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Simple analytical results for harmonically trapped quantum gases

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Abstract
By making use of the generating function for the associated Laguerre polynomials, we derive new analytical results for harmonically trapped quantum gases in arbitrary dimensions. These exact expressions prove to be very numerically efficient, and possess a much simpler mathematical form than those previously reported in the literature. As a direct consequence of our work, new summation relations for Laguerre polynomials are also established.

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1. Introduction

Sophisticated magneto-optical trapping and cooling techniques have finally made it possible to reliably fabricate trapped degenerate quantum gases in the laboratory. Remarkably, in these systems the inter-particle interactions between the neutral atoms can be 'tuned' by either adjusting the trapping geometry, using different atomic isotopes, and/or utilizing the so-called Feshbach resonance [1]. In the case of trapped degenerate Fermi gases, the ability to effectively tune the inter-particle interactions has led to an entirely new area of ultra-cold atoms research, in which detailed studies of the BEC-BCS crossover, and unitary regime, can be undertaken. For both fermions and bosons, there also exists a regime in which the inter-particle interactions can be taken to be weak. This results in a particularly attractive situation from a theoretical point of view because the non-interacting gas can serve as a useful starting point for investigating the weakly interacting quantum many-body system. Not surprisingly, several papers in the last few years have appeared where exact, analytical results for ideal, harmonically trapped quantum gases at finite temperatures and arbitrary dimensionality, d, have been presented [2–18].

In spite of the apparent simplicity of the problem, exact closed form results are in fact not trivial to obtain. Indeed, when the particles are fermions, closed form expressions for the thermodynamic properties of the system are difficult to calculate owing to the low-temperature analytic properties of the Fermi distribution function [11]. Regardless of the species of atoms under consideration however, the usefulness of such exact results (e.g., in density-functional theory (DFT) and the theory of trapped Bose gases) is now well established, and illustrates that theoretical investigations of this kind are not just academic in nature.

Arguably, the central theoretical tool that has permitted the most analytical progress is the connection between inverse Laplace transform (ILT) of the Bloch density matrix (BDM) and the first-order density matrix (FDM), from which the thermodynamic properties of the ideal quantum gases can be derived [19]. In the ILT technique, explicit expressions for the single-particle wavefunctions and eigenvalue spectrum are replaced by only knowledge of the BDM. In this way, it is possible to avoid the evaluation of finite or infinite summations (over single-particle levels) usually required for determining the quantum thermodynamic properties of the system. Moreover, the ILT approach provides a universal scheme to address either Fermi or Bose quantum statistics at finite temperatures, and arbitrary dimensions, in a *single* calculation. Consequently, analytical results (e.g., kinetic energy density, particle density, structure factors, momentum distributions, etc) for the trapped quantum gases exhibit a common mathematical form in which the dimensionality and quantum statistics are encoded in Fermi- or Bose-like distribution functions.

Unfortunately, it turns out that for all but the special case of $d = 2$, the dimensional dependence encoded in these functions is complicated. As a result, mathematical manipulations for other dimensions can become quite involved. For example, the work in [14] has provided a rigorous demonstration that the exact 2D zero-temperature fermionic expressions for the particle and kinetic energy densities reduce to their Thomas–Fermi (TF) forms in the large-N limit. Establishing this result for arbitrary dimensions, however, was not presented owing to the non-trivial way in which the dimensionality is encoded into the densities. The more recent work of Brack and Murthy [15] has managed to generalize these results to arbitrary dimensions, but their mathematical analysis is quite technical. In addition to the increased mathematical complexity, numerical implementations of the exact densities in, e.g., DFT or perturbative treatments of interparticle interactions, are not optimal, again because of the way in which dimensionality is treated within the usual ILT approach.

The goal of this paper is to then motivate further theoretical and computational investigations by providing new, exact, analytical results for harmonically trapped quantum gases, which are both numerically efficient and mathematically simpler than results previously reported. To this end, the rest of our paper is organized as follows. In the following section, we briefly review the mathematical formalism of the ILT approach, which serves to set the stage for the presentation of our new analytical results in section 3. Finally, in section 4 we present our summary and concluding remarks.

