

## Thermodynamics of partially confined Fermi gases at low temperature

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2004 J. Phys. A: Math. Gen. 37 3111

(<http://iopscience.iop.org/0305-4470/37/9/004>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.66

The article was downloaded on 02/06/2010 at 20:00

Please note that [terms and conditions apply](#).

# Thermodynamics of partially confined Fermi gases at low temperature

**David J Toms**

School of Mathematics and Statistics, University of Newcastle Upon Tyne,  
Newcastle Upon Tyne, NE1 7RU, UK

E-mail: [d.j.toms@newcastle.ac.uk](mailto:d.j.toms@newcastle.ac.uk)

Received 10 October 2003

Published 18 February 2004

Online at [stacks.iop.org/JPhysA/37/3111](http://stacks.iop.org/JPhysA/37/3111) (DOI: 10.1088/0305-4470/37/9/004)

## Abstract

We examine the behaviour of non-interacting Fermi gases at low temperature. If there is a confining potential present the thermodynamic behaviour is altered from the familiar results for the unconfined gas. The role of de Haas–van Alphen type oscillations that are a consequence of the confining potential is considered. Attention is concentrated on the behaviour of the chemical potential and the specific heat. Results are compared and contrasted with those for an unconfined and a totally confined gas.

PACS numbers: 03.75.Ss, 05.30.Fk, 71.10.Ca

## 1. Introduction

A gas of free (non-self-interacting) fermions is a simple model of great value, useful for illustrating the fundamental differences between Bose and Fermi systems at finite temperature in elementary statistical mechanics [1–4]. With the rapid advances that have been made in the cooling and trapping of atomic gases (see [5] for a review) the emphasis has shifted to systems confined by simple harmonic oscillator potentials. The presence of a confining potential can lead to considerable alterations in the behaviour of the system when compared to the free gas.

There have been a number of theoretical studies of confined Fermi gases. Butts and Rokhsar [6] presented an analysis based around approximating the sums over the discrete energy levels that occur with integrals. A numerical study of Schneider and Wallis [7] (see also [8]) showed that thermodynamic quantities, such as the specific heat, exhibited step-like behaviour. The analysis of the particle density and kinetic energy density for one and higher dimensional gases has been presented at both zero and finite temperatures [9–14] using Green's function or density matrix methods. An extensive analysis using a symmetrized density matrix approach has been given in [15–21]. Finally, we mention recent work by the present author [22, 23] that presents an analytical approach to the thermodynamics of confined Fermi gases,

pointing out the analogy with the de Haas–van Alphen effect. The purpose of the present paper is to apply the analysis of [22, 23] to partially confined gases.

The de Haas–van Alphen effect is concerned with the low temperature behaviour of a gas of charged particles obeying Fermi–Dirac statistics in a constant magnetic field of strength  $B$ . When the magnetic field is varied, instead of a monotonic dependence of thermodynamic quantities such as the magnetic susceptibility on the magnetic field  $B$ , what is observed [24] is an oscillatory behaviour whose period of oscillation is determined by  $1/B$ . These oscillations are now referred to as de Haas–van Alphen oscillations, or the de Haas–van Alphen effect. An early theoretical study of this [25] showed how the oscillations could be found from the thermodynamic potential. Because the de Haas–van Alphen oscillations manifest themselves directly in the thermodynamic potential, they will be present in other thermodynamic quantities such as the specific heat. A classic analysis of the thermodynamic potential, that we make use of, was given by Sondheimer and Wilson [26]. The de Haas–van Alphen effect provides a valuable technique for studying the Fermi surface in condensed matter physics [27].

The outline of our paper is the following. In section 2 we evaluate the thermodynamic potential for a three-dimensional gas of fermions with confinement of the particles in one or two dimensions by a harmonic oscillator potential. (The formalism is set up for any number of dimensions.) The chemical potential is evaluated in section 3, and the application to the specific heat is given in section 4. A brief summary of the results is given in section 5. Two brief appendices summarize the results for the free gas in  $D$  dimensions, and the two-dimensional partially confined gas.

## 2. Thermodynamic potential

Consider the noninteracting Fermi gas in  $D$ -dimensional space, and assume that there is a confining potential of the form

$$V(\mathbf{x}) = \frac{1}{2}m \sum_{j=1}^p \omega_j^2 x_j^2 \quad (2.1)$$

with  $\mathbf{x} = (x_1, \dots, x_D)$  being the  $D$ -dimensional Cartesian coordinates,  $\omega_j$  the frequencies that characterize the trapping potential,  $m$  the fermion mass and  $p \leq D$  a number describing the dimension of the trap. The case of full trapping ( $p = D$ ) has been dealt with elsewhere for both isotropic [22] and anisotropic traps [23], so we will concentrate only on partial confinement ( $p < D$ ) here. To deal with the unconfined spatial directions we will impose box normalization with periodic boundary conditions and the large box limit taken. In this case the single-particle energy eigenvalues read (with  $\hbar = 1$  units used)

$$E_{\mathbf{n}\mathbf{k}} = \sum_{j=1}^p \left( n_j + \frac{1}{2} \right) \omega_j + \frac{1}{2m} \sum_{j=p+1}^D \left( \frac{2\pi k_j}{L_j} \right)^2 \quad (2.2)$$

where  $L_j$  is the dimension of the box in the  $j$ th direction,  $n_j = 0, 1, \dots$  and  $k_j = 0, \pm 1, \dots$

The single-particle canonical partition function reads (with  $\beta = T^{-1}$  in units with the Boltzmann constant set equal to 1)

$$Z(\beta) = \sum_{\mathbf{n}=0}^{\infty} \sum_{\mathbf{k}=-\infty}^{\infty} e^{-\beta E_{\mathbf{n}\mathbf{k}}}. \quad (2.3)$$

The sums over  $\mathbf{n}$  are recognized as geometric series and are easily performed. To make the following analysis easier we will assume that the harmonic oscillator frequencies are all equal, meaning that the confining potential is isotropic in the  $p$ -dimensional confinement subspace.

