the formulae we shall derive will also allow us to study in a simple manner the half-full shell and the problem of a system of almost degenerate fermions at some finite temperature T , for which the structure in F may be appreciably damped (Prakash *et al* 1981, Heller 1976).

2. Integral expressions for \bar{F}_M^N

It may be shown (Shlomo and Prakash 1981) that the Wigner function defined in equation (1.6) may be related to the Wigner function of a *single* shell in a system of *higher* dimensionality by the expression

$$F_M^N(\varepsilon) = \frac{2\pi}{\omega} \int_{\varepsilon}^{\infty} f_M^{N+1}(\varepsilon') d\varepsilon'. \quad (2.1)$$

In terms of the quantities \bar{F}_M^N and γ this may be written

$$\bar{F}_M^N(\varepsilon) = \frac{\gamma}{\varepsilon_F} \int_{\varepsilon}^{\infty} \bar{f}_M^{N+1}(\varepsilon') d\varepsilon' \quad (2.2)$$

and we may now consider if this is suitable for obtaining analytic approximations. The great advantage of this integral is that it contains a single value of the oscillator shell number unlike the sum in equation (1.6) which contains all shells $K = 0$ to M . For large M we may, therefore, replace \bar{f}_M^{N+1} by some asymptotic approximation and Balazs and Zipfel (1973) have used an Airy function in the above formula. In terms of the Airy function (Abramowitz and Stegun 1965) we may write for large γ

$$\begin{aligned} \bar{f}_M^{N+1}(\varepsilon) &= (-1)^K 2^N \exp(-2\gamma z) L_K^N(4\gamma z) \\ &\approx 2^{2/3} \gamma^{-1/3} \text{Ai}((2\gamma)^{2/3}(z-1)) \end{aligned} \quad (2.3)$$

and thus obtain

$$\begin{aligned} \bar{F}_M^N(\varepsilon) &\approx (2\gamma)^{2/3} \int_{\varepsilon/\varepsilon_F}^{\infty} \text{Ai}((2\gamma)^{2/3}(z-1)) dz \\ &\approx \int_{x_0}^{\infty} \text{Ai}(x) dx, \end{aligned} \quad (2.4)$$

with $x_0 = (2\gamma)^{2/3}(\varepsilon/\varepsilon_F - 1)$. This approximation is, however, unsatisfactory since the Airy function expression is valid only in the region $|1 - \varepsilon/\varepsilon_F| \leq (2\gamma)^{-2/3}$ whereas the integral contains values of the argument outside this range and fails to reproduce correctly the oscillatory structure in \bar{F} . However, the expression may be used (Balazs and Zipfel 1973, 1974) to derive the asymptotic value of \bar{F} at $\varepsilon = \varepsilon_F$

$$\bar{F}_M^N(\varepsilon_F) \approx \int_0^{\infty} \text{Ai}(x) dx = \frac{1}{3} \quad (2.5)$$

since at the positive values of $\varepsilon - \varepsilon_F$ for which the Airy function is not a good approximation, the exact $\bar{f}_M^{N+1}(\varepsilon)$ is small.

We may also differentiate equation (2.2) to obtain

$$\partial \bar{F}_M^N(\varepsilon) / \partial \varepsilon = -(\gamma/\varepsilon_F) \bar{f}_M^{N+1}(\varepsilon) \quad (2.6)$$

and for $\epsilon \approx \epsilon_F$ we may use the Airy function expression (2.3) to obtain a good approximation to this derivative. In particular

$$\partial \bar{F}_M^N(\epsilon) / \partial \epsilon |_{\epsilon_F} = -((2\gamma)^{2/3} / \epsilon_F) \text{Ai}(0) = -0.355((2\gamma)^{2/3} / \epsilon_F) \tag{2.7}$$

which is exact in the limit of large γ , when F falls rapidly to zero for $\epsilon > \epsilon_F$.

We see, therefore, that the problem of finding an approximation to $\bar{F}_M^{N+1}(\epsilon)$ for all $\epsilon > 0$ makes equation (2.2) unsuitable for our purposes. We shall now derive an alternative integral formula which is more amenable to approximations and which has the further advantage of naturally separating \bar{F} into its 'classical' value plus a term which produces oscillations about this.

By introducing a convergence factor $\exp(-\alpha K)$ we may write the sum in equation (1.12) in the form

$$\bar{F}_M^N(\epsilon) = \lim_{\alpha \rightarrow 0} \left(\sum_{K=0}^{\infty} \bar{f}_K^N(\epsilon) e^{-\alpha K} - \sum_{K=M+1}^{\infty} \bar{f}_K^N(\epsilon) e^{-\alpha K} \right), \tag{2.8}$$

where $\bar{f}_K^N(\epsilon)$ is given by (1.13). Using the generating function (Magnus *et al* 1966)

$$\sum_{K=0}^{\infty} L_K^{N-1}(x) y^K = (1-y)^{-N} \exp\left(\frac{xy}{y-1}\right) \tag{2.9}$$

with $y = -e^{-\alpha}$ we then find

$$\lim_{\alpha \rightarrow 0} \sum_{K=0}^{\infty} \bar{f}_K^N(\epsilon) e^{-\alpha K} = 1 \tag{2.10}$$

which is the 'classical' value of \bar{F} mentioned in § 1. Therefore, we have

$$\bar{F}_M^N(\epsilon) = 1 + \tilde{F}_M^N(\epsilon), \tag{2.11}$$

where we shall find that

$$\tilde{F}_M^N(\epsilon) = -\lim_{\alpha \rightarrow 0} \sum_{K=M+1}^{\infty} \bar{f}_K^N(\epsilon) e^{-\alpha K} \tag{2.12}$$

is responsible for the oscillatory structure in F (quantal oscillations) for $\epsilon < \epsilon_F$ and vanishes for large γ as $\gamma^{-1/2}$. Of course for $\epsilon > \epsilon_F$ the full Wigner function decreases rapidly to zero and we must, therefore, have $\tilde{F} \approx -1$ in this region.