2. Mathematical formalism

The theoretical tool that we use to investigate either the trapped Fermi or Bose gas is the zero temperature BDM, $C_0(\mathbf{r}, \mathbf{r}'; \beta)$. The zero temperature BDM is defined by [19]

$$C_0(\mathbf{r}, \mathbf{r}'; \beta) = \sum_{\text{all i}} \psi_i^\star(\mathbf{r}')\psi_i(\mathbf{r}) \exp(-\beta\epsilon_i), \tag{1}$$

where the ψ_i's and the one-particle energies ϵ_i are the solutions of the time-independent Schrödinger equation. The constant β above is to be interpreted as a mathematical variable which in general is taken to be complex, and not the inverse temperature $1/k_B T$. The BDM satisfies the so-called Bloch equation

$$H_r C_0(\mathbf{r}, \mathbf{r}'; \beta) = -\frac{\partial C_0(\mathbf{r}, \mathbf{r}'; \beta)}{\partial \beta}, \tag{2}$$

subject to the initial condition

$$C_0(\mathbf{r}, \mathbf{r}'; 0) = \delta(\mathbf{r} - \mathbf{r}'). \tag{3}$$

While equation (1) suggests that one does need to know the single-particle wavefunctions and energies, this is not the case. Typically, an *ansatz* for the functional form of the BDM is made, with the exact expression determined from a solution to equations (2) and (3) [20]. Note also that the BDM is independent of the quantum statistics of the problem, meaning that we have a unified treatment for either Fermi or Bose gases. The Hamiltonian, H_r, that we use in the majority of this paper is the isotropic harmonic oscillator (HO) potential in d dimensions: $V(r) = \frac{1}{2}m\omega_0^2 r^2$, with $r = \sqrt{x_1^2 + \cdots + x_d^2}$ being the radial variable, and ω_0 the trapping frequency. When dealing exclusively with the 2D trapped *charged* quantum gas (cf section 3.4), the Hamiltonian takes the more specific form

$$H_r = \frac{(\mathbf{p} - e\mathbf{A}/c)^2}{2m} + \frac{1}{2}m\omega_0^2(x^2 + y^2), \tag{4}$$

where we now include a uniform, finite magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, directed along the z-axis, and use the symmetric gauge

$$\mathbf{A} = \left(-\tfrac{1}{2}By, \tfrac{1}{2}Bx, 0\right). \tag{5}$$

Assuming that we have found an explicit solution to the Bloch equation, we may determine the FDM via an inverse Laplace transform. For the case of finite temperatures, the ILT must be taken to be two-sided (i.e., so that the chemical potential μ can take on negative values), and we have [19]

$$\rho(\mathbf{r}, \mathbf{r}'; T) = \mathcal{L}_\mu^{-1}\left[\frac{2}{\beta}C_T(\mathbf{r}, \mathbf{r}'; \beta)\right], \tag{6}$$

where

$$\begin{aligned} C_T(\mathbf{r}, \mathbf{r}'; \beta) &= C_0(\mathbf{r}, \mathbf{r}'; \beta)\frac{\pi\beta T}{\sin(\pi\beta T)} \quad \text{(fermions)}, \\ &= C_0(\mathbf{r}, \mathbf{r}'; \beta)\frac{\pi\beta T}{\tan(\pi\beta T)} \quad \text{(bosons)}. \end{aligned} \tag{7}$$

The factor of 2 in equation (6) accounts for the spin degeneracy; in the case of spin-polarized fermions, or spinless bosons, the factor of 2 should be dropped. Equations (6) and (7) are the fundamental equations used to determine all of the theromodynamic properties of the d-dimensional trapped quantum gas at finite temperature. Of course, zero-temperature quantities can be obtained by taking the $T \to 0$ limit of the finite-T results.

