Exact results for a charged harmonically trapped quantum gas at arbitrary temperature and magnetic field strength

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An analytical expression for the first-order density matrix of a charged, two-dimensional, harmonically confined quantum gas, in the presence of a constant magnetic field is derived. Our approach is nonpertabative, and is therefore exact for any temperature and magnetic field strength. We also present a useful factorization of the Bloch density matrix in the form of a simple product with a clean separation of the zero-field and field-dependent parts. This factorization provides an alternative way of analytically investigating the effects of the magnetic field on the system, and also permits the extension of our analysis to other dimensions, and/or anisotropic confinement.

I. INTRODUCTION

Theoretical investigations of harmonically trapped ideal Fermi gases have seen a renewed interest in recent years owing to the remarkable experimental advances made in the area of trapped, ultracold atoms.[1] Indeed, theorists now have an experimental realization of what is close to being an ideal, inhomogeneous, quantum many-body Fermi system. Sophisticated magneto-optical traps now allow for the possibility of "tuning" the dimensionality of these gases from three dimensions (3D) to quasi-2D or quasi-1D. Thus, studying the properties of essentially ideal, lower-dimensional many-body Fermi systems is now firmly in the realm of experimental fact, and not simply a matter of academic interest. Furthermore, analytical results for these systems can be of great use in the density-functional theory (DFT) of inhomogeneous Fermi systems, whereby one can bypass the numerically expensive one-particle Schrödinger equations.[2]

The ideal charged Bose gas (CBG) is the Bose analog of a charged Fermi system. This model consists of a gas of spinless, charged bosons, coupled to an external, homogeneous magnetic field, and was investigated in 3D by Osborne,[3] Kosevitch,[4] and later by Schafroth.[5] The uniform 2D CBG has also been analytically studied quite extensively in the literature in light of its possible connection to the theory of high-T_c in the cuprates.[6–11] To date, no detailed analytical analysis has been performed for the inhomogeneous case. Since the confined 2D CBG is no longer forbidden from undergoing a Bose-Einstein condensation (BEC) transition at low temperatures (i.e., the Bogoliubov $1/k^2$ theorem is no longer applicable),[12] an exact analytical investigation of the thermodynamic and magnetic properties [e.g., the Meissner-Ochsenfeld (MO) effect] of the inhomogeneous system would be of great interest.

The fundamental quantity from which the thermodynamic and magnetic properties of the ideal quantum gases are derived is the first-order density matrix (FDM), $\rho(\mathbf{r}, \mathbf{r}')$. However, it is highly nontrivial to obtain an exact expression for the FDM (even at zero temperature) for all but the simplest of cases, viz., the homogeneous ideal charged quantum gas. The introduction of a magnetic field further complicates the problem, and it is only relatively recently that an exact ana-

lytical expression for the zero temperature FDM of a *uniform* Fermi system coupled to a homogeneous magnetic field has become available.[13] Extensions of these results (i.e., to include the case of the CBG and finite temperatures), have only been given in the last few years.[10] For the inhomogeneous ideal charged quantum gas, even the field-free case at zero temperature is difficult. Indeed, exact results for nonuniform systems at zero[14–17] and finite temperature[18–20] are limited to the case of harmonic confinement. Not surprisingly, closed form, exact results for $\rho(\mathbf{r}, \mathbf{r}')$ for an ideal charged Fermi or Bose gas under general confinement, finite temperatures, and arbitrary magnetic field strength, are exceedingly difficult to obtain.

The purpose of the present work is to help fill in this gap by providing an analytical expression for $\rho(\mathbf{r}, \mathbf{r}')$, generalized to treat *exactly* the presence of a uniform external magnetic field and confining potential. Our focus will be on providing results for the 2D harmonically confined quantum gas, although the general approach of our analysis does allow for an extension to other dimensions, and anisotropic traps, should the need arise.[21] The exact results of this paper should prove useful in the areas of current-density-functional theory[22,23] (CDFT) which is a rigorous extension of DFT to inhomogeneous systems immersed in an external magnetic field, and for the analytical investigation of the magnetic and thermodynamic properties of the CBG in the case of nonuniform systems.