We may now write this sum as an integral in the complex K -plane

$$\tilde{F}_M^N = 2^{N-1} e^{-2\gamma z} i \lim_{\alpha \rightarrow 0} \int_C \frac{L_K^{N-1}(4\gamma z) e^{-\alpha K} dK}{\cos \pi(K - \frac{1}{2})} \tag{2.13}$$

where the contour C encloses the positive real axis from a point between M and $M+1$ and $+\infty$. The convergence factor now merely ensures that we have no contribution from large $\text{Re } K$ and since the function L_K^{N-1} has no singularities for $\text{Re } K > 0$ we may simply take C to be a line parallel to the imaginary K -axis. Crossing the real axis at $K = M + \frac{1}{2}$ we then obtain

$$\tilde{F}_M^N(\epsilon) = (-1)^M 2^{N-1} e^{-2\gamma z} \int_{-\infty}^{\infty} \frac{L_{M+1/2+iy}^{N-1}(4\gamma z)}{\cosh \pi y} dy. \tag{2.14}$$

This expression now provides a means of employing a large- M approximation valid for fixed ϵ and has the further advantage that the limits of integration are not variable as in (2.1).

3. Properties of $\bar{F}_M^N(\epsilon)$

We show in appendix 1 that an asymptotic expression suitable for our purposes is given by

$$\bar{f}_K^N(\epsilon) = (-1)^K 2^N e^{-2\alpha\epsilon} L_K^{N-1}(4\alpha\xi) = (2/\pi\alpha)^{1/2} [\xi^{(N-1/2)/2}]^{-1} (1-\xi)^{-1/4} \cos \omega, \quad (3.1)$$

where

$$\alpha = \alpha(K, N) = K + \frac{1}{2}N, \quad \xi = \tilde{\epsilon}/\alpha = \gamma z/\alpha, \quad (3.2a, b)$$

$$\omega = 2\alpha \{ \sin^{-1}(1-\xi)^{1/2} - [\xi(1-\xi)]^{1/2} \} - \frac{1}{4}\pi. \quad (3.2c)$$

This expression is the first term in an asymptotic expansion of f for large α and fixed ξ in the region $0 < \xi < 1$. For a given value of α , however, it is a good approximation to $\bar{f}_K^N(\epsilon)$ for $\xi \gg \alpha^{-2}$ and $(1-\xi) \geq (2\alpha)^{-2/3}$. Our approximation and the exact \bar{f}_K^N are compared in figure 1 for $N = 3, K = 5$.

It is interesting at this point to reflect on the importance of the quantity $\gamma = \epsilon_F/\hbar\omega$ introduced in § 1. We have seen (equation (2.6)) that the derivative $\partial\bar{F}_M^N(\epsilon)/\partial\epsilon$ is exactly proportional to $\bar{F}_M^{N+1}(\epsilon)$ and we now see that for the latter combination of shell number and dimensionality we have from equation (3.2a)

$$\alpha(M, N + 1) = M + \frac{1}{2}(N + 1) = \gamma = \epsilon_F/\hbar\omega \quad (3.3a)$$

and thus from (3.2b)

$$\xi = \tilde{\epsilon}/\gamma = z = \epsilon/\epsilon_F \quad (3.3b)$$

and from (3.2c)

$$\omega = 2\gamma \{ \sin^{-1}(1-z)^{1/2} - [z(1-z)]^{1/2} \} - \frac{1}{4}\pi. \quad (3.3c)$$

Therefore, all the maxima and minima in the full Wigner function \bar{F}_M^N occur (within our approximation) at values of $z = \epsilon/\epsilon_F$ for which

$$2\gamma \{ \sin^{-1}(1-z)^{1/2} - [z(1-z)]^{1/2} \} = (n + \frac{3}{4})\pi, \quad (3.4)$$

with $n = 0, 1, 2, \dots$. In particular the last maximum (see figure 2) occurs for $z \approx 1$ in which region we may write

$$\omega \approx \frac{2}{3} [(2\gamma)^{2/3}(1-z)]^{3/2} - \frac{1}{4}\pi. \quad (3.5)$$

Thus for $z \approx 1$ the positions of the oscillations depend on the same combination $(2\gamma)^{2/3}(1-z)$ as the Airy function and give the last maximum at

$$z_{\max} = \frac{\epsilon_{\max}}{\epsilon_F} = 1 - \left(\frac{9\pi}{16\gamma} \right)^{2/3} = 1 - \frac{2.32}{(2\gamma)^{2/3}} \quad (3.6)$$

compared with $1 - 2.33/(2\gamma)^{2/3}$ for the Airy function (Balazs and Zipfel 1973, 1974). Note, however, that for smaller values of z our approximation (unlike the Airy function) no longer depends simply on the above parameters and reproduces the oscillatory structure in \bar{F} rather well (see figure 2).

In addition to \bar{f}_M^{N+1} giving the combination $\alpha(M, N + 1) = M + \frac{1}{2}(N + 1) = \gamma$ we see from equation (2.14) that in order to evaluate \bar{F}_M^N we must expand the Laguerre function about the point $K = M + \frac{1}{2}$ and thus we again obtain $\alpha(M + \frac{1}{2}, N) = M + \frac{1}{2}(N + 1) = \gamma$. The evaluation of the resulting integral is performed in appendix 2 and

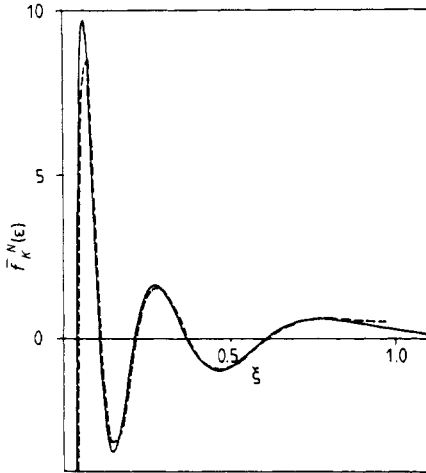


Figure 1. The exact 'normalised' Wigner function $\bar{f}_K^N(\epsilon)$ for a single full shell ($K=5$ in three dimensions) is shown by the full curve. The broken curve shows the approximation of (3.1) to this quantity which is plotted as a function of $\xi = \epsilon/(K + \frac{1}{2}N)\hbar\omega$.