3. Trapped quantum gases

3.1. Fermi gas at finite temperatures

Let us define the center-of-mass and relative coordinates

$$\mathbf{q} = \frac{\mathbf{r} + \mathbf{r}'}{2}, \qquad \mathbf{s} = \mathbf{r} - \mathbf{r}', \tag{8}$$

respectively. Unless stated otherwise, $k_B = 1$, and all lengths and energies are scaled by the oscillator length and the oscillator energy, respectively. The d-dimensional zero-temperature BDM then takes the form [21]

$$C_0^{(d)}(\mathbf{q}, \mathbf{s}; \beta) = \left(\frac{1}{2\pi\sinh(\beta)}\right)^{d/2} \exp\{-q^2\tanh(\beta/2) - s^2/4\coth(\beta/2)\}. \tag{9}$$

Now, utilizing the generating function for the associated Laguerre polynomials [22]

$$\frac{\exp\left(-x\frac{t}{1-t}\right)}{(1-t)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x) t^n, \tag{10}$$

and making use of this expression with $t = \mathrm{e}^{-\beta}$ and $t = -\mathrm{e}^{-\beta}$, the following new identities

$$\begin{aligned} \mathrm{e}^{-q^2\tanh(\beta/2)} &= \sum_{n=0}^{\infty}(-1)^n L_n^{d/2-1}(2q^2)\,\mathrm{e}^{-q^2}\,\mathrm{e}^{-(n+d/4)\beta}(\mathrm{e}^{\beta/2}+\mathrm{e}^{-\beta/2})^{d/2} \\ \mathrm{e}^{-s^2/4\coth(\beta/2)} &= \sum_{k=0}^{\infty} L_k^{d/2-1}(s^2/2)\,\mathrm{e}^{-s^2/4}\,\mathrm{e}^{-(k+d/4)\beta}(\mathrm{e}^{\beta/2}-\mathrm{e}^{-\beta/2})^{d/2}, \end{aligned} \tag{11}$$

can be established, respectively. The above expressions can be used to write a new form for the BDM:

$$C_0^{(d)}(\mathbf{q},\mathbf{s};\beta) = \frac{1}{\pi^{d/2}}\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}(-1)^n L_n^{d/2-1}(2q^2) L_k^{d/2-1}(s^2/2)\,\mathrm{e}^{-(q^2+s^2/4)}\,\mathrm{e}^{-(d/2+n+k)\beta}. \tag{12}$$

The FDM can now be determined by putting equation (12) into equation (7) (for fermions) and explicitly evaluating the ILT in equation (6). Equipped with the two-sided ILTs given in [16], the result of this calculation is

$$\rho^{(d)}(\mathbf{q},\mathbf{s};T) = \frac{2}{\pi^{d/2}}\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}(-1)^n L_n^{d/2-1}(2q^2) L_k^{d/2-1}(s^2/2)\,\mathrm{e}^{-(q^2+s^2/4)}\,\frac{1}{\exp\left(\frac{\varepsilon_n+k-\mu}{T}\right)+1}, \tag{13}$$

where $\varepsilon_n = (n + d/2)$ is the noninteracting eigenvalue spectrum. Equation (13) is one of our main new results. The utility of this expression can be better appreciated upon comparison with the FDM obtained previously [16]:

$$\rho^{(d)}(\mathbf{q},\mathbf{s};T) = \frac{2}{\pi^{d/2}}\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}(-1)^n L_n(2q^2) L_k(s^2/2)\,\mathrm{e}^{-(q^2+s^2/4)}\,F_{n,k}^{(d)}(\mu), \tag{14}$$

where

$$F_{n,k}^{(d)}(\mu) \equiv \left(\frac{1}{\exp[(\varepsilon_n+k-\mu)/T]+1} + \sum_{m=1}^{\infty}\frac{g_m^{(d)}}{\exp[(\varepsilon_n+k+2m-\mu)/T]+1}\right), \tag{15}$$