For a description of how the anisotropic case can be dealt with, see [23]. We will also assume that the box used for normalization purposes is isotropic, so that  $L_j = L$  for all  $j$ . The sums over  $\mathbf{k}$  can be expressed in terms of  $\theta$ -functions, but if we take the limit where  $L$  is very large (specifically  $mTL^2 \gg 1$ ) the sums over  $\mathbf{k}$  can be approximated with integrals leading to

$$Z(\beta) = \left( \frac{mL^2}{2\pi\beta} \right)^{(D-p)/2} \frac{e^{-p\beta\omega/2}}{(1 - e^{-\beta\omega})^p}. \quad (2.4)$$

Because our aim is to examine the role of de Haas–van Alphen type terms in the thermodynamics, we will adopt the classic analysis of Sondheimer and Wilson [26]. Using Laplace transform theory, it can be shown that the thermodynamic potential of the system,  $\Omega$ , can be expressed as

$$\Omega = -\frac{1}{4}\beta \int_0^\infty dE \frac{\mathfrak{Z}(E)}{\cosh^2 \frac{1}{2}\beta(E - \mu)} \quad (2.5)$$

where

$$\mathfrak{Z}(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta e^{\beta E} \beta^{-2} Z(\beta) \quad (2.6)$$

with  $Z(\beta)$  being the canonical partition function, given in this case by equation (2.4) ( $c > 0$  is an arbitrary constant). The analysis now consists of evaluating equation (2.6) by closing the contour in the complex plane. The nature of how this is done depends on whether  $D - p$  in equation (2.4) is an even or odd integer. If  $(D - p)/2$  is an integer, then the integrand of equation (2.6) is a meromorphic function of  $\beta$  with poles at  $\beta = 2\pi ik/\omega$  for  $k = 0, \pm 1, \dots$ . The contour can be closed in this case with a semi-circle extended to infinity and the result evaluated by residues. When  $D - p$  is an odd integer, then  $\beta = 0$  is a branch point for the integrand in equation (2.6) and we introduce a branch cut along the negative real  $\beta$ -axis extending from the origin. The contour can be closed in the left-hand side of the complex  $\beta$ -plane with a deformation around the branch cut. The portion of the contour integral around the branch cut can be related to the generalized, or Hurwitz,  $\zeta$ -function [28] resulting in a closed form expression for  $\mathfrak{Z}(E)$  that we will give below. In either case (branch cut or not) provided that  $p \neq 0$ , there are a series of poles along the imaginary  $\beta$ -axis that, as in the de Haas–van Alphen case [26], are responsible for an oscillatory part of  $\Omega$ .

To keep the analysis simple, we will now specialize to  $D = 3$  and look at the evaluation of  $\Omega$  for  $p = 1, 2$ . The application to the particle number, chemical potential and specific heat will be given in sections 3 and 4. The case of general  $D$  with  $p = 0$  is given in appendix A for comparison. We also outline the results for  $D = 2$  in appendix B.

### 2.1. One-dimensional trapping

We will take  $D = 3$  and  $p = 1$  here and refer to this case as one-dimensional trapping since the confining potential is only non-zero in one spatial dimension. From equations (2.4) and (2.6) we have

$$\mathfrak{Z}(E) = \frac{mL^2}{4\pi^2 i} \int_{c-i\infty}^{c+i\infty} d\beta \beta^{-3} \frac{e^{\beta(E-\omega/2)}}{(1 - e^{-\beta\omega})}. \quad (2.7)$$

There is a pole of order 4 at  $\beta = 0$  and simple poles at  $\beta = 2\pi ik/\omega$  for  $k = \pm 1, \pm 2, \dots$ . If we close the contour in the left-hand side of the complex  $\beta$ -plane as described above it can be shown that

$$\mathfrak{Z}(E) = \mathfrak{Z}_0(E) + \mathfrak{Z}_r(E) \quad (2.8)$$

with

$$\mathfrak{Z}_0(E) = \frac{mL^2}{48\pi\omega} E(4E^2 - \omega^2) \tag{2.9}$$

the contribution coming from the  $\beta = 0$  pole, and

$$\mathfrak{Z}_r(E) = -\frac{mL^2\omega^2}{8\pi^4} \sum_{k=1}^{\infty} \frac{\sin\left[2\pi k\left(\frac{E}{\omega} - \frac{1}{2}\right)\right]}{k^3} \tag{2.10}$$

the contribution coming from the rest of the poles away from the origin along the imaginary axis.

We may substitute equations (2.9) and (2.10) into equation (2.5) and obtain  $\Omega_0$  and  $\Omega_r$  with an obvious notation. Making a change of variable in the integration results in

$$\Omega_{0,r} = -\frac{1}{2} \int_{-\frac{1}{2}\beta\mu}^{\infty} d\theta \frac{\mathfrak{Z}_{0,r}\left(\mu + \frac{2}{\beta}\theta\right)}{\cosh^2 \theta}. \tag{2.11}$$

If we assume that the temperature is low enough so that  $\beta\mu \gg 1$  (or  $T \ll \mu$ ) then up to exponentially small terms we can replace the lower limit of the integral with  $-\infty$ . This approximation enables us to evaluate

$$\Omega_0 \simeq -\frac{mL^2}{48\pi\omega} (4\mu^3 - \omega^2\mu + 4\pi^2\mu T^2) \tag{2.12}$$

in a straightforward way. For  $\Omega_r$  we find

$$\Omega_r \simeq \frac{mL^2\omega}{4\pi^2\beta} \sum_{k=1}^{\infty} \frac{\sin\left[2\pi k\left(\frac{\mu}{\omega} - \frac{1}{2}\right)\right]}{k^2 \sinh\left(\frac{2\pi^2 k}{\beta\omega}\right)}. \tag{2.13}$$

The term of  $\Omega$  that we have called  $\Omega_r$  shows the oscillations in  $\mu/\omega$  familiar from the de Haas–van Alphen effect (although the detailed expression is different here).

### 2.2. Two-dimensional trapping

We will refer to the  $D = 3, p = 2$  case as two-dimensional trapping since the confining potential is only non-zero in two of the spatial directions. From equations (2.4) and (2.6) we have

$$\mathfrak{Z}(E) = \frac{L}{2\pi i} \left(\frac{m}{2\pi}\right)^{1/2} \int_{c-i\infty}^{c+i\infty} d\beta \beta^{-5/2} \frac{e^{\beta(E-\omega)}}{(1 - e^{-\beta\omega})^2}. \tag{2.14}$$