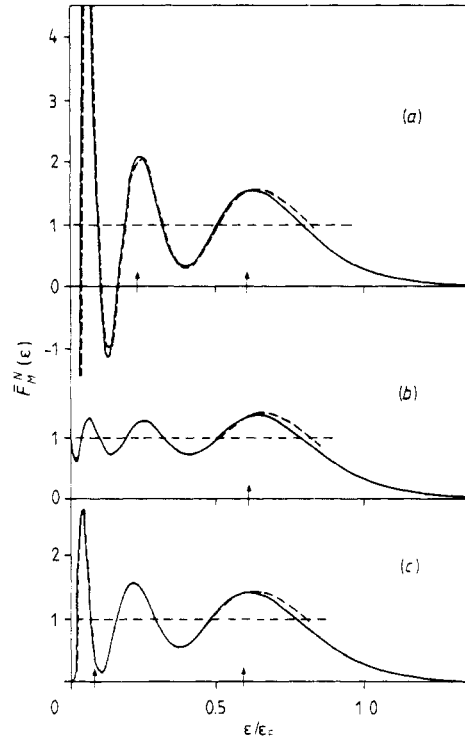


Figure 2. (a) The exact (full curve) and approximate (broken curve) normalised Wigner functions $\bar{F}_M^N(\epsilon)$ are shown for $M=5$, $N=3$ as a function of ϵ/ϵ_F (equations (1.12) and (3.7)). Also indicated is the position at which the last maximum occurs (as calculated from equation (3.6)) and the point below which the oscillating contribution may exceed unity (as calculated by (3.11)). The height of the first maximum which is cut off in this figure is about 6.7. (b) As (a) but for $M=6$, $N=1$. Note that both (a) and (b) correspond to $\gamma = M + \frac{1}{2}(N+1) = 7$ and thus the structure occurs in both cases at almost exactly the same points. However since (b) is two dimensions lower than (a) the magnitude of the structure is reduced by approximately a factor of ϵ/ϵ_F . (c) As (a) and (b) but for $M=5$, $N=2$. This figure corresponds, therefore, to only half filling the 5th shell in three dimensions (see equation (4.4)) and the structure seen in figure 1(a) is reduced here by about a factor of $(\epsilon/\epsilon_F)^{1/2}$.

leads to our central result

$$\bar{F}_M^N(\epsilon) \approx 1 + [\cos \phi / (2\pi\gamma)^{1/2} z^{(N-1/2)/2} (1-z)^{3/4}] \tag{3.7}$$

(where now $\gamma = M + \frac{1}{2}(N+1)$ and $z = \epsilon/\epsilon_F$) with

$$\phi = \phi(\gamma, z) = 2\gamma\{\sin^{-1}(1-z)^{1/2} - [z(1-z)]^{1/2}\} - \frac{3}{4}\pi. \tag{3.8}$$

This is valid asymptotically for fixed z in the region $0 < z < 1$ as $\gamma \rightarrow \infty$. However, for

a given γ it is a good approximation for $z \gg \gamma^{-2}$ and $(1-z) \gg (2\gamma)^{-2/3}$. Since we are principally concerned with the oscillations in F the fact that our formulae are not valid for $\varepsilon \gg \varepsilon_F$ is no real problem.

We saw above that for $z \approx 1$ the positions of the oscillations in \bar{F} depended only on $(2\gamma)^{2/3}(1-z)$ and we now see that this is also true of their magnitude since we may write for $z \approx 1$

$$\bar{F}_M^N(\varepsilon) \approx 1 + \left\{ \cos\left[\frac{4}{3}\gamma(1-z)^{3/2} - \frac{3}{4}\pi\right] / \pi^{1/2} [(2\gamma)^{2/3}(1-z)]^{3/4} \right\} \tag{3.9}$$

though again this ceases to be true for smaller z for which our full approximation is more correct.

In particular there is a dependence on the dimensionality N through the term $z^{-(N-1/2)/2}$ which gives stronger oscillations for systems of higher dimensionalities. We find though the height of the last maximum as

$$\begin{aligned} \bar{F}(z_{\max}) &\approx 1 + \frac{4}{3\pi 2^{1/2}} \left[1 + \frac{1}{2}(N - \frac{1}{2}) \left(\frac{9\pi}{16\gamma} \right)^{2/3} \right] \\ &= 1 + 0.30 \left[1 + \frac{1}{2}(N - \frac{1}{2}) \left(\frac{9\pi}{16\gamma} \right)^{2/3} \right] = 1.30 + O(\gamma^{-2/3}) \end{aligned} \tag{3.10}$$

which is actually independent of N and γ in the limit $\gamma \rightarrow \infty$. The above dependence means, however, that in higher dimensionalities the oscillations in the Wigner function may become of order unity at larger values of $\varepsilon/\varepsilon_F$ (and thus F may become negative over a greater region for larger N). Equation (3.7) shows that for dimensionality N this may occur for

$$\varepsilon < \varepsilon_0 = z_0 \varepsilon_F = \varepsilon_F (2\pi\gamma)^{-1/(N-1/2)} \tag{3.11}$$

which is valid only for $N > 1$ since for $N = 1$ this formula predicts a value of z_0 in a region where our approximation is not valid.

Some of the above points are demonstrated in figure 2. In figures 2(a) and 2(b) we show \bar{F}_M^N for $M = 5, N = 3$ and $M = 6, N = 1$. Both of these combinations correspond to $\gamma = 7$ and we see that even for this relatively small value of γ our expression (3.7) (broken curve) is already a rather good approximation to the exact \bar{F}_M^N of equation (1.6) (full curve). Although both these Wigner functions have $\gamma = 7$ they correspond to very different particle numbers $A = 56$ and 6 respectively.

As predicted by equations (3.7) and (3.8) we see that the positions of the oscillations depend only on γ but that their magnitude also depends explicitly on N . The position of the last maximum as predicted by equation (3.6) is shown in these figures and for $N = 3$ we also show the point below which the magnitude of the oscillating term will exceed unity and may render the Wigner function negative. These values are seen to be in good agreement with the numerical calculations.

As M and hence γ increase, the quality of our approximation improves and we see, therefore, that in the 'classical' limit the oscillations in the Wigner function vanish as $\gamma^{-1/2}$ for any fixed value of $\varepsilon/\varepsilon_F$. However, since the frequency of the oscillations increases with γ we see that the structure in quantities such as the density

$$\rho(\mathbf{q}) = \int F_M^N(\mathbf{q}, \mathbf{p}) \, d\mathbf{p}^N \tag{3.12}$$

decreases rather faster than this. For a three-dimensional system we have

$$\rho(q) = \frac{4\pi}{(2\pi\hbar)^3} \int_0^\infty \bar{F}(\epsilon) p^2 dp \tag{3.13}$$

or using equation (1.5)

$$\rho(q) = \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} \int_{V(q)}^\infty \bar{F}(\epsilon)(\epsilon - V(q))^{1/2} d\epsilon \tag{3.14}$$