The rest of our paper is organized as follows. In the next section, we introduce the central theoretical tool used in our analysis, viz., the Bloch density matrix (BDM). In Sec. III we provide a derivation of the inverse Laplace transform of the BDM, which leads directly to the exact FDM for a Fermi or Bose gas at any finite temperature and magnetic field strength. Section IV summarizes our main results and offers a discussion of how they may be applied in the context of CDFT and the inhomogeneous 2D CBG.

II. THE BLOCH DENSITY MATRIX

The central theoretical tool used in our analysis is the zero temperature BDM, $C_0(\mathbf{r}, \mathbf{r}'; \beta)$, which is related to the FDM

through an inverse Laplace transform.[24] One of the key reasons for working with the BDM is that one does not require explicit knowledge of the one-particle wave functions of the associated trapping potential. In addition, the zero temperature BDM is independent of the quantum statistics of the system, thereby allowing for an extremely robust approach for treating either the Fermi or Bose gas. Since a detailed discussion of the BDM has already been given in our previous work, we will only present here the essential formalism required for a self-contained statement of the problem, and refer the reader to Refs. 10, 14, 18, and 19 for additional details.

The zero temperature BDM is defined by

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

where the ψ_i's and the one-particle energies ϵ_i are solutions of the 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 $1/k_BT$. 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

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

In this paper,

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

is the specific Hamiltonian we work with, where the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, is applied along the z axis, and

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

Note that while $C_0(\mathbf{r},\mathbf{r}';\beta)$ is gauge dependent, any physical observable is necessarily gauge invariant. By choosing a general functional form for $C_0(\mathbf{r},\mathbf{r}';\beta)$, the solution to Eqs. (2) and (3), with the Hamiltonian (4), can be obtained without having to specify the single-particle wave functions or energies. Such a solution has already been obtained by March and Tosi,[25] which we now present in a more explicit form:

$$C_0(\mathbf{r},\mathbf{r}';\beta) = \frac{m\omega_{\text{eff}}}{2\pi\hbar} \frac{1}{\sinh(\hbar\omega_{\text{eff}}\beta)} e^{-(im\omega_{\text{eff}}/\hbar)[\sinh(\hbar\omega_c\beta)/\sinh(\hbar\omega_{\text{eff}}\beta)](xy'-yx')}$$

$$\times e^{-[(x-x')^2+(y-y')^2](m\omega_{\text{eff}}/4\hbar)\{\coth(\hbar\omega_{\text{eff}}\beta)+[\cosh(\hbar\omega_c\beta)/\sinh(\hbar\omega_{\text{eff}}\beta)]\}}$$

$$\times e^{-[(x+x')^2+(y+y')^2](m\omega_{\text{eff}}/4\hbar)\{\coth(\hbar\omega_{\text{eff}}\beta)-[\cosh(\hbar\omega_c\beta)/\sinh(\hbar\omega_{\text{eff}}\beta)]\}}, \tag{6}$$

where

$$\omega_c = \frac{eB}{2mc}, \quad \omega_0 = \sqrt{\frac{k}{m}}, \quad \omega_{\text{eff}} = \sqrt{\omega_0^2 + \omega_c^2}. \tag{7}$$

Introducing the center-of-mass and relative coordinates $\mathbf{q}$ and $\mathbf{s}$, respectively,

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

allows us to write the BDM as

$$C_0(\mathbf{q},\mathbf{s};\beta) = \frac{m\omega_{\text{eff}}}{2\pi\hbar} \frac{1}{\sinh(\hbar\omega_{\text{eff}}\beta)} e^{-i(m\omega_{\text{eff}}/\hbar)(q_ys_x-q_xs_y)[\sinh(\hbar\omega_c\beta)/\sinh(\hbar\omega_{\text{eff}}\beta)]} e^{-(m\omega_{\text{eff}}/\hbar)(q^2\{\coth(\hbar\omega_{\text{eff}}\beta)-[\cosh(\hbar\omega_c\beta)/\sinh(\hbar\omega_{\text{eff}}\beta)]\})}$$

$$\times e^{-m\omega_{\text{eff}}/\hbar(s^2/4\{\coth(\hbar\omega_{\text{eff}}\beta)+[\cosh(\hbar\omega_c\beta)/\sinh(\hbar\omega_{\text{eff}}\beta)]\})}. \tag{9}$$