This time we introduce a branch cut along the negative  $\beta$ -axis as described above. The contour is deformed around the branch cut resulting in a contribution of the Hankel type to  $\mathfrak{Z}(E)$  that we will call  $\mathfrak{Z}_0(E)$ , as well as contributions coming from double poles at  $\beta = 2\pi ik/\omega$  for  $k = \pm 1, \pm 2, \dots$  that we will call  $\mathfrak{Z}_r(E)$ . An elementary manipulation enables us to express  $\mathfrak{Z}_0(E)$  as

$$\mathfrak{Z}_0(E) = \frac{L}{3\pi} (2\omega)^{3/2} m^{1/2} \left[ \zeta\left(-\frac{5}{2}, 1 + \frac{E}{\omega}\right) - \frac{E}{\omega} \zeta\left(-\frac{3}{2}, 1 + \frac{E}{\omega}\right) \right] \tag{2.15}$$

where  $\zeta(s, a)$  is the generalized, or Hurwitz,  $\zeta$ -function [28]. For  $\mathfrak{Z}_r(E)$  we find

$$\mathfrak{Z}_r(E) = \frac{L(m\omega)^{1/2}}{16\pi^4} \sum_{k=1}^{\infty} \left\{ \frac{5\omega}{k^{7/2}} \sin\left(2\pi k \frac{E}{\omega} - \frac{\pi}{4}\right) - \frac{4\pi E}{k^{5/2}} \cos\left(2\pi k \frac{E}{\omega} - \frac{\pi}{4}\right) \right\}. \tag{2.16}$$

We still have equation (2.11) holding; however, this time the evaluation of  $\Omega_0$  is not quite so trivial. Making the approximation  $\beta\mu \gg 1$  as before, so that the temperature is low, it can be

seen because of the  $\cosh^2 \theta$  present in the denominator, that the dominant contribution to the integral will come from small values of  $\theta$ . The numerator can be developed in a power series around  $\theta = 0$  and the first few terms integrated without difficulty to give

$$\Omega_0 \simeq -\mathfrak{Z}_0(\mu) - \frac{\pi^2}{6} T^2 \mathfrak{Z}_0''(\mu) - \frac{7\pi^4}{360} T^4 \mathfrak{Z}_0^{iv}(\mu) + \dots \tag{2.17}$$

This can be recognized as the Sommerfeld expansion [2, 4, 27]. For  $\Omega_r$  we find

$$\Omega_r \simeq \frac{L(m\omega)^{1/2}}{8\pi^2\beta} \sum_{k=1}^{\infty} \left\{ \frac{4\pi\mu \cos\left(2\pi k \frac{E}{\omega} - \frac{\pi}{4}\right)}{\omega k^{3/2} \sinh \theta_k} - \frac{1}{k^{5/2}} \left( \frac{3}{\sinh \theta_k} + 2\theta_k \frac{\cosh \theta_k}{\sinh^2 \theta_k} \right) \sin\left(2\pi k \frac{E}{\omega} - \frac{\pi}{4}\right) \right\} \tag{2.18}$$

where to save writing we have defined

$$\theta_k = \frac{2\pi^2 k}{\beta\omega}. \tag{2.19}$$

Again the oscillatory de Haas–van Alphen type of terms are present in  $\Omega$ , although the result is more complicated than for one-dimensional trapping.

So far the only approximation that we have made is the low temperature approximation  $T \ll \mu$  used to simplify the evaluation of certain integrals. If we now make the further assumption that  $\mu \gg \omega$ , then it is possible to obtain a more friendly expression for  $\Omega_0$  than that found by a straightforward substitution of equation (2.15) into equation (2.17). A short calculation results in

$$\frac{\Omega_0}{L(m\omega)^{1/2}} \simeq -\frac{16\omega}{105\sqrt{2}\pi} \left(\frac{\mu}{\omega}\right)^{7/2} + \left[ \frac{\omega}{9\sqrt{2}\pi} - \frac{2\pi T^2}{9\sqrt{2}\omega} \right] \left(\frac{\mu}{\omega}\right)^{3/2} + \dots \tag{2.20}$$

The next term in equation (2.20) is of order  $(\mu/\omega)^{-1/2}$  so the neglected terms will be negligible for large  $\mu/\omega$ .

### 3. Particle number and chemical potential

In this section we will use the expressions obtained for the thermodynamic potential in section 2 to study the relationship between the particle number and the chemical potential. Generally the particle number is expressed in terms of the thermodynamic potential by

$$N = - \left( \frac{\partial \Omega}{\partial \mu} \right) \Big|_{T, \omega, L}. \tag{3.1}$$

Given the natural split of  $\Omega = \Omega_0 + \Omega_r$  as described in section 2 we have a similar split

$$N = N_0 + N_r \tag{3.2}$$

with  $N_0$  and  $N_r$  obtained from equation (3.1) with  $\Omega = \Omega_0$  and  $\Omega_r$ , respectively.

#### 3.1. One-dimensional trapping

From equation (2.13) we find that

$$N_0 \simeq \frac{mL^2}{48\pi\omega} (12\mu^2 - \omega^2 + 4\pi^2 T^2) \tag{3.3}$$

and from equation (2.13) that

$$N_r \simeq -\frac{mL^2}{2\pi\beta} \sum_{k=1}^{\infty} \frac{\cos\left[2\pi k \left(\frac{\mu}{\omega} - \frac{1}{2}\right)\right]}{k \sinh\left(\frac{2\pi^2 k}{\beta\omega}\right)}. \tag{3.4}$$

The term  $N_r$  has its origin in the de Haas–van Alphen part of the thermodynamic potential. If we temporarily ignore  $N_r$ , then by setting  $N = N_0$  in equation (3.3) we can solve for

$$\frac{\mu}{\omega} \simeq \left( \frac{4\pi N}{m\omega L^2} + \frac{1}{12} - \frac{\pi^2 T^2}{3\omega^2} \right)^{1/2}. \quad (3.5)$$

In order to get some idea of the magnitude of  $\mu$ , we will take some typical values for  $m$  and  $\omega$ . We use [5]  $\omega \sim 10^2\text{--}10^3 \text{ s}^{-1}$  and  $m \sim 10^{-26} \text{ kg}$  as reasonable orders of magnitude. (We take a typical atomic mass to be about 10 times that of hydrogen.) Restoring the factors of  $\hbar$  results in  $\hbar/(m\omega) \sim 10^{-11} \text{ m}^{-2}$ . For the neglect of interactions to be valid we require  $L^2/N \gg r_0^2$  where  $r_0 \sim 10^{-9} \text{ m}$  is the size of a typical atom. (This allows the gas to be dilute.) We then find (restoring  $\hbar = 1$  units) that

$$\frac{N}{m\omega L^2} \ll 10^7. \quad (3.6)$$

This still allows large values of  $\mu/\omega$  from equation (3.5). We have already assumed that  $\beta\mu \gg 1$  in deriving the thermodynamic potential. If we also require  $\mu/\omega$  to be large, this allows us to have  $T$  as small as we like, so our approximations are perfectly consistent for examining the low temperature limit.