and

$$g_m^{(d)} = \frac{1}{m!}\frac{\Gamma(d/2+m-1)}{\Gamma(d/2-1)}. \tag{16}$$

Note that it is only for the special case of $d = 2$ where equations (13) and (14) agree in the functional form (i.e., $g_m^{(2)} = 0, \forall m$). For all other dimensions, the explicit mathematical structure of equation (14) changes with dimensionality (via $F_{n,k}^{(d)}(\mu)$), and we have an additional infinite sum over the m index. In contrast, equation (13) is truly universal in form, in that there is only a single-Fermi distribution function (i.e., avoiding the additional infinite m summation) regardless of the dimensionality. Equation (13) is rather remarkable in its mathematical simplicity, but this fact should not be used to conclude that the result is trivial. Indeed, the form of equation (13) suggests that we have done nothing more than to write down the definition of the FDM in terms of the single-particle states weighted by their statistical occupancy. We emphatically wish to point out that this is not the case; it would be exceedingly difficult to obtain equation (13) starting from the single-particle wavefunctions for the HO in d dimensions. In fact, if one were to go this route, non-trivial summation relations for the associated Laguerre polynomials would need to be established. It is also important to realize that equation (13) is much more numerically efficient than equation (14). In our simple benchmark tests for $N \sim \mathcal{O}(10^3)$ particles and $T \sim 0.5$ (T denotes the dimensionless quantity $(k_B T/\hbar\omega_0)$), we saw at least an order of magnitude improvement in computational speed when comparing equation (13) with equation (14).

The particle density in arbitrary dimensions now also takes on a particularly simple form. Explicitly, setting $\mathbf{s} = 0$ immediately yields the single-particle density

$$\rho^{(d)}(\mathbf{q}, T) = \frac{2}{\pi^{d/2}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} (-1)^n \binom{k + d/2 - 1}{k} L_n^{d/2-1}(2q^2)\, \mathrm{e}^{-q^2} \frac{1}{\exp\left(\frac{\varepsilon_n + k - \mu}{T}\right) + 1}, \tag{17}$$

where we have used $L_k^{\alpha}(0) = \binom{k+\alpha}{k}$ [22]. Again, obtaining this d-dimensional result by starting with the single-particle wavefunctions may not be practically possible.

3.2. Fermi gas at zero temperature

Our new expression for the FDM also readily admits the construction of zero-temperature results. Specifically, in the $T \to 0$ limit, the Fermi function becomes the Heaviside step function, namely,

$$\frac{1}{\exp\left(\frac{(\varepsilon_n + k) - \mu)}{T}\right) + 1} \to \Theta(\varepsilon_f - (\varepsilon_n + k)), \tag{18}$$

and when filling $M + 1$ oscillator shells, the Fermi energy is given by $\varepsilon_f = M + d/2$ [15]. Hence, the zero temperature FDM becomes

$$\begin{aligned}
\rho^{(d)}(\mathbf{q}, \mathbf{s}) &= \frac{2}{\pi^{d/2}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} (-1)^n L_n^{d/2-1}(2q^2) L_k^{d/2-1}(s^2/2)\, \mathrm{e}^{-(q^2+s^2/4)}\, \Theta(\varepsilon_f - (\varepsilon_n + k)) \\
&= \frac{2}{\pi^{d/2}} \sum_{n=0}^{M} \sum_{k=0}^{M-n} (-1)^n L_n^{d/2-1}(2q^2) L_k^{d/2-1}(s^2/2)\, \mathrm{e}^{-(q^2+s^2/4)} \\
&= \frac{2}{\pi^{d/2}} \sum_{n=0}^{M} (-1)^n L_n^{d/2-1}(2q^2) L_{M-n}^{d/2}(s^2/2)\, \mathrm{e}^{-(q^2+s^2/4)},
\end{aligned} \tag{19}$$

where the summation relation $\sum_{n=0}^{m} L_n^{\alpha}(x) = L_m^{\alpha+1}(x)$ has been used [22]. What is particularly noteworthy is the trivial way in which the zero temperature result follows from equation (13); namely, one has to simply replace the Fermi function by the Heaviside step function in the first line of equation (19). In contrast, if one starts from the finite-T expression given by equation (14) and proceeds to take the $T \to 0$ limit, the resulting expression is much more complicated and involves an additional m-summation which must be evaluated with some care (see, e.g., [5]).