For later convenience, we now introduce the following definitions:

$$A = q^2 + \frac{s^2}{4}, \quad B = \frac{1}{2}\left(\frac{s^2}{4} - q^2\right) - \frac{i}{2}(q_ys_x - q_xs_y), \quad \omega = \frac{\omega_c}{\omega_{\text{eff}}}, \tag{10}$$

and scale all lengths and energies by $\ell_{\text{eff}} = \sqrt{\hbar/m\omega_{\text{eff}}}$ and $\hbar\omega_{\text{eff}}$, respectively. The zero temperature BDM can then be written in the more compact form

$$C_0(\mathbf{q},\mathbf{s};\beta) = \frac{1}{2\pi\sinh(\beta)}\exp\left(-A\coth(\beta) - B\frac{e^{-\omega\beta}}{\sinh(\beta)}\right.$$
$$\left. - B^\star\frac{e^{\omega\beta}}{\sinh(\beta)}\right), \tag{11}$$

where B^* denotes complex conjugation. Equation (11) serves as the starting point for the rest of our study, but it is worthwhile pointing out that a useful factorization of the BDM can be performed.

First, let us rewrite the BDM as

$$C_0(\mathbf{q},\mathbf{s};\beta) = \frac{1}{2\pi\sinh(\beta)}\exp\left\{-\left(q^2 + \frac{s^2}{4}\right)\coth(\beta)\right.$$
$$+ \left(q^2 - \frac{s^2}{4}\right)\frac{\coth(\omega\beta)}{\sinh(\beta)} + i(q_y s_x$$
$$\left. - q_x s_y)\frac{\sinh(\omega\beta)}{\sinh(\beta)}\right\}. \tag{12}$$

Making use of the trigonometric identities

$$\frac{\cosh(\beta) - \cosh(\omega\beta)}{\sinh(\beta)} = \tanh(\beta/2) - 2\frac{\sinh^2(\omega\beta/2)}{\sinh(\beta)},$$

$$\frac{\cosh(\beta) + \cosh(\omega\beta)}{\sinh(\beta)} = \coth(\beta/2) + 2\frac{\sinh^2(\omega\beta/2)}{\sinh(\beta)} \tag{13}$$

in Eq. (12) gives

$$C_0(\mathbf{q},\mathbf{s};\beta) = \frac{1}{2\pi\sinh(\beta)}e^{\{-q^2\tanh(\beta/2)-(s^2/4)\coth(\beta/2)\}}e^{U_c(\mathbf{q},\mathbf{s};\beta)}, \tag{14}$$

where

$$U_c(\mathbf{q},\mathbf{s};\beta) \equiv 2\left(q^2 - \frac{s^2}{4}\right)\frac{\sinh^2(\omega\beta/2)}{\sinh(\beta)} + i(q_x s_x$$
$$- q_x s_y)\frac{\sinh(\omega\beta)}{\sinh(\beta)}. \tag{15}$$

The "effective potential" $U_c(\mathbf{q},\mathbf{s};\beta)$ explicitly includes all of the magnetic field dependence, and there is a clean separation of the BDM into field free and field dependent parts. In particular, setting $\omega_c = 0$ in Eq. (15) immediately gives $U_c = 0$ and the BDM (14) reduces to that of a 2D harmonically trapped system.[14,18,19] This factorization is reminiscent of the introduction of an effective potential in Ref. 26, which was motivated by the desire to improve the Thomas-Fermi approximation to potentials which are varying too rapidly in some regions of space.[27] Viewing the magnetic field as an additional 1D confining potential suggests a similar interpretation in the present context; that is, going beyond $\omega_c = 0$ may be achieved through the introduction of some effective potential U_c which encodes the magnetic field dependence. Irrespective of this suggestive connection, however, Eq. (14) here should be viewed as a more direct route to generalizing our results below to other dimensions, and allowing for a more transparent analytical investigation of the effects of the

magnetic field in the weak/high field limits, along with anisotropic confinement, should this be desired.