For large values of  $N/(m\omega L^2)$ , we see from equation (3.5) that we can further approximate (for  $T/\omega$  not too large)

$$\frac{\mu}{\omega} \simeq \left( \frac{4\pi N}{m\omega L^2} \right)^{1/2} \quad (3.7)$$

showing that  $\mu$  scales like  $N^{1/2}$ . This contrasts with the result for the unconfined gas that scales like  $N^{2/3}$  (see equation (A.6)). The  $N$ -dependence in equation (3.7) is the same as that for the unconfined gas in four spatial dimensions.

It now remains to see if the de Haas–van Alphen part of  $\Omega$  has any effect on the result for  $\mu$ . This requires knowledge of the sum in equation (3.4). For large values of  $T/\omega$ , where large can mean  $T/\omega \simeq 1$ , it is clear that the presence of the factor of  $\sinh(2\pi^2 kT/\omega)$  in the denominator of the summand suppresses any contribution that  $N_r$  could make to the total particle number. (Since  $\mu$  is assumed to be large, the  $\mu^2$  contribution from  $N_0$  will be the dominant term.) Thus if the de Haas–van Alphen oscillations are to affect the value we have found for  $\mu$  in equation (3.7) they can only do so as  $T \rightarrow 0$ . As  $T \rightarrow 0$ , the sum in equation (3.4) becomes more slowly convergent; however, it is possible to obtain an analytical approximation that is valid at low temperatures as follows. (Similar expressions were obtained previously for fully trapped gases in [22, 23].) Add and subtract terms in the sum to obtain

$$N_r = -\frac{mL^2}{2\pi}(S_1 + S_2) \quad (3.8)$$

where

$$S_1 = \frac{1}{\beta} \sum_{k=1}^{\infty} \frac{\cos\left(\frac{2\pi k\mu}{\omega} - \pi k\right) - 1}{k \sinh \theta_k} \quad (3.9)$$

$$S_2 = \frac{1}{\beta} \sum_{k=1}^{\infty} \frac{1}{k \sinh \theta_k}. \quad (3.10)$$

The most complete way to analyse  $S_1$  is to use the Poisson summation formula to give a result that is valid for all temperatures; however, if we are only interested in low temperatures,

we can use the simpler Euler–Maclaurin formula [29]. By adding in the  $k = 0$  term to the sum in  $S_1$  it is possible to show that

$$S_1 \simeq -T \ln \cosh \left\{ \frac{\omega}{4T} \left( 2 \frac{\mu}{\omega} - 2 \left[ \frac{\mu}{\omega} \right] - 1 \right) \right\} + \frac{\omega}{8} \left( 2 \frac{\mu}{\omega} - 2 \left[ \frac{\mu}{\omega} \right] - 1 \right)^2 \tag{3.11}$$

where  $[x]$  denotes the largest integer less than or equal to  $x$ . For  $S_2$ , the low temperature expansion is most easily obtained by making use of the inverse Laplace transform of the  $\Gamma$ -function to obtain

$$S_2 = \frac{T}{\pi i} \int_{c-i\infty}^{c+i\infty} dz \Gamma(z) \left( \frac{2\pi^2 T}{\omega} \right)^{-z} \zeta(z+1)(1-2^{-z})\zeta(z) \tag{3.12}$$

where  $\zeta(z)$  is the Riemann  $\zeta$ -function, and  $c > 1$ . Closing the contour in the left-hand side of the complex plane, noting the contributions from poles at  $z = 1, 0, -1$  results in the asymptotic expansion

$$S_2 \simeq \frac{\omega}{12} - T \ln 2 + \frac{\pi^2 T^2}{6\omega}. \tag{3.13}$$

In this way we obtain a simple analytical approximation for the sum in equation (3.4) defining  $N_r$  that is valid as  $T \rightarrow 0$ . It is then straightforward to show that because  $N_r$  really only involves  $\mu/\omega - [\mu/\omega]$ ,  $N_r$  makes a negligible contribution to  $N$ .

We have verified conclusions based on the analytical approximations just described by solving  $N = N_0 + N_r$  numerically for  $\mu$  for a range of values for  $N/(m\omega L^2)$  consistent with equation (3.6). Even as  $T \rightarrow 0$  the step-like features that were so prominent in the fully trapped gas [22, 23] are virtually absent here. The behaviour for  $\mu/\omega$  as a function of  $N/(m\omega L^2)$  followed the simple result of equation (3.7) to a very good approximation.

### 3.2. Two-dimensional trapping

If we take  $\Omega = \Omega_0$  in equation (3.1) with equation (2.20) used for  $\Omega_0$ , it is easily seen that

$$\frac{N_0}{L(m\omega)^{1/2}} \simeq \frac{8}{15\sqrt{2}\pi} \left( \frac{\mu}{\omega} \right)^{5/2} - \frac{1}{6\sqrt{2}\pi} \left( 1 - \frac{2\pi^2 T^2}{\omega^2} \right) \left( \frac{\mu}{\omega} \right)^{1/2}. \tag{3.14}$$

With equation (2.18) used for  $\Omega_r$ , we find

$$N_r \simeq \frac{L(m\omega)^{1/2}}{4\pi\beta\omega} \sum_{k=1}^{\infty} \left\{ \frac{4\pi\mu \sin\left(2\pi k \frac{\mu}{\omega} - \frac{\pi}{4}\right)}{\omega k^{1/2} \sinh \theta_k} + \frac{1}{k^{3/2}} \left( \frac{1}{\sinh \theta_k} + 2\theta_k \frac{\cosh \theta_k}{\sinh^2 \theta_k} \right) \cos\left(2\pi k \frac{\mu}{\omega} - \frac{\pi}{4}\right) \right\}. \tag{3.15}$$

( $\theta_k$  was defined in equation (2.19).) Unlike the one-dimensional trapped case,  $N_r$  contains an explicit factor of  $\mu$  this time, so the importance of  $N_r$  in the evaluation of  $\mu$  is not so obvious.