The $T = 0$ particle density is obtained by setting $\mathbf{s} = 0$ in equation (19), which reads

$$\rho^{(d)}(\mathbf{q}) = \frac{2}{\pi^{d/2}} \sum_{n=0}^{M} (-1)^n \binom{M - n + d/2}{M - n} L_n^{d/2-1}(2q^2)\, \mathrm{e}^{-q^2}. \tag{20}$$

As expected, equation (20) has a much simpler mathematical form than the $T = 0$ d-dimensional results presented in [5].

To close this zero-temperature subsection, we wish to also present new analytical expressions for the kinetic energy densities. Our focus here on $T = 0$ is motivated by the fact that it is the regime most relevant to applications in DFT. For the kinetic energy density, we investigate three expressions, all of which can be evaluated from the $T = 0$ FDM given by equation (19) (hereby, we drop the superscript as it is understood that our results are for general dimensions):

$$\tau(\mathbf{q}) = -\frac{1}{2}\left(\frac{1}{4}\nabla_{\mathbf{q}}^2 + \nabla_{\mathbf{s}}^2\right)\rho(\mathbf{q},\mathbf{s})|_{\mathbf{s}=0} \tag{21}$$

$$\tau_1(\mathbf{q}) = \frac{1}{2}\left(\frac{1}{4}\nabla_{\mathbf{q}}^2 - \nabla_{\mathbf{s}}^2\right)\rho(\mathbf{q},\mathbf{s})|_{\mathbf{s}=0} \tag{22}$$

$$\xi(\mathbf{q}) = \frac{\tau(\mathbf{q}) + \tau_1(\mathbf{q})}{2} = -\frac{1}{2}\nabla_{\mathbf{s}}^2\rho(\mathbf{q},\mathbf{s})|_{\mathbf{s}=0}. \tag{23}$$

All three quantities integrate to the exact same kinetic energy, and since $\tau(\mathbf{q})$ and $\tau_1(\mathbf{q})$ have oscillations exactly opposite in phase, their mean $\xi(\mathbf{q})$ is a smooth function of q. To proceed, we first write our differential operators in d dimensions as

$$\nabla_{\mathbf{q}}^2 = \frac{\mathrm{d}^2}{\mathrm{d}q^2} + \frac{(d-1)}{q}\frac{\mathrm{d}}{\mathrm{d}q} = 4x\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2d\frac{\mathrm{d}}{\mathrm{d}x}, \qquad x = q^2 \tag{24}$$

$$\nabla_{\mathbf{s}}^2 = \frac{\mathrm{d}^2}{\mathrm{d}s^2} + \frac{(d-1)}{q}\frac{\mathrm{d}}{\mathrm{d}s} = 4y\frac{\mathrm{d}^2}{\mathrm{d}y^2} + 2d\frac{\mathrm{d}}{\mathrm{d}y}, \qquad y = s^2. \tag{25}$$

It is straightforward to show that

$$\nabla_{\mathbf{q}}^2\rho(\mathbf{q},\mathbf{s})|_{\mathbf{s}=0} = \frac{2}{\pi^{d/2}}\sum_{n=0}^{M}(-1)^n\binom{M-n+d/2}{M-n}(-2d-8n+4q^2)L_n^{d/2-1}(2q^2)\,\mathrm{e}^{-q^2}, \tag{26}$$

$$\nabla_{\mathbf{s}}^2\rho(\mathbf{q},\mathbf{s})|_{\mathbf{s}=0} = \frac{2}{\pi^{d/2}}\sum_{n=0}^{M}(-1)^n\binom{M-n+d/2}{M-n}\left(-\frac{d}{2} - \frac{2d}{2+d}(M-n)\right)L_n^{d/2-1}(2q^2)\,\mathrm{e}^{-q^2}, \tag{27}$$

where we have tacitly used the differential equation for the associated Laguerre polynomials [22],