where $V(q) = \frac{1}{2}m\omega^2q^2$. Applying the above results we may approximately write, for $V(q) < \epsilon_F$ (since for large γ , $\bar{F} \rightarrow 0$ rapidly for $\epsilon > \epsilon_F$),

$$\begin{aligned} \rho(q) &= \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} \left(\int_{V(q)}^{\epsilon_F} (\epsilon - V(q))^{1/2} d\epsilon + \int_{V(q)}^{\epsilon_F} \tilde{F}(\epsilon)(\epsilon - V(q))^{1/2} d\epsilon \right) \\ &= \rho_{TF}(q) + \tilde{\rho}(q) \end{aligned} \tag{3.15}$$

where

$$\rho_{TF} = \frac{2}{3\pi^2} \left(\frac{2m(\epsilon_F - \frac{1}{2}m\omega^2q^2)}{\hbar^2} \right)^{3/2} \tag{3.16}$$

is the Thomas–Fermi approximation to the density and $\tilde{\rho}$ is an oscillating term involving the oscillatory part of the Wigner function. The function \tilde{F} decreases as $\gamma^{-1/2}$ except near to ϵ_F , where the maximum period of the oscillations decreases as $\gamma^{-2/3}$ (see equation (3.5)) and we may write, therefore,

$$\rho(q) \approx \rho_{TF}(q) + O(\gamma^{-2/3}). \tag{3.17}$$

Note that in the limit $\omega \rightarrow 0$ at constant Fermi energy, ρ_{TF} tends to the Fermi gas value $2k_F^3/3\pi^2$ for finite q . Also the ‘radius’ R of the system (defined as the point at which $\rho_{TF}(R) = 0$) is given by

$$R = (2\epsilon_F/m\omega^2)^{1/2} = 2\gamma/k_F \tag{3.18}$$

and so in three dimensions with a fixed Fermi energy (as in the nuclear physics case) we have

$$R = R_0 A^{1/3}. \tag{3.19}$$

All the above discussions have been based on a system of degenerate fermions completely filling the first M shells of an oscillator potential. We shall now relax this constraint to consider firstly the case of the half-full shell and secondly a system of almost degenerate fermions at a finite temperature T such that $kT \ll \epsilon_F$.

4. The half-full shell

Our definition of the half-full shell is that the occupation numbers for all states of the (degenerate) M th oscillator shell are $\frac{1}{2}$ and all lower shells are full. This essentially corresponds, therefore, to a *thermal* distribution with $kT \ll \hbar\omega$ and $\epsilon_F = (M + \frac{1}{2}N)\hbar\omega$ since the spacing of the levels in a given shell is zero. In this case we denote our

Wigner function by $\bar{F}_{M(1/2)}^N(\epsilon)$ and write

$$\bar{F}_{M(1/2)}^N(\epsilon) = \sum_{K=0}^{M-1} \bar{f}_K^N(\epsilon) + \frac{1}{2} \bar{f}_M^N(\epsilon) = \frac{1}{2} \sum_{K=0}^M \bar{f}_K^N(\epsilon) + \frac{1}{2} \sum_{K=0}^{M-1} \bar{f}_K^N(\epsilon) = \frac{1}{2}(\bar{F}_M^N(\epsilon) + \bar{F}_{M-1}^N(\epsilon)). \tag{4.1}$$

In other words the Wigner function, if the last shell is only half full, is just the arithmetic mean for the two adjacent closed shells. Balazs and Zipfel (1973) use such an arithmetic mean to damp out the oscillations in the case of $N = 1$. Using equation (2.1) we may write

$$\bar{F}_{M(1/2)}^N(\epsilon) = \frac{1}{\hbar\omega} \int_{\epsilon}^{\infty} \frac{1}{2}(\bar{f}_M^N(\epsilon') + \bar{f}_{M-1}^N(\epsilon')) d\epsilon' \tag{4.2}$$

and since (Magnus *et al* 1966)

$$L_M^{N-1}(x) - L_{M-1}^{N-1}(x) = L_M^{N-2}(x) \tag{4.3}$$

we then obtain using equation (1.13)

$$\bar{F}_{M(1/2)}^N(\epsilon) = \frac{1}{\hbar\omega} \int_{\epsilon}^{\infty} \bar{f}_M^{N-1}(\epsilon') d\epsilon' = \bar{F}_M^{N-1}(\epsilon). \tag{4.4}$$

Therefore, the Wigner function for a system with the last shell half full is just proportional to the Wigner function for the same shell closed but in one dimension *lower*. In figure 2(c) we show $\bar{F}_5^2(\epsilon)$ and we see from the above results that this is also equal to $\bar{F}_{5(1/2)}^3(\epsilon)$. Thus the oscillations seen in figure 2(a) with the 5th shell filled are reduced to those seen in figure 2(c) if the 5th is only half filled. Note, that $F_M^{N-1}(\epsilon)$ corresponds to a Fermi energy $\epsilon_F = (M + \frac{1}{2}N)\hbar\omega$ but that this is exactly what we require in N dimensions if we only wish the M th shell to be half full (see also § 5). Note also from equation (3.7) that the above ‘reduction of dimensionality’ essentially damps the oscillations by a factor $z^{1/2}$.

Since the half-full shell behaves somewhat more ‘classically’ than the full shell then the smooth approximations taken to nuclear Wigner functions in the study of deep-inelastic reactions may be more appropriate for nuclei between closed shells (though the degree of damping is not very great). We shall now show, however, that the introduction of a finite temperature can produce substantially more damping than that given by choosing our last shell to be half full.