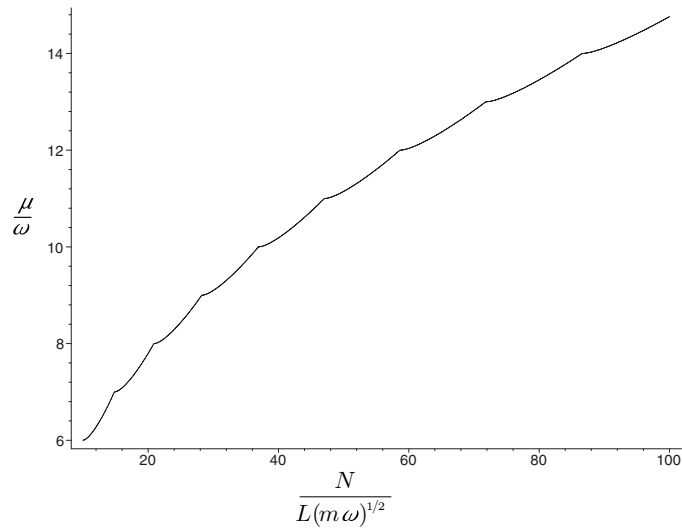
If we temporarily ignore  $N_r$  and set  $N = N_0$  in equation (3.14), then we can solve for  $\mu = \mu_0$  with

$$\frac{\mu_0}{\omega} \simeq \left( \frac{15\sqrt{2}\pi N}{8L(m\omega)^{1/2}} \right)^{2/5}. \tag{3.16}$$

This gives a dependence on  $N$  proportional to  $N^{2/5}$  in place of  $N^{1/2}$  for one-dimensional trapping, and  $N^{2/3}$  for the free gas. This is the same as the  $N$ -dependence for the five-dimensional unconfined gas. To estimate the size of  $\mu$  a repeat of the estimate in section 3.1, this time assuming  $L/N \gg 10^{-9}$  results in

$$\frac{N}{L(m\omega)^{1/2}} \ll 10^4. \tag{3.17}$$





**Figure 1.** The chemical potential scaled by the trap frequency plotted as a function of the dimensionless combination  $\frac{N}{L(m\omega)^{1/2}}$ . The temperature is given by  $T = 0.001\omega$ .

We now examine the contribution of  $N_r$  to  $N$ . Because of the dependence of the summand of equation (3.15) on fractional powers of  $k$  it is not possible to obtain such a simple analytical expression as we had before. If we look at the  $T \rightarrow 0$  limit of  $N_r$  and keep only the leading order term for large  $\mu/\omega$ , it can be shown that

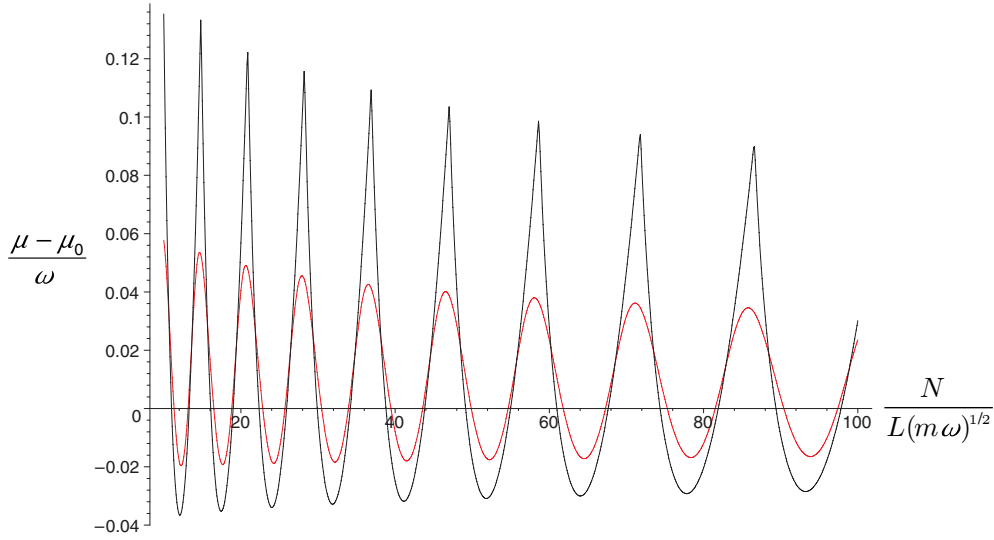
$$N_r \simeq \frac{L(m\omega)^{1/2}\mu}{2\pi^2\omega} \sum_{k=1}^{\infty} \frac{\sin\left(2\pi k \frac{\mu}{\omega} - \frac{\pi}{4}\right)}{k^{3/2}}. \quad (3.18)$$

The remaining sum in equation (3.18) can be expressed in terms of polylogarithms to give a closed form expression

$$N_r \simeq \frac{L(m\omega)^{1/2}\mu}{2\pi^2\omega} \operatorname{Im}\{e^{-i\pi/4} \operatorname{Li}_{3/2}(e^{2\pi i\mu/\omega})\}. \quad (3.19)$$

(Here  $\operatorname{Im}$  denotes the imaginary part, and  $\operatorname{Li}_s(z) = \sum_{n=1}^{\infty} z^n/n^s$  defines the polylogarithm.) The other terms in equation (3.15) can be approximated in a similar way if desired, but equation (3.19) turns out to be sufficiently accurate as  $T \rightarrow 0$ .

We have examined the importance of the de Haas–van Alphen contribution to the chemical potential by solving  $N = N_0 + N_r$  numerically for  $\mu$  and comparing the result with equation (3.16). The results are shown in figure 1. As the temperature was reduced oscillations were clearly visible in the result, showing that the de Haas–van Alphen contributions do have an effect on the result in contrast to the case of one-dimensional trapping. However the results did not show the dramatic step-like behaviour found for the fully trapped gas [7, 22, 23]. This is attributable to the different  $\mu$ -dependence of the de Haas–van Alphen part of  $\Omega$  for the fully and partially trapped gases. The general shape of the curve follows equation (3.16). In order to show the oscillations more clearly, we have plotted the difference between the true result and the approximation of equation (3.16) in figure 2 for two different temperatures. The oscillations become more pronounced as the temperature is reduced (as expected) and the result found analytically in equation (3.19) becomes a very good approximation.



**Figure 2.** The difference between the approximation in equation (3.16) for the chemical potential and the actual value plotted as a function of the particle number. This difference shows the contribution that the de Haas–van Alphen part of the thermodynamic potential makes to the chemical potential. The lower curve is for  $T = 0.01\omega$  (red online) and the upper curve is for  $T = 0.001\omega$  (black online).

#### 4. Specific heat

To compute the specific heat we first need the internal energy  $U$  defined in terms of the thermodynamic potential  $\Omega$  by

$$U = \left. \frac{\partial}{\partial \beta} (\beta \Omega) \right|_{\beta, \mu, \omega, L}. \quad (4.1)$$

With the decomposition  $\Omega = \Omega_0 + \Omega_r$  this allows us to identify the de Haas–van Alphen contribution to the internal energy. The specific heat at constant volume (fixed box size)  $C$  is then defined in terms of  $U$  by

$$C = \left. \left( \frac{\partial U}{\partial T} \right) \right|_{N, \omega, L}. \quad (4.2)$$

$$= \left. \left( \frac{\partial U}{\partial T} \right) \right|_{\mu, \omega, L} - \frac{\left. \left( \frac{\partial U}{\partial \mu} \right) \right|_{T, \omega, L} \left. \left( \frac{\partial N}{\partial T} \right) \right|_{\mu, \omega, L}}{\left. \left( \frac{\partial N}{\partial \mu} \right) \right|_{T, \omega, L}}. \quad (4.3)$$

Although the internal energy  $U$  has a simple representation as  $U = U_0 + U_r$ , the same is not true for the specific heat because of  $N$  being held fixed in equation (4.2). This complicates the identification of de Haas–van Alphen contributions to the specific heat.