We are now in a position to see why the BDM provides such a universal scheme to investigate either the Fermi or Bose gases. While the zero temperature BDM is independent of the quantum statistics, at finite temperature, the BDM for the Fermi system is obtained via $(k_B = 1)$[24]

$$C_T(\mathbf{q},\mathbf{s};\beta) = C_0(\mathbf{q},\mathbf{s};\beta)\frac{\pi\beta T}{\sin(\pi\beta T)} \quad \text{(fermions)}, \tag{16}$$

whereas for bosons, it is given by

$$C_T(\mathbf{q},\mathbf{s};\beta) = C_0(\mathbf{q},\mathbf{s};\beta)\frac{-\pi\beta T}{\tan(\pi\beta T)} \quad \text{(bosons)}. \tag{17}$$

Therefore, aside from the different temperature dependent factors in Eqs. (16) and (17), it is clear that only the $T=0$ BDM is required to study either quantum gas.

III. THE FIRST-ORDER DENSITY MATRIX

A. Fermi gas

The (spin-averaged) FDM at finite temperature is obtained by a two-sided inverse Laplace transform of the finite temperature BDM. The inverse Laplace transform must be two-sided to allow for the dual variable to go negative. Specifically, we have[28]

$$\rho(\mathbf{q},\mathbf{s};T) = \mathcal{L}_\mu^{-1}\left[\frac{2}{\beta}C_T(\mathbf{q},\mathbf{s};\beta)\right], \tag{18}$$

where μ is the chemical potential, which at fixed ω_c, is determined by particle number conservation. As we have discussed before,[14,18,19] it is very difficult to perform the inverse Laplace transform by simply substituting the finite temperature BDM, as given by Eqs. (11) and (16), into Eq. (18). In order to proceed any further analytically, one requires the following identities

$$\exp[-A\coth(\beta)] = \sum_{k=0}^{\infty} L_k(2A)e^{-A}\{e^{-2k\beta} - e^{-2(k+1)\beta}\}, \tag{19}$$

$$\exp\left(-\frac{Be^{-\omega\beta}}{\sinh(\beta)}\right) = \sum_{m=0}^{\infty}\sum_{i=0}^{m}\frac{(-2Be^{-(\omega-1)\beta})^i}{i!}\binom{m}{m-i}$$
$$\times\{e^{-2m\beta} - e^{-2(m+1)\beta}\}, \tag{20}$$

$$\exp\left(-\frac{B^\star e^{\omega\beta}}{\sinh(\beta)}\right) = \sum_{n=0}^{\infty}\sum_{j=0}^{n}\frac{(-2B^\star e^{(\omega+1)\beta})^j}{j!}\binom{n}{n-j}$$
$$\times\{e^{-2n\beta} - e^{-2(n+1)\beta}\}, \tag{21}$$

where $L_l(x)$ is a Laguerre polynomial. Utilizing these identities in Eq. (11) gives

$$C_0(\mathbf{q},\mathbf{s};\beta) = \frac{1}{2\Pi}\frac{1}{\sinh(\beta)}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{i=0}^{m}\sum_{j=0}^{n}L_l(2A)e^{-A}\frac{(-2B)^i}{i!}\frac{(-2B^{\star})^j}{j!}\binom{m}{m-i}\binom{n}{n-j}\times\{e^{(-2l-2m-2n+i+j)\beta+(j-i)\omega\beta}$$

$$-3e^{(-2l-2m-2n+i+j-2)\beta+(j-i)\omega\beta}+3e^{(-2l-2m-2n+i+j-4)\beta+(j-i)\omega\beta}-e^{(-2l-2m-2n+i+j-6)\beta+(j-i)\omega\beta}\}. \tag{22}$$