5. Temperature smoothing of \bar{F}

At a finite temperature T and for a Fermi energy $\epsilon_F = (\lambda + \frac{1}{2}N)\hbar\omega$ we may write the normalised Wigner function as

$$\bar{F}^N(\lambda, \beta, \epsilon) = \sum_{K=0}^{\infty} n_K \bar{f}_K^N(\epsilon), \tag{5.1}$$

where

$$n_K = \{1 + \exp[(K - \lambda)/\beta]\}^{-1} \tag{5.2}$$

with

$$\beta = kT/\hbar\omega = (kT/\epsilon_F)(\lambda + \frac{1}{2}N). \tag{5.3}$$

By introducing the convergence factor $e^{-\alpha K}$ again we may write equation (5.1) in the form

$$\begin{aligned} \bar{F}^N(\lambda, \beta, \varepsilon) &= \lim_{\alpha \rightarrow 0} \left(n_0 \sum_{K=0}^{\infty} \bar{f}_K^N(\varepsilon) e^{-\alpha K} + \sum_{K=1}^{\infty} \left[(n_{K-1} - n_K) \sum_{j=K}^{\infty} \bar{f}_j^N(\varepsilon) e^{-\alpha j} \right] \right) \\ &= n_0 + \sum_{K=0}^{\infty} (n_K - n_{K+1}) \tilde{F}_K^N(\varepsilon) \end{aligned} \tag{5.4}$$

which is just an exact rearrangement of the sum (5.1) and $\tilde{F}_K^N(\varepsilon)$ is defined in (2.12). Note that for the full-shell case we have $n_K - n_{K+1} = \delta_{K,M}$. If our fermions are almost degenerate we have $\beta \ll \lambda$ (i.e. $kT \ll \varepsilon_F$) and thus $n_0 \approx 1$ and also the coefficients $(n_K - n_{K+1})$ in equation (5.4) are non-zero only for values of K such that

$$|K - \lambda| \approx \beta \ll \lambda. \tag{5.5}$$

Thus we see that the period of the oscillations in the finite temperature problem must be characteristic of the shell number corresponding to the Fermi energy. In appendix 3 we use equation (5.4) to derive a simple approximation to the temperature-smoothed Wigner function. We find that for $\beta \gg 1/2\pi^2$ (cf Bohr and Mottelson 1975) and for ε not too near ε_F

$$\begin{aligned} \bar{F}^N(\lambda, \beta, \varepsilon) &= 1 + \{D(\beta, z)/(2\pi\gamma)^{1/2} z^{(N-1/2)/2} (1-z)^{3/4}\} \\ &\quad \times [\cos \phi - \cos(\phi - 2\pi\lambda) \exp(-4\pi\beta z^{1/2})] \end{aligned} \tag{5.6}$$

where ϕ and z are defined as in (3.8) but now with $\gamma = \varepsilon_F/\hbar\omega = \lambda + \frac{1}{2}N$ and the 'damping function' D is given by

$$D(\beta, z) = 2\pi\beta(1-z)^{1/2}/\sinh[2\pi\beta \sin^{-1}(1-z)^{1/2}] \tag{5.7}$$

and is independent of both λ and N . We see from (5.6) that for $z \gg (4\pi\beta)^{-2}$ the second term in square brackets may be neglected and we have simply

$$\bar{F}^N(\lambda, \beta, \varepsilon) = 1 + \tilde{F}_\lambda^N(\varepsilon)D(\beta, z), \tag{5.8}$$

i.e. the oscillations are given by the closed shell expression (3.7) (but note that λ is now a *continuous* variable) modified simply by the function D . We have seen, however, that for $T = 0$ the oscillations in the Wigner function depend quite sensitively on the choice of λ ; in particular if we choose λ to be an integer then we obtain a half-full shell. In this case F suffers a 'reduction of dimensionality' and the oscillations are essentially damped by a factor $z^{1/2}$. The remnants of this effect at finite temperature can be seen from the term in square brackets in equation (5.6). If λ is an integer then this becomes $4\pi\beta z^{1/2} \cos \phi$ for small z , whereas for half-integral values of λ we obtain $2 \cos \phi$.

It is clear from equation (5.7) that we obtain little change in the Wigner function in the region of the Fermi energy ($D(\beta, z) \rightarrow 1$ for $z \rightarrow 1$) whereas at small energies the damping may be large $D(\beta, 0) = 4\pi\beta \exp(-\pi^2\beta)$. For $\beta \approx 0.3$ this gives $D(\beta, 0) \approx 20\%$ and for $\beta \approx 0.6$ we have $D(\beta, 0) \approx 2\%$.

In figures 3(a) and (b) we show by the full curves the exact temperature-smoothed Wigner function (5.1) for $\lambda = 5.5$ with (a) $\beta = 0.3$ and (b) $\beta = 0.6$ for a three-dimensional system. The broken curves in these figures show the approximation (5.6) to these functions. The full curve in figure 4 shows the same quantity for $\lambda = 20.5$ and $\beta = 0.6$ and the broken curves show the envelopes of the oscillations for $\beta = 0.3$ and $\beta = 0$.

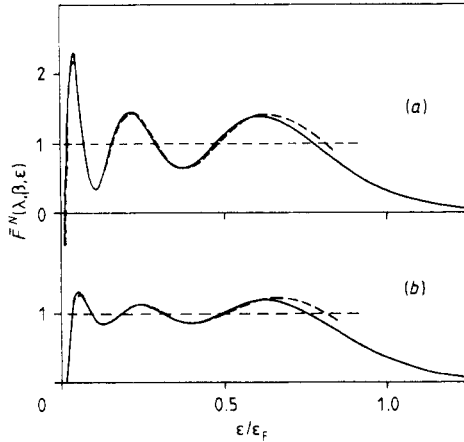


Figure 3. (a) The normalised Wigner function $\bar{F}^N(\lambda, \beta, \epsilon)$ is shown for $N = 3$, $\lambda = 5.5$ and $\beta = kT/\hbar\omega = 0.3$ as a function of ϵ/ϵ_F with $\epsilon_F = (\lambda + \frac{1}{2}N)\hbar\omega$. The broken curve shows the approximation of (5.6). Although the structure is considerably reduced from that seen in figure 1(a) (corresponding to $\beta = 0$) it is by no means negligible. (b) As (a) but for a higher temperature $\beta = 0.6$. In a nuclear problem these figures would roughly correspond to $A = 224$ ($N = Z = 112$) and to temperatures of about 2.5 and 5 MeV respectively.

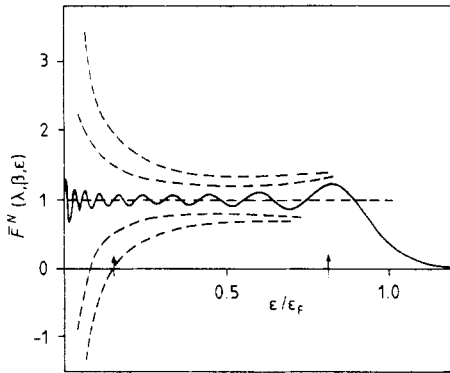


Figure 4. As figure 3 but with $\lambda = 20.5$ and $\beta = 0.6$. The broken curves show the envelopes of the oscillations for $\beta = 0.3$ and the largest case of $\beta = 0$.