##### 4.1. One-dimensional trapping

By taking  $\Omega = \Omega_0$  in equation (4.1) with  $\Omega_0$  given by equation (2.12), it is easy to see that

$$U_0 = m\omega L^2 \left( \frac{\mu^3}{6\pi\omega^2} + \frac{\pi\mu T^2}{6\omega^2} \right). \quad (4.4)$$

Before computing the de Haas–van Alphen contribution to the internal energy we will calculate the specific heat with any de Haas–van Alphen contributions ignored. If we use equation (4.4) for  $U$  and equation (3.3) for  $N$  in equation (4.3) it can be shown that the specific heat is given by

$$C_0 \simeq \frac{\pi m L^2 \mu T}{6\omega}. \quad (4.5)$$

This gives the linear temperature dependence familiar from the free gas at low temperature (see equation (A.8) or [2, 3, 4, 27]). Elimination of  $\mu$  using equation (3.7) results in

$$C_0 \simeq \frac{\pi}{3} (\pi N m \omega L^2)^{1/2} \frac{T}{\omega}. \quad (4.6)$$

We now need to examine the specific heat when the de Haas–van Alphen contributions are present. Their contribution to the internal energy can be found by using  $\Omega = \Omega_r$  with  $\Omega_r$  given by equation (2.13) in equation (4.1). The result is

$$U_r = \frac{m L^2}{2\pi} \sum_{k=1}^{\infty} \left\{ -\frac{\mu T \cos(2\pi k \mu / \omega - \pi k)}{k \sinh \theta_k} + \frac{\pi T^2 \cosh \theta_k}{k \sinh^2 \theta_k} \sin(2\pi k \mu / \omega - \pi k) \right\}. \quad (4.7)$$

Although it is not possible to write  $C$  as a simple sum with the de Haas–van Alphen contribution clearly displayed, we can look at the leading behaviour for large  $\mu$ . Using  $\mu/\omega$  as the expansion parameter, and taking  $U = U_0 + U_r$ , it can be shown that

$$\frac{1}{m\omega L^2} \left( \frac{\partial U}{\partial T} \right) \Big|_{\mu, \omega, L} \simeq \frac{\mu}{\omega} \left\{ \frac{\pi T}{3\omega} - \frac{1}{2\pi} \sum_{k=1}^{\infty} (1 - \theta_k \coth \theta_k) \frac{\cos(2\pi k \mu / \omega - \pi k)}{k \sinh \theta_k} \right\} \quad (4.8)$$

$$\frac{1}{m\omega L^2} \left( \frac{\partial U}{\partial \mu} \right) \Big|_{T, \omega, L} \simeq \frac{1}{2\pi} \left( \frac{\mu}{\omega} \right)^2 \quad (4.9)$$

as the leading terms. A similar calculation applied to  $N = N_0 + N_r$  with  $N_0$  and  $N_r$  given by equations (3.3) and (3.4) respectively results in

$$\frac{1}{m\omega L^2} \left( \frac{\partial N}{\partial T} \right) \Big|_{\mu, \omega, L} \simeq \frac{\pi T}{6\omega^2} - \frac{1}{2\pi\omega} \sum_{k=1}^{\infty} (1 - \theta_k \coth \theta_k) \frac{\cos(2\pi k \mu / \omega - \pi k)}{k \sinh \theta_k} \quad (4.10)$$

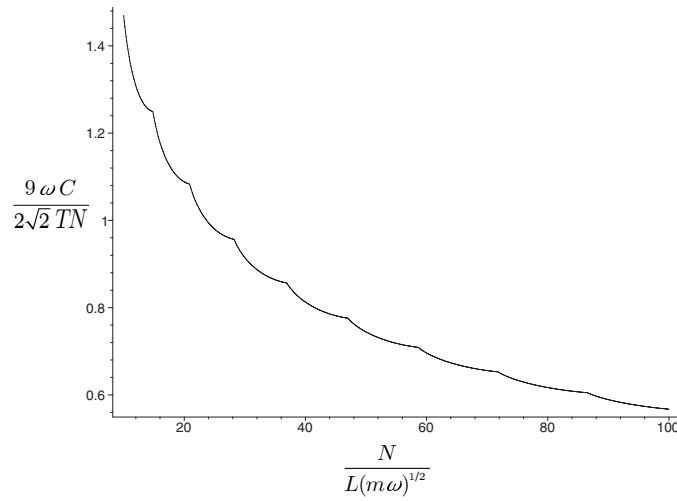
$$\frac{1}{m\omega L^2} \left( \frac{\partial N}{\partial \mu} \right) \Big|_{T, \omega, L} \simeq \frac{1}{2\pi\omega} \left( \frac{\mu}{\omega} \right). \quad (4.11)$$

If the results of equations (4.8)–(4.11) are used in equation (4.3) it can be seen that despite the fact that the de Haas–van Alphen contributions alter the individual terms that contribute to the specific heat, a cancellation occurs and we recover equation (4.5) to leading order in  $\mu$ . Since we found that equation (3.7) was a reliable approximation for  $\mu$  even with the de Haas–van Alphen contributions included, we can conclude that equation (4.6) provides a good approximation to the specific heat. The de Haas–van Alphen contributions do not vanish identically for the specific heat, but because they only show up below leading order the specific heat will be dominated by equation (4.6), and they would not be expected to be observable even at very low temperatures.