$$x\frac{\mathrm{d}^2}{\mathrm{d}x^2}L_n^{\alpha}(x) + (1+\alpha-x)\frac{\mathrm{d}}{\mathrm{d}x}L_n^{\alpha}(x) + nL_n^{\alpha} = 0, \tag{28}$$

to simplify our expressions. Using equations (26) and (27) in the expressions for the kinetic energy densities above yields

$$\tau(\mathbf{q}) = \frac{1}{\pi^{d/2}}\sum_{n=0}^{M}(-1)^n\binom{M-n+d/2}{M-n}\left(d + \frac{2dM+4n}{d+2} - q^2\right)L_n^{d/2-1}(2q^2)\,\mathrm{e}^{-q^2} \tag{29}$$

$$\tau_1(\mathbf{q}) = \frac{1}{\pi^{d/2}}\sum_{n=0}^{M}(-1)^n\binom{M-n+d/2}{M-n}\left(\frac{2dM-4(d+1)n}{d+2} + q^2\right)L_n^{d/2-1}(2q^2)\,\mathrm{e}^{-q^2} \tag{30}$$

$$\xi(\mathbf{q}) = \frac{1}{\pi^{d/2}}\sum_{n=0}^{M}(-1)^n\binom{M-n+d/2}{M-n}\left(\frac{d}{2} + \frac{2d}{d+2}(M-n)\right)L_n^{d/2-1}(2q^2)\,\mathrm{e}^{-q^2}. \tag{31}$$

To our knowledge, the d-dimensional kinetic energy densities given by equations (29)–(31) have not yet appeared in the literature. It is also now easy to verify our earlier assertion that all three kinetic energy densities integrate to the exact same kinetic energy, namely,

$$E_{\mathrm{kin}}(M) = \frac{1}{2}E_{\mathrm{tot}}(M) = \frac{d}{2}\frac{2M+d+1}{d+1}\binom{M+d}{d}, \tag{32}$$

where M is related to the number of particles, N, by

$$N(M) = 2\binom{M+d}{M}. \tag{33}$$

3.3. Bose gas at finite temperatures

The ILT approach allows us to immediately write down the FDM for the trapped (spinless) Bose gas in arbitrary dimensions. Remarkably, all that is required is the replacement of the '+1' in the denominator of equation (13) by '−1' and the removal of the spin-degeneracy pre-factor of 2:

$$\rho(\mathbf{q},\mathbf{s};T) = \frac{1}{\pi^{d/2}}\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}(-1)^n L_n^{d/2-1}(2q^2)L_k^{d/2-1}(s^2/2)\,\mathrm{e}^{-(q^2+s^2/4)}\frac{1}{\exp\left(\frac{\varepsilon_n+k-\mu}{T}\right)-1}. \tag{34}$$

Thus, as advertised, the ILT approach requires no extra effort to construct the appropriate FDM for the trapped Bose gas in arbitrary dimensions. Equation (34) is a new result and serves to highlight the power of the ILT approach.

3.4. Trapped 2D charged quantum gas in a uniform magnetic field

In a very recent paper [18], we have presented for the first time a closed form expression for the FDM applicable to a 2D harmonically trapped charged quantum gas in the presence of a uniform magnetic field of arbitrary strength (see equation (4)). Scaling all lengths and energies by $\sqrt{\frac{m\omega_{\mathrm{eff}}}{\hbar}}$ and $\hbar\omega_{\mathrm{eff}}$, respectively, it was shown that the zero-temperature BDM takes the form

$$\begin{aligned}C_0(\mathbf{q},\mathbf{s};\beta) &= \frac{1}{2\pi\sinh(\beta)}\exp\left\{-(q^2+s^2/4)\coth(\beta)+(q^2-s^2/4)\frac{\cosh(\omega\beta)}{\sinh(\beta)}\right.\\ &\qquad\left.-\,\mathrm{i}(q_xs_y-q_ys_x)\frac{\sinh(\omega\beta)}{\sinh(\beta)}\right\}\\ &= \frac{1}{2\pi\sinh(\beta)}\exp\left\{-A\coth(\beta)+B\frac{\mathrm{e}^{\omega\beta}}{\mathrm{e}^{\beta}-\mathrm{e}^{-\beta}}+B^{\star}\frac{\mathrm{e}^{-\omega\beta}}{\mathrm{e}^{\beta}-\mathrm{e}^{-\beta}}\right\},\end{aligned} \tag{35}$$