In dynamical nuclear calculations it is common to use a smoothed Wigner function as input (see the references cited in § 1) on the grounds that the temperature induced by the reaction will damp out much of the structure in F . In this respect the quantities in figure 3 are relevant since they correspond to a particle number of 224 (including a factor 4 for spin and isospin degeneracy) and thus correspond to what one might expect for a heavy nucleus. In this mass region we have $\hbar\omega \approx 8$ MeV and thus at a nuclear temperature $kT \approx 2.5$ MeV ($\beta \approx 0.3$) the Wigner function still possesses a considerable degree of structure and one should be careful to check that this does not seriously affect the conclusions of any calculations made using a smooth approximation. Of course in this mass region the oscillator potential is not really appropriate though one might expect a similar amount of structure from other potentials.

We have seen in § 3 that for any fixed value of $\epsilon/\epsilon_F < 1$ the structure in F vanishes as $\gamma^{-1/2}$ as $\gamma \rightarrow \infty$. We have also seen, however, that the height of the last maximum in \bar{F} is about 1.30 (the difference being that this maximum is not at a fixed value of z but occurs at the point where $(1 - \epsilon/\epsilon_F)(2\gamma)^{2/3} \approx 2.32$) and it is interesting, therefore, to speculate on the temperature \tilde{T} at which even the oscillations in this region are damped. Near the last maximum we have $1 - z \sim \gamma^{-2/3}$ and thus D simply becomes

$$D \approx 2x e^{-x} \tag{5.9}$$

with $x \sim 2\pi\tilde{\beta}\gamma^{-1/3}$. To obtain significant damping we clearly require $x \gg 1$ and thus $\tilde{\beta} \gg \gamma^{1/3}/2\pi$. Thus $\tilde{\beta}$ is an increasing function of γ . However, we have $\tilde{\beta} = k\tilde{T}/\hbar\omega$ whereas the quantity which determines whether our fermions are degenerate or not is $k\tilde{T}/\epsilon_F = \tilde{\beta}/\gamma$. We thus find that for large particle numbers the value of the temperature at which the Wigner function has no quantal oscillations is given by

$$k\tilde{T} = \epsilon_F \tilde{\beta}/\gamma \gg \epsilon_F/2\pi\gamma^{2/3} \tag{5.10}$$

which vanishes as $A^{-2/9}$ for a three-dimensional system.

6. Particle number and Fermi energy at finite temperature

At a finite temperature we must, of course, choose the Fermi energy (or in our notation λ) to reproduce the correct particle number A for the system. Writing A as a function of β and λ we have

$$A(\beta, \lambda) = \sum_{K=0}^{\infty} n_K(\beta, \lambda) g_K. \tag{6.1}$$

Since we shall only consider the three-dimensional system in this section we have

$$g_K = \binom{K+N-1}{K} = \frac{1}{2}(K+1)(K+2) \tag{6.2}$$

in the above equation. For a reason which will become apparent later we now formally include the term $K = -1$ in the above sum (note that $g_{-1} = 0$) to obtain

$$A(\beta, \lambda) = \sum_{K=-1}^{\infty} n_K(\beta, \lambda) g_K = \sum_{K=0}^{\infty} n_{K-1}(\beta, \lambda) g_{K-1}. \tag{6.3}$$

This sum may now be written (exactly) using the Poisson summation formula (Lighthill 1958) as

$$\begin{aligned} A(\beta, \lambda) &= \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} n_{K-3/2}(\beta, \lambda) g_{K-3/2} \exp(2\pi m i K) dK \\ &= \sum_{m=-\infty}^{\infty} \int_{-3/2}^{\infty} n_K(\beta, \lambda) g_K \exp(2\pi m i K) dK. \end{aligned} \tag{6.4}$$

The terms $m \neq 0$ may now be evaluated by contour integration. For $m > 0$ we integrate upwards parallel to the imaginary axis and then close the contour around the first quadrant picking up half the poles of $n_K(\beta, \lambda)$ which occur at $K = \lambda + (2n + 1)\pi i\beta$. Similarly for $m < 0$ we close around the fourth quadrant. The advantage of having $K = -\frac{3}{2}$ as the lower limit in equation (6.4) is that it may be readily shown that all the background integrals (sections parallel to the imaginary axis) now cancel pairwise

for the terms in m and $-m$, and this was the reason for including $K = -1$ in equation (6.3). The sum of all the pole terms obtained in this way is discontinuous for integral λ in the limit $\beta \rightarrow 0$ and this simply corresponds to the abrupt addition of a further shell as λ increases at zero temperature. However, for finite β the sum is well defined for all λ and generates a term of order $\exp(-2\pi^2\beta)$. We are, therefore, left with the expression

$$A(\beta, \lambda) = \int_{-3/2}^{\infty} n_K g_K dK + O(\exp(-2\pi^2\beta))$$

which on integrating by parts yields

$$\begin{aligned} A(\beta, \lambda) &= \left[\frac{1}{6} n_K (K^3 + \frac{9}{2} K^2 + 6K) \right]_{-3/2}^{\infty} \\ &+ \frac{1}{6} \int_{-3/2}^{\infty} \frac{(K^3 + \frac{9}{2} K^2 + 6K)}{4\beta \cosh^2((K - \lambda)/2\beta)} dK + O(\exp(-2\pi^2\beta)) \\ &= \frac{1}{6}(\lambda + \frac{1}{2})(\lambda + \frac{3}{2})(\lambda + \frac{5}{2}) + \frac{1}{6}(\pi^2\beta^2 + \frac{1}{4})(\lambda + \frac{3}{2}) + O(\exp(-2\pi^2\beta)) \end{aligned} \tag{6.5}$$

which is valid for any temperature satisfying $0 < \beta \ll \lambda$. Note that the number of particles contained in a system where all shells up to the M th are full is just $\frac{1}{6}(M + 1) \times (M + 2)(M + 3)$ and this is reproduced exactly by the first term in equation (6.5) if we choose $\lambda = M + \frac{1}{2}$ i.e. if we take the Fermi energy exactly between two levels. The second term, therefore, gives the correction to the particle number due to the finite temperature. For example in our case $\lambda = 5.5$, $\beta = 0.6$ (see figure 3) we have a contribution of 4.43 to the particle number due to the second term in equation (6.5). This is in addition to the 56 particles in the system in the case of a closed shell.