Notice that all of the β dependence is now contained in the exponential factors and the (two-sided) inverse Laplace transform is now tractable. The mathematical details of this transform closely follows our earlier work,[10,18,19] so here we will simply give the final result, namely,

$$\rho(\mathbf{q},\mathbf{s};T) = \frac{2}{\pi}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{i=0}^{m}\sum_{j=0}^{n}\sum_{k}L_l(2A)e^{-A}\frac{(-2B)^i}{i!}\frac{(-2B^{\star})^j}{j!}\binom{m}{m-i}\binom{n}{n-j}\times F_k(l,m,n,i,j), \tag{23}$$

where all of the temperature dependence is encoded in the Fermi-like function

$$F_k(l,m,n,i,j) \equiv \frac{n(k)}{\exp\left(\dfrac{k+2(l+m+n)-i-j-(j-i)\omega-\mu}{T}\right)+1} \quad \text{(fermions)}, \tag{24}$$

and the k summation is over $k=1,3,5$ with $n(1)=n(5)=1$ and $n(3)=-2$. Equation (23) is the central result of this paper and gives the exact FDM for an ideal, harmonically trapped 2D Fermi gas at arbitrary temperature and magnetic field strength. Putting $\mathbf{s}=0$ immediately yields the spatial density of the system. It is certainly worthwhile reemphasizing that Eq. (23) is completely general, and readily recovers previous results pertaining to this system by taking various limits. For example, in the uniform case at zero temperature, Eq. (23) can be shown to reduce to (with dimensional constants recovered)[10,13]

$$\rho\left(\mathbf{q}+\frac{\mathbf{s}}{2},\mathbf{q}-\frac{\mathbf{s}}{2}\right) = \frac{2m\omega_c}{\pi\hbar}e^{-i(m\omega_c/\hbar)(x'y-y'x)}e^{-(m\omega_c/2\hbar)s^2}L_{n_F-1}^{(1)}$$

$$\times\left(\frac{m\omega_c}{\hbar}s^2\right). \tag{25}$$

As an illustrative numerical example, we present in Fig. 1, the spatial density for $N=110$ particles at zero-temperature and various magnetic field strengths. It is important to note that while the summations at finite temperature in Eq. (23) look somewhat formidable, any practical numerical imple-

mentation requires only a relatively small number of terms. Figure 1, for example, required only a few minutes to plot using a nominally equipped PC running a generic flavor of Unix. Consequently, finite temperature effects are readily studied, should the need arise.[29] Note also that the relative ease for which we were able to write down $\rho(\mathbf{q},\mathbf{s};T)$ should not be used to conclude that the calculation is trivial. In particular, it is notoriously difficult to treat finite temperature effects exactly in the Fermi gas owing to the fact that one cannot express the Fermi distribution function as a convergent power series, except at very high temperatures.[20] Rather, one should view our almost immediate statement of the FDM as a testament to the utility of the inverse Laplace transform technique.

B. Bose gas

The power of the inverse Laplace transform technique is also apparent if one wishes to extend our results to the case of a harmonically confined 2D CBG. Indeed, one can immediately write down the final expression for the FDM, with the only changes being a change in the sign in front of unity in the denominator of Eq. (24), viz.,

$$F_k(l,m,n,i,j) \equiv \frac{n(k)}{\exp\left(\dfrac{k+2(l+m+n)-i-j-(j-i)\omega-\mu}{T}\right)-1} \quad \text{(bosons)}, \tag{26}$$

and the elimination of the factor of two in Eq. (18) (i.e., the bosons are spinless). Thus, with no additional work, we also have an exact, closed form expression for the FDM of thetrapped 2D CBG at arbitrary temperature