#### 4.2. Two-dimensional trapping

With  $\Omega_0$  given by equation (2.20) and  $\Omega_r$  given by equation (2.18) we find

$$\frac{1}{L(m\omega)^{1/2}} U_0 \simeq \frac{4\sqrt{2}\omega}{21\pi} \left( \frac{\mu}{\omega} \right)^{7/2} - \frac{\omega}{18\sqrt{2}\pi} \left( 1 - \frac{10\pi^2 T^2}{\omega^2} \right) \left( \frac{\mu}{\omega} \right)^{3/2} + \dots \quad (4.12)$$



**Figure 3.** The specific heat scaled by the particle number and temperature plotted as a function of the particle number with  $T = 0.001\omega$  held fixed.

$$\frac{1}{L(m\omega)^{1/2}} U_r \simeq \frac{\mu^2}{\beta\omega^2} \sum_{k=1}^{\infty} \frac{\sin(2\pi k\mu/\omega - \pi/4)}{\sqrt{k} \sinh \theta_k} + \dots \quad (4.13)$$

Only the terms that contribute to the specific heat at leading order have been included here for brevity. From these two expressions we can compute

$$C \simeq \frac{2\sqrt{2}\pi T}{9\omega} \left(\frac{\mu}{\omega}\right)^{3/2} L(m\omega)^{1/2} \quad (4.14)$$

as the leading order behaviour of the specific heat. Although there is no explicit dependence on the oscillatory terms (unlike the case of complete trapping [22, 23]) there can still be an implicit dependence through the oscillatory behaviour of  $\mu$ . This was discussed in section 3. We show the specific heat in figure 3.

## 5. Discussion and conclusions

We have examined the possible role of de Haas–van Alphen type oscillations in partially confined gases of fermions. Although our efforts were concentrated on three-dimensional gases (the two-dimensional case is outlined in appendix B), it is clear how the analysis could be applied to any spatial dimension. For two-dimensional trapping we only examined the case of an isotropic potential, but it would be quite straightforward to adapt the approach of [23] to deal with anisotropic potentials. Experience gained from [23] indicates that the maximal effect for the de Haas–van Alphen oscillations occurs for isotropic potentials, or those for which the frequencies are rational multiples of each other.

Although we established the existence of oscillatory de Haas–van Alphen type oscillations in the thermodynamic potential for partially trapped gases (and hence in derived thermodynamic expressions) their overall contribution turned out to be small. This contrasts with fully trapped gases where there can be quite marked oscillations present in expressions such as the chemical potential and specific heat at low temperature [7, 22, 23]. The dependence of the chemical potential and specific heat on the particle number was altered from that of

the unconfined gas due to the trapping potential. If  $p$  denotes the dimension of the confining potential and  $D$  is the spatial dimension, it was found that the confined gas (to leading order in  $\mu$  at low temperature) behaved like the unconfined gas in  $D + p$  spatial dimensions.

### Appendix A. Unconfined gas in any dimension

In this appendix we wish to summarize the application of the analysis described in the main part of the paper to the case where the gas is not trapped. We will keep the dimension  $D$  general here to demonstrate the dimensional dependence of the results for comparison with the partially trapped gas. The results for  $D = 3$  are standard and are covered in a number of standard textbooks [2–4, 27].

In keeping with the approach and notation of section 2 we will confine the gas to a cubical box of side  $L$ . The partition function for the  $\mu = 0$  gas is found by taking  $p = 0$  in equation (2.4). Using this result in equation (2.6) gives us

$$\mathfrak{Z}(E) = \left(\frac{mL^2}{2\pi}\right)^{D/2} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta \beta^{-2-D/2} e^{\beta E} \quad (\text{A.1})$$

and the thermodynamic potential is recovered from equation (2.5).  $\beta = 0$  is a branch point of the integrand and, as in section 2.2, we choose a branch cut along the negative real  $\beta$ -axis and close the contour in the left-hand side of the complex  $\beta$ -plane with a deformation around the branch cut. This enables us to relate equation (A.1) to the standard Hankel representation for the  $\Gamma$ -function [28]. After a short calculation, the result for  $\mathfrak{Z}(E)$  is found to be

$$\mathfrak{Z}(E) = \left(\frac{mL^2}{2\pi}\right)^{D/2} \frac{E^{1+D/2}}{\Gamma(2 + D/2)}. \quad (\text{A.2})$$

This is related to the density of states and equivalent results can be obtained in a variety of other more elementary ways. Making use of the Sommerfeld expansion, assuming  $\beta\mu \gg 1$  as usual, we obtain

$$\left(\frac{2\pi}{mL^2}\right)^{D/2} \Omega \simeq -\frac{\mu^{1+D/2}}{\Gamma(2 + D/2)} - \frac{\pi^2 T^2 \mu^{D/2-1}}{6\Gamma(D/2)} + \dots \quad (\text{A.3})$$

The particle number  $N$ , defined by equation (3.1), becomes

$$\left(\frac{2\pi}{mL^2}\right)^{D/2} N \simeq \frac{\mu^{D/2}}{\Gamma(1 + D/2)} + \frac{\pi^2 T^2 \mu^{D/2-2}}{6\Gamma(D/2 - 1)} + \dots \quad (\text{A.4})$$

(For  $D = 2$  the second term vanishes, as is clear from equation (A.3), and the next to leading order term is of order  $T^4$ .) We can solve equation (A.4) for  $\mu$  with the result

$$\mu \simeq \mu_0 \left[ 1 - \left(\frac{D}{2} - 1\right) \frac{\pi^2 T^2}{6\mu_0^2} \right] \quad (\text{A.5})$$

where

$$\mu_0 = \frac{2\pi}{mL^2} [\Gamma(1 + D/2) N]^{2/D} \quad (\text{A.6})$$

is the chemical potential at  $T = 0$ . This shows the scaling  $\mu \propto N^{2/D}$  for general dimension  $D$ .

The internal energy is easily computed using equation (4.1) to be

$$U \simeq \frac{D}{2} \left(\frac{mL^2}{2\pi}\right)^{D/2} \left\{ \frac{\mu^{1+D/2}}{\Gamma(2 + D/2)} + \frac{\pi^2 T^2 \mu^{D/2-1}}{6\Gamma(D/2)} + \dots \right\}. \quad (\text{A.7})$$

With  $\mu \propto N^{2/D}$  this shows  $U \propto N^{1+2/D}$ .

The specific heat follows from equation (4.3) as

$$C \simeq \frac{\pi^2}{3\Gamma(D/2)} \left( \frac{mL^2}{2\pi} \right)^{D/2} T \mu^{D/2-1}. \quad (\text{A.8})$$

For low  $T$  we can replace  $\mu$  in equation (A.8) with  $\mu_0$ , so it can be seen that the dependence of the specific heat on the particle number behaves like  $N^{1-2/D}$ .

## Appendix B. Partially confined gas in two dimensions

In this appendix we summarize the main results for the case of a two-dimensional partially trapped gas. The results are contrasted with those for the unconfined gas (as found in appendix A) and fully confined gas found in [22].