where $\omega = \omega_c/\omega_{\mathrm{eff}}$, $\omega_c = eB/2mc$, $\omega_{\mathrm{eff}} = \sqrt{\omega_0^2+\omega_c^2}$ and

$$A = q^2+s^2/4 \qquad B = q^2-s^2/4+\mathrm{i}(q_ys_x-q_xs_y). \tag{36}$$

In the above, $B^{\star}$ denotes the complex conjugation. Our purpose here is to develop a new expression for the FDM, which is both mathematically and numerically more efficient than our previous result. To this end, we first write the second two exponential terms in the last line of equation (35) in terms of their Taylor series expansions, and then make use of the second identity in equation (11) for the first term to give

$$C_0(\mathbf{q},\mathbf{s};\beta) = \frac{1}{\pi}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}L_l^{m+n}(2A)\,\mathrm{e}^{-A}\frac{B^m(B^{\star})^n}{m!n!}\exp(-(1+2l+(1-\omega)m+(1+\omega)n)\beta). \tag{37}$$

Proceeding now exactly as for the zero field case, the FDM for fermions becomes

$$\rho(\mathbf{q},\mathbf{s};T)=\frac{2}{\pi}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\mathrm{L}_l^{m+n}(2A)\,\mathrm{e}^{-A}\,\frac{B^m(B^*)^n}{m!n!}\,\frac{1}{\exp\left(\frac{1+2l+(1-\omega)m+(1+\omega)n-\mu}{T}\right)+1},\tag{38}$$

where again, the FDM for the corresponding Bose system may be obtained by simply exchanging the '+1' for a '−1' in the denominator of the Fermi function and dropping the pre-factor of 2. For the sake of comparison, we recall that our previous result for the FDM for fermions is given by [18]

$$\rho(\mathbf{q},\mathbf{s};T)=\frac{2}{\pi}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{i=0}^{m}\sum_{j=0}^{n}\sum_{k}L_l(2A)\,\mathrm{e}^{-A}\,\frac{(-2B)^i}{i!}\,\frac{(-2B^\star)^j}{j!}$$
$$\times\begin{pmatrix}m\\ m-\mathrm{i}\end{pmatrix}\begin{pmatrix}n\\ n-\mathrm{j}\end{pmatrix}F_k(l,m,n,i,j),\tag{39}$$

where all of the temperature dependence is encoded in the function

$$F_k(l,m,n,i,j)=\frac{n(k)}{\exp\left(\frac{k+2(l+m+n)-i-j-(j-i)\omega-\mu}{T}\right)+1},$$

and the k summation is over $k=1,3,5$, with $n(1)=n(5)=1$ and $n(3)=-2$. Clearly equation (38) is a substantial improvement in terms of its mathematically simplicity over equation (39) and also proves to be much more numerically efficient.

To further illustrate how this alternative expression for the FDM may be useful, we now consider the much studied *uniform* charged quantum gas subjected to a homogeneous magnetic field (see [17] and references cited therein). In the present case, this amounts to taking the $\omega_0\to 0$ limit in equation (38), so that $\omega\to\omega_c/\omega_c=1$. We readily obtain the result (for fermions)

$$\rho(\mathbf{q},\mathbf{s};T)=\frac{2}{\pi}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}L_l^{m+n}(2A)\,\mathrm{e}^{-A}\,\frac{(B)^m(B^\star)^n}{m!n!}\,\frac{1}{\exp\left(\frac{1+2l+2n-\mu}{T}\right)+1},\tag{40}$$

which should be contrasted with the FDM obtained in [17], namely,

$$\rho(\mathbf{q},\mathbf{s};T)=\frac{2}{\pi}\sum_{n=0}^{\infty}L_n(s^2)\,\mathrm{e}^{-s^2/2-\mathrm{i}(q_xs_y-q_ys_x)}\,\frac{1}{\exp\left(\frac{1+2n-\mu}{T}\right)+1}.\tag{41}$$