In order to obtain our original 56 particles once more we must change λ by an amount

$$\delta\lambda \approx -\frac{1}{6}(\pi^2\beta^2 + \frac{1}{4})(\lambda + \frac{3}{2})/(\partial A/\partial\lambda) \tag{6.6}$$

where $\partial A/\partial\lambda \approx g_\lambda$. Inserting the above values into this equation we find $\delta\lambda \approx -0.16$ giving $\lambda = 5.34$.

The largest of the pole terms in equation (6.5) comes from the Poisson terms $m = \pm 1$ and yields explicitly an oscillatory correction to A

$$A_{osc} \approx 4\pi g_\lambda \beta \sin(2\pi\lambda) \exp(-2\pi^2\beta) \tag{6.7}$$

from which we see that the particle number still increases most rapidly when λ is integral (though of course this effect is entirely negligible for $2\pi^2\beta \gg 1$). An analysis similar to that given above may be performed for the total energy of the system at finite temperature. We now find an oscillatory contribution of the form

$$E_{osc} \approx 4\pi g_\lambda (\lambda + \frac{3}{2}) \hbar\omega\beta \sin(2\pi\lambda) \exp(-2\pi^2\beta). \tag{6.8}$$

Bohr and Mottelson (1975) refer to such terms as shell contributions to the energy and they are again negligible for $\beta \gg 1/2\pi^2$.

7. Conclusions

We have derived some simple closed-form approximations to the N -dimensional oscillator Wigner function which are valid in the region where F is strongly oscillatory.

Unfortunately, our approximations break down for ϵ near to and greater than ϵ_F in which region, however, F decreases monotonically. For these values of ϵ , other approximations are more suitable e.g. the Airy function approximation (Balazs and Zipfel 1973, 1974).

We have been able to isolate the importance of the quantity $\gamma = \epsilon_F/\hbar\omega$ on both the magnitude and period of the oscillatory structure and were able to show that for $(1 - \epsilon/\epsilon_F)(2\gamma)^{2/3} \gg 1$ the structure decreases, in the 'macroscopic' limit as $\gamma^{-1/2}$ even for totally degenerate fermions. We have also shown that the magnitude of the oscillatory structure increases with the dimensionality of the system and that half-filling the last oscillator shell essentially reduces this structure to that corresponding to a system in one dimension lower.

Our formulae have also allowed us to generalise to the case of almost degenerate fermions ($kT \ll \epsilon_F$) and we have seen that for $kT/\hbar\omega \approx 0.3$ and 0.6 the structure is reduced to about 20% and 2% of its value for the degenerate closed-shell problem. This implies, however, that for deep-inelastic nuclear reactions at a temperature of 2 to 3 MeV a considerable degree of structure may still be present in F (see figure 3).

In the macroscopic limit, however, smaller and smaller values of kT/ϵ_F are capable of completely damping even the structure in the region of the last maximum and under these conditions the Wigner function may approach closer and closer to its classical value for all values of ϵ .

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Appendix 1

The function $L_K^{N-1}(x)$ may be written in the form (Abramowitz and Stegun 1965)

$$e^{-x/2} L_K^{N-1}(x) = (1/\pi^{1/2} \alpha^{3/4})(\alpha/x)^{N/2} H(x), \tag{A1.1}$$

where H is a solution of the differential equation

$$d^2H/dx^2 = -(\alpha/x - N(N-2)/4x^2 - \frac{1}{4})H(x) \tag{A1.2}$$

with $\alpha = K + \frac{1}{2}N$. A frequently quoted asymptotic expression for H (see e.g. Szegő 1939) is then given by

$$H(x) \sim x^{1/4} \cos[2(\alpha x)^{1/2} - \frac{1}{2}\pi(N - \frac{1}{2})], \tag{A1.3}$$

which is valid for fixed $x > 0$ in the limit $\alpha \rightarrow \infty$. We wish, however, to find an asymptotic expression valid for fixed $\xi = x/4\alpha$ with $\alpha \rightarrow \infty$. In terms of this variable equation (A1.2) becomes

$$\frac{1}{16\alpha^2} \frac{d^2H}{d\xi^2} = -\frac{1}{4} \left(\frac{1}{\xi} - \frac{N(N-2)}{16\xi^2\alpha^2} - 1 \right) H(\xi). \tag{A1.4}$$

For $\xi \gg |N(N-2)|/16\alpha^2$ we then obtain the Ricatti equation

$$\frac{1}{4\alpha} (dg/d\xi) + g^2 = -\frac{1}{4}[(1-\xi)/\xi] \tag{A1.5}$$

where $g = d(\ln H)/d\xi$. For fixed $0 < \xi < 1$ we may then solve for g as an expansion in powers of α^{-1} and obtain

$$4\alpha g \sim 2i\alpha [(1-\xi)/\xi]^{1/2} + [1/4\xi(1-\xi)] + O(\alpha^{-1}) \tag{A1.6}$$

giving

$$H(\xi) \approx \left(\frac{\xi}{1-\xi}\right)^{1/4} \exp[i(2\alpha \{\sin^{-1} \xi^{1/2} + [\xi(1-\xi)]^{1/2}\} - \phi_0)]. \tag{A1.7}$$

Taking the real part of this expression with a normalisation of $(4\alpha)^{1/4}$ and with $\phi_0 = \frac{1}{2}\pi(N - \frac{1}{2})$ clearly reproduces (A1.3) for fixed $x = 4\alpha\xi$ as $\alpha \rightarrow \infty$ since then $\xi \rightarrow 0$ and we have

$$\begin{aligned} & [4\alpha\xi/(1-\xi)]^{1/4} \cos(2\alpha \{\sin^{-1} \xi^{1/2} + [\xi(1-\xi)]^{1/2}\} - \frac{1}{2}\pi(N - \frac{1}{2})) \\ & \sim (4\alpha\xi)^{1/4} \cos[4\alpha\xi^{1/2} - \frac{1}{2}\pi(N - \frac{1}{2})] \sim H(x). \end{aligned} \tag{A1.8}$$

Inserting the improved approximation into equation (A1.1) we then obtain

$$\begin{aligned} 2^N \exp(-2\alpha\xi) L_K^{N-1}(4\alpha\xi) & \sim (2/\pi\alpha)^{1/2} \frac{1}{\xi^{(N-1/2)/2}} \frac{1}{(1-\xi)^{1/4}} \\ & \times \cos(2\alpha \{\sin^{-1} \xi^{1/2} + [\xi(1-\xi)]^{1/2}\} - \frac{1}{2}\pi(N - \frac{1}{2})). \end{aligned} \tag{A1.9}$$

Including the factor $(-1)^K$ in $\tilde{f}_K^N(\varepsilon)$ as $-\pi K$ in the argument of the cosine and writing $\sin^{-1} \xi^{1/2} = \frac{1}{2}\pi - \sin^{-1}(1-\xi)^{1/2}$, this then simply leads to the expression (3.1) in the text for $\tilde{f}_K^N(\varepsilon)$.