The partition function is obtained by setting  $D = 2$  and  $p = 1$  in equation (2.4). Because this results in a  $\beta^{-1/2}$  factor, when we use the result for  $Z(\beta)$  in equation (2.6) and close the contour it is necessary to deform the contour around a branch cut as described in section 2.2. For  $\Omega_0$ , assuming  $\beta\mu \gg 1$  and  $\mu/\omega \gg 1$ , we find

$$\Omega_0 \simeq \frac{Lm^{1/2}(2\omega)^{3/2}}{3\pi} \left\{ -\frac{2}{5} \left( \frac{\mu}{\omega} \right)^{5/2} + \frac{1}{16} \left( 1 - \frac{4\pi^2 T^2}{\omega^2} \right) \left( \frac{\mu}{\omega} \right)^{1/2} + \dots \right\}. \quad (\text{B.1})$$

For  $\Omega_r$  we find

$$\Omega_r \simeq -\frac{L(m\omega)^{1/2}}{2\pi\beta} \sum_{k=1}^{\infty} \frac{(-1)^k \sin(2\pi k\mu/\omega - 3\pi/4)}{k^{3/2} \sinh \theta_k} \quad (\text{B.2})$$

with  $\theta_k$  being defined in equation (2.19). The results of equations (B.1) and (B.2) can then be used to find

$$N_0 \simeq \frac{2L(2m\omega)^{1/2}}{3\pi} \left\{ \left( \frac{\mu}{\omega} \right)^{3/2} - \frac{1}{32} \left( 1 - \frac{4\pi^2 T^2}{\omega^2} \right) \left( \frac{\mu}{\omega} \right)^{-1/2} + \dots \right\} \quad (\text{B.3})$$

$$N_r \simeq L(m\omega)^{1/2} \frac{T}{\omega} \sum_{k=1}^{\infty} \frac{(-1)^k \cos(2\pi k\mu/\omega - 3\pi/4)}{k^{1/2} \sinh \theta_k}. \quad (\text{B.4})$$

(It is necessary to keep the second term indicated in  $N_0$  because it gives the leading order contribution to  $(\partial N/\partial T)|_{\mu,L,\omega}$ , needed to compute the specific heat using equation (4.3).)

We can now solve  $N = N_0 + N_r$  for  $\mu$ . Because  $N_r$  has no explicit factors of  $\mu$ , the situation is very similar to that discussed in section 3.1. In this case we find

$$\frac{\mu}{\omega} \simeq \left( \frac{3\pi N}{2\sqrt{2}L(m\omega)^{1/2}} \right)^{2/3}. \quad (\text{B.5})$$

The de Haas–van Alphen part of  $N$ , which we have called  $N_r$ , is negligible in comparison with  $N_0$ , and equation (B.5) is a very good approximation even for very low values of  $T \ll \omega$ . We verified this conclusion by solving for  $\mu$  numerically over a range of different temperatures.

The internal energy can be computed as described earlier. With only the leading order term in the specific heat kept, it can be shown using equation (4.3) that

$$C \simeq L(m\omega)^{1/2} \frac{\sqrt{2}\pi}{3} \left( \frac{\mu}{\omega} \right)^{1/2} \frac{T}{\omega}. \quad (\text{B.6})$$

This gives the familiar linear temperature dependence. Because the oscillations are invisible in  $\mu/\omega$ , they do not show up in the specific heat either. Combining equation (B.5) with equation (B.6) shows that  $C \propto N^{1/3}$ , a result that is typical of the unconfined three-dimensional gas. Once again we see that it is as if the confined spatial direction has increased the effective total spatial dimension by one, from 2 to 3. This is also true for the chemical potential found in equation (B.5).

## References

- [1] Wilson A H 1957 *Thermodynamics and Statistical Mechanics* (London: Cambridge University Press)
- [2] Huang K 1987 *Statistical Mechanics* 2nd edn (New York: Wiley)
- [3] Feynman R P 1972 *Statistical Mechanics* (New York: Addison-Wesley)
- [4] Pathria R K 1972 *Statistical Mechanics* (London: Pergamon)
- [5] Pethick C J and Smith H 2002 *Bose–Einstein Condensation in Dilute Gases* (Cambridge: Cambridge University Press)
- [6] Butts D A and Rokhsar D S 1997 *Phys. Rev. A* **55** 4346
- [7] Schneider J and Wallis H 1998 *Phys. Rev. A* **57** 1253
- [8] Bruun G M and Burnett K 1998 *Phys. Rev. A* **58** 2427
- [9] Vignolo P, Minguzzi A and Tosi M P 2000 *Phys. Rev. Lett.* **85** 2850
- [10] Gleisberg F, Wonneberger W, Schlöder U and Zimmermann C 2000 *Phys. Rev. A* **62** 063602
- [11] Brack M and van Zyl B P 2001 *Phys. Rev. Lett.* **86** 1574
- [12] Wang X Z 2002 *J. Phys. A: Math. Gen.* **35** 9601
- [13] van Zyl B P, Bhaduri R K S, Suzuki A and Brack M 2003 *Phys. Rev. A* **67** 023609
- [14] Brack M and Murthy M V N 2003 *J. Phys. A: Math. Gen.* **36** 1111
- [15] Brosens F, Devreese J T and Lemmens L F 1997 *Phys. Rev. E* **55** 227
- [16] Brosens F, Devreese J T and Lemmens L F 1997 *Phys. Rev. E* **55** 6795
- [17] Luczak F, Brosens F, Devreese J T and Lemmens L F 1998 *Phys. Rev. E* **57** 2411
- [18] Brosens F, Devreese J T and Lemmens L F 1998 *Phys. Rev. E* **57** 3871
- [19] Foulon S, Brosens F, Devreese J T and Lemmens L F 1999 *Phys. Rev. E* **59** 3911
- [20] Lemmens L F, Brosens F and Devreese J T 2000 *Phys. Rev. E* **61** 3358
- [21] Foulon S, Brosens F, Devreese J T and Lemmens L F 2001 *Phys. Rev. E* **63** 016111
- [22] Toms D J 2003 *Preprint cond-mat/0309399*
- [23] Toms D J Periodic structure of trapped Fermi gases in anisotropic potentials (in preparation)
- [24] de Haas W J and van Alphen P M 1930 *Leiden Commun.* **209a** 212a
- [25] Landau L D 1930 *Z. Phys.* **64** 629
- [26] Sondheimer E H and Wilson A H 1951 *Proc. R. Soc. A* **210** 173
- [27] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (Philadelphia, PA: Holt, Rinehart and Winston)
- [28] Whittaker E T and Watson G N 1928 *Modern Analysis* (London: Cambridge University Press)
- [29] Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards, Applied Mathematics Series)