and magnetic field strength. Of course, setting $\omega_0=0$ reproduces the recently obtained finite temperature results corresponding to the uniform 2D CBG found in Ref. 10.
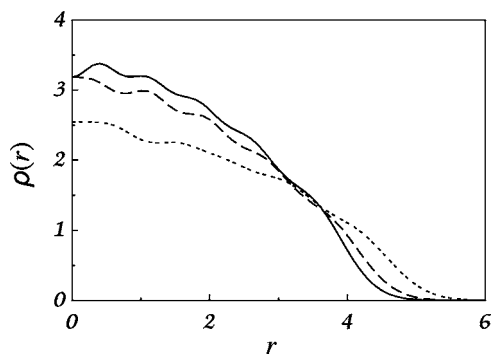
FIG. 1. Plot of the spatial density for $N=110$ fermions at zerotemperature and various magnetic field strengths. The solid curve is for $\omega=0$, the dashed curve for $\omega=0.45$, and the dotted curve for $\omega=0.70$. All lengths and energies have been scaled as discussed in the text

IV. SUMMARY AND FUTURE WORK

We have derived an analytical expression for the FDM of an ideal, harmonically trapped charged 2D Fermi or Bose gas at finite temperature and arbitrary magnetic field strength. This work therefore provides one more addition to the short list of inhomogeneous quantum systems for which an exact expression for the FDM can be obtained. Apart from their inherent technical merit, we believe that our results now open up several other fruitful avenues of investigation, which are outside the intended scope of this paper.

First it would be interesting to investigate the properties of the 2D Thomas-Fermi kinetic energy functional for the case of finite magnetic field. The motivating factor behind this suggestion lies in the remarkable fact that for zerofield, the 2D Thomas-Fermi kinetic energy functional leads to the *exact* quantum mechanical kinetic energy (i.e., without gradient corrections) when integrated over all space. This nontrivial result was only recently discovered by Brack and one of us.[14] From Eq. (25), it can be shown that the local-density approximation (LDA)[2] of the magnetic 2D kinetic energy functional is identical in form to the zero-field case, but now the magnetic field is encoded implicitly by the density.[10,13] Thus, determining whether the 2D magnetic-Thomas-Fermi kinetic energy functional is also exact (i.e., similar to its zero-field counterpart without gradient corrections) would be very interesting. It would also be illustrative to study the 2D exchange energy (i.e., suitable for the study of parabolically confined quantum dots in a magnetic field) via the exact FDM and compare the integrated, and spatial properties against the commonly used LDA of CDFT. This type of comparison has already been undertaken for the zero magnetic field case,[19] and would be an equally worthwhile endeavor for the finite-field case. Furthermore, having an exact expression for $\rho(\mathbf{r}, \mathbf{r}'; T)$ also allows for the perturbative study of the effects of particle-particle interactions, similar to what has already been performed for the $\omega_c=0$ case in Ref. [18].

As for the CBG, the most obvious application of our results will be in investigating the thermodynamic and magnetic properties of the inhomogeneous system. In contrast to the uniform 2D CBG, the trapping potential stabilizes the system to density and phase fluctuations and allows for the possibility of a transition to a BEC.[12] We recall here that the uniform 2D CBG does exhibit an essentially perfect MO effect, in spite of the *absence* of a BEC state.[10] Thus, analytically studying the connection between the onset of the MO effect and the BEC phase in the trapped system is, in our opinion, an important problem.

ACKNOWLEDGMENTS

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[21] Our restriction to 2D is for the following reasons: (i) the 2D calculation is the most transparent application of the inverse Laplace transform technique and (ii) we expect that the most relevant applications of our work will be to the inhomogeneous 2D Fermi and charged Bose gases.

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[27] The work in Ref. 26 does provide results for the inhomogeneous Fermi gas in a magnetic field of arbitrary strength. However, their *analytical* results are limited to zero temperature, and are only valid in weak and high field limits within the local-density approximation. For intermediate field strengths, the authors rely on a numerical inverse Laplace transform.

[28] At zero temperature, Eq. (18) still holds, but with C_0 instead of C_T, and the inverse Laplace transform is now one sided.

[29] Of course, at high temperatures, quantum effects (i.e., shell effects) are already washed out, and it makes no sense to continue using Eq. (23). See e.g., Ref. 18 for an illustrative example of this scenario.