Now, it is certainly not obvious that equations (40) and (41) are in fact mathematically equivalent. However, note that the m-sum can be evaluated by using the well-known identity between Laguerre polynomials [22]

$$L_n^{\alpha}(x+y)\,\mathrm{e}^{-y}=\sum_{k=0}^{\infty}L_n^{\alpha+k}(x)\frac{(-y)^k}{k!}.\tag{42}$$

Thus, equation (40) simplifies to

$$\rho(\mathbf{q},\mathbf{s};T)=\frac{2}{\pi}\sum_{l=0}^{\infty}\sum_{n=0}^{\infty}L_l^n(2A-B)\,\mathrm{e}^{B-A}\,\frac{(B^\star)^n}{n!}\,\frac{1}{\exp\left(\frac{1+2l+2n-\mu}{T}\right)+1}.\tag{43}$$

The above sums can be rearranged by using $l+n=k$, whence

$$\rho(\mathbf{q},\mathbf{s};T)=\frac{2}{\pi}\sum_{k=0}^{\infty}\sum_{n=0}^{k}L_{k-n}^n(2A-B)\,\mathrm{e}^{B-A}\,\frac{(B^\star)^n}{n!}\,\frac{1}{\exp\left(\frac{1+2k-\mu}{T}\right)+1}.\tag{44}$$

At this point, equations (44) and (41) can only be equivalent provided the following summation theorem for Laguerre polynomials is true:

$$L_n^{\alpha}(x-y) = \sum_{k=0}^{n} L_{n-k}^{\alpha+k}(x)\frac{y^k}{k!}. \tag{45}$$

We have been able to prove this summation theorem, and applying it to equation (44) finally yields

$$\begin{aligned}\rho(\mathbf{q},\mathbf{s};T) &= \frac{2}{\pi}\sum_{k=0}^{\infty} L_k(2A-B-B^\star)\,\mathrm{e}^{(B-A)/2}\frac{1}{\exp\left(\frac{1+2k-\mu}{T}\right)+1} \\ &= \frac{2}{\pi}\sum_{k=0}^{\infty} L_k(s^2)\,\mathrm{e}^{-s^2/2-\mathrm{i}(q_x s_y - q_y s_x)}\frac{1}{\exp\left(\frac{1+2k-\mu}{T}\right)+1},\end{aligned} \tag{46}$$

which is, of course, identical to equation (41). Thus, a comparison of equation (40), with an alternative expression in the literature, has led to (what we believe is) a new summation theorem for Laguerre polynomials, which is a useful addition to the limited inventory of such results in the mathematical literature.

4. Summary and conclusions

We have made use of the generating function for the associated Laguerre polynomials to develop new analytical results for d-dimensional harmonically trapped quantum gases. These new results have proven to be both mathematically and numerically more efficient than those previously reported, and will be of value in other areas of physics such as DFT and the physics of trapped Bose gases. As an immediate application, we foresee the work of Brack and Murthy being substantially simplified by making use of our $T=0$ d-dimensional results. For example, equation (34) (relating the densities τ, ρ, and ξ) in their paper [15] is now essentially a trivial consequence of the results presented in section 3.2. In fact, it is straightforward to derive additional equations of this kind by simply manipulating the explicit expressions given by equations (20) and (29)–(31). Moreover, equation (38) also allows for the calculation of a simple, closed form expression for the finite-T kinetic energy density of a 2D trapped Fermi gas in a magnetic field, which, to our knowledge, has not yet explicitly appeared in the literature[1]. Such an expression would be of great interest to workers in the field of magnetic-DFT [23], as it would permit a detailed comparison of the widely used local density approximation with an exact result. We have also established new summation relations for Laguerre polynomials, namely, equations (11) and (45), which we believe will be of use in future analytical studies beyond those which have been considered in this paper (e.g., in information entropies of orthogonal polynomials [24]).

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