Appendix 2

We may now use the above expression in (2.14) to obtain an approximation to $\tilde{F}_M^N(\varepsilon)$. Inserting equation (A1.9) we have

$$\tilde{F}_M^N(\varepsilon) \approx \frac{(-1)^M}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \frac{h(y) \cos(g(y)) dy}{\cosh \pi y}, \tag{A2.1}$$

where

$$h = [\alpha^{1/2} \xi^{(N-1/2)/2} (1-\xi)^{1/4}]^{-1} \tag{A2.2}$$

and

$$g(y) = 2\alpha \{\sin^{-1} \xi^{1/2} + [\xi(1-\xi)]^{1/2}\} - \frac{1}{2}\pi(N - \frac{1}{2}) \tag{A2.3}$$

with

$$\alpha = M + \frac{1}{2}(N + 1) + iy = \gamma + iy \tag{A2.4}$$

and

$$\xi = \tilde{\varepsilon}/\alpha = \gamma z/\alpha. \tag{A2.5}$$

From these equations we readily obtain

$$\partial h / \partial y|_{y=0} = -(h/\gamma)\{[z/4(1-z)] + \frac{1}{2}(N - \frac{3}{2})\} \tag{A2.6}$$

and

$$\partial g / \partial y|_{y=0} = 2 \sin^{-1} z^{1/2}, \quad \partial^2 g / \partial y^2|_{y=0} = -(1/\gamma)[z/(1-z)]^{1/2}. \tag{A2.7}$$

For z not too close to 1 (i.e. ϵ not too close to ϵ_F) we may ignore the first derivative of h and the second derivative of g which are both of order γ^{-1} and write

$$\begin{aligned} \tilde{F}_M^N(\epsilon) &\approx \frac{(-1)^M}{(2\pi)^{1/2}} h(0) \int_{-\infty}^{\infty} \frac{\cos(g(0) + 2iy \sin^{-1} z^{1/2})}{\cosh \pi y} dy \\ &= \frac{(-1)^M}{(2\pi)^{1/2}} \frac{h(0) \cos(g(0))}{(1-z)^{1/2}}. \end{aligned} \tag{A2.8}$$

Inserting the values of $h(0)$ and $g(0)$ and including the term $(-1)^M$ as $-M\pi$ in the argument of the cosine then yields equation (3.7) in the text.

Appendix 3

The sum in equation (5.4) may be exactly rewritten using the Poisson summation formula (Lighthill 1958) as

$$\sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} (n_{K-1/2} - n_{K+1/2}) \tilde{F}_{K-1/2}^N(\epsilon) \exp(2\pi m i K) dK. \tag{A3.1}$$

As in appendix 2 we may expand \tilde{F}_K^N about $K = \lambda$ and for ϵ not too close to ϵ_F retain only the variation of the argument of the cosine. Thus we write

$$\tilde{F}_K^N(\epsilon) = \frac{1}{(2\pi\gamma)^{1/2} z^{(N-1/2)/2} (1-z)^{3/4}} \cos[\phi(\gamma) + \phi'(K - \lambda)]. \tag{A3.2}$$

We need, therefore, to evaluate an expression of the form

$$\begin{aligned} \text{Re} \sum_{m=-\infty}^{\infty} (-1)^m \exp[i(\phi + 2\pi m \lambda)] \int_0^{\infty} (n_{K-1/2} - n_{K+1/2}) \exp[i(\phi' + 2\pi m)(K - \lambda)] dK \\ = \text{Re} \sum_{m=-\infty}^{\infty} (-1)^m \frac{\exp[i(\phi + 2\pi m \lambda)]}{i(\phi' + 2\pi m)} \int_{-\infty}^{\infty} \left(\frac{\partial n}{\partial K} \Big|_{K-1/2} - \frac{\partial n}{\partial K} \Big|_{K+1/2} \right) \\ \times \exp[i(\phi' + 2\pi m)(K - \lambda)] dK \\ = 2 \text{Re} \sum_{m=-\infty}^{\infty} \frac{\exp[i(\phi + 2\pi m \lambda)] \sin \frac{1}{2} \phi'}{(\phi' + 2\pi m)} \\ \times \int_{-\infty}^{\infty} \frac{\partial n}{\partial K} \exp[i(\phi' + 2\pi m)(K - \lambda)] dK. \end{aligned} \tag{A3.3}$$

Using the fact that $n_K = \{1 + \exp[(K - \lambda)/\beta]\}^{-1}$ this becomes

$$\pi\beta \sin \frac{1}{2} \phi' \sum_{m=-\infty}^{\infty} \frac{\cos(\phi + 2\pi m \lambda)}{\sinh[\pi\beta(\phi' + 2\pi m)]}. \tag{A3.4}$$

From equation (3.8) we see that

$$\phi' = 2 \sin^{-1}(1-z)^{1/2}$$

and thus $0 < \phi' < \pi$. Therefore, for $2\pi^2\beta \gg 1$, we only need to retain $m = 0, -1$ in equation (A3.4) giving

$$\frac{\pi\beta(1-z)^{1/2}}{\sinh[2\pi\beta \sin^{-1}(1-z)^{1/2}]} \left(\cos \phi - \cos(\phi - 2\pi\lambda) \frac{\sinh[2\pi\beta \sin^{-1}(1-z)^{1/2}]}{\sinh[2\pi\beta[\pi - \sin^{-1}(1-z)^{1/2}]]} \right). \quad (\text{A3.5})$$

The second term in equation (A3.5) is important only near $z \approx 0$ for which we may write

$$\begin{aligned} \frac{\sinh[2\pi\beta \sin^{-1}(1-z)^{1/2}]}{\sinh[2\pi\beta(\pi - \sin^{-1}(1-z)^{1/2})]} &\sim \exp[4\pi\beta(\sin^{-1}(1-z)^{1/2} - \frac{1}{2}\pi)] \\ &= \exp(-4\pi\beta \sin^{-1} z^{1/2}) \approx \exp(-4\pi\beta z^{1/2}). \end{aligned} \quad (\text{A3.6})$$

Formula (A3.5) then simply leads to equation (5.6).

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