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Finite-Temperature Evaluation of the Fermi Density Operator

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A rational expansion of the Fermi density operator is proposed. This approach allows us to calculate efficiently the physical properties of fermionic systems at finite temperatures without solving an eigenvalue problem. Using N evaluations of the Green's function, the Fermi density operator can be approximated, subject to a given precision, in the energy interval $[-\beta, \infty]$ with $\beta \propto$ N. The presented method may become especially useful for electronic structure calculations involving the calculation of charge densities, but it may also find other applications in, e.g., signal processing and numerical linear algebra. © 1998 Academic Press

Key Words: Fermi distribution; density operator (density matrix); fractional expansion; numerical methods; electronic structure calculations; finite temperature; charge density; Green's function.

1. INTRODUCTION

Quantum systems are most generally described in terms of their density operator ρ. Once ρ is known, the expectation values of physical quantities are obtained as

$$\langle A \rangle = \mathrm{Tr}(\rho \mathbf{A}), \tag{1}$$

where **A** is the associated operator of the quantity under consideration. For instance, for the calculation of the charge density, **A** becomes a projector and the charge density is simply given by the diagonal elements of ρ in the site representation. In the following we consider fermionic systems in the grand-canonical ensemble, where

$$\rho(\mu, T) = f\left(\frac{\mathbf{H} - \mu}{kT}\right), \tag{2}$$

with $\mathbf{H}$, T, and μ being the Hamiltonian, the temperature, and the chemical potential

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respectively, and

$$f(x) = \frac{1}{1 + e^x} \tag{3}$$

being the Fermi function. The Fermi function has been studied extensively, and effective approximation schemes for the case of scalar arguments, e.g. the Sommerfeld expansion, have been developed [1].

However, for the calculation of, e.g. ρ, one is faced with f applied to operators. For large scale applications, it cannot be switched into the eigen representation of H in order to evaluate Eq. (2), since in general full diagonalization of $\mathbf{H}$ is practically impossible. Because only polynomial and fractional functions of operators can be evaluated, corresponding decompositions of $f(x)$ are highly desirable. A recent approach is due to Goedecker [2] who proposed using systematically complex line integrals over the Green's function, and similar approaches in electronic structure calculations have been employed since then [3]. In the following a fractional expansion is presented which does not depend on the calculation of line integrals. It will be shown that physical quantities like the charge density, which is at the base of many methods in electronic structure calculations, can be obtained effectively *without* solving an eigenvalue problem, necessitating only evaluations of the Green's function at selected points. While the method is *a priori* constructed for finite temperatures, it is also well adapted to approximate charge densities at zero temperature since the range of the approximation can be arbitrarily extended toward lower temperatures.

2. FRACTIONAL EXPANSION

It is well known, that the Matsubara expansion [4] of the Fermi function,

$$f(x) = 1/2 - 2\sum_{m=0}^{\infty} \frac{x}{x^2 + [(2m+1)\pi]^2}, \tag{4}$$

shows very poor convergence properties when truncated to degree $m = N$. Although being the exact fractional series of $f(x)$, the Matsubara expansion is therefore not suited for numerical applications.

Let us consider the function

$$f_\alpha(x) := f(x - \alpha) f(-x - \alpha) = \frac{e^\alpha}{2[\cosh(\alpha) + \cosh(x)]}, \tag{5}$$

which is depicted in Fig. 1 for $\alpha = 20$. It is readily seen that for sufficiently high $\alpha > 0$, $f_\alpha(x + \alpha)$ will approximate $f(x)$ for all $x > -\alpha$, subject to a given precision. We now truncate the series in the denominator,

$$f_\alpha(x) \approx g_N(x;\alpha) := \frac{e^\alpha}{2 p_N(x;\alpha)}, \tag{6}$$

where

$$p_N(x;\alpha) = \cosh(\alpha) + \sum_{j=0}^{N} \frac{x^{2j}}{(2j)!}. \tag{7}$$

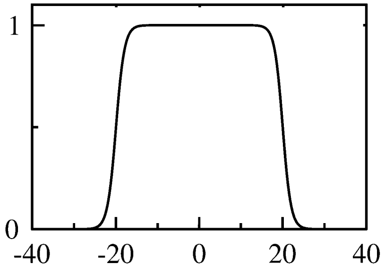

FIG. 1. The symmetric function $f_\alpha(x)$ for $\alpha = 20$.

It is readily seen than $p_N(x;\alpha)$ has no real zeros. For the fractional expansion of Eq. (6), we need all zeros z_ν, $\nu = 1, \ldots, N$, of $q(z) := p_N(x;\alpha)|_{x^2=z}$ (see [7]). For this purpose we define

$$y_1 = 1 + \cosh(\alpha); \quad y_i(z) = \frac{z^{i-1}}{[2(i-1)]!}, \quad i = 2, \ldots, N-1. \tag{8}$$

Then, it can be seen that

$$\mathbf{y}(z) \equiv (y_1(z), \ldots, y_N(z))^T$$

satisfies a matrix equation $\mathbf{A}\mathbf{y}(z_\nu) = z_\nu \mathbf{y}(z_\nu)$, with the $N \times N$ matrix $\mathrm{A} \equiv (a_{i,j})$,

$$a_{i,j} = \begin{cases} 2 + 2\cosh(\alpha) & \text{if } (i,j) = (1,2); \\ 2l(2l-1) & \text{if } (i,j) = (l, l+1), l = 2, \ldots, N-1; \\ 2N(1-2N) & \text{if } i = N; \\ 0 & \text{else.} \end{cases} \tag{9}$$

One easily shows that the z_ν are given by the eigenvalues of the matrix $\mathbf{A}$. It is well known that the zeros of a given polynomial can be obtained from an eigenvalue problem for a related Hessenberg matrix [5]. Goedecker [6] already has proposed to use this fact for the numerical evaluation of all zeros of a polynomial as eigenvalues. The usual scheme corresponds to the implicit choice of $y_i = z^{i-1}$; here the point is to avoid the explicit use of any factorial by using Eq. (8) leading to Eq. (9). The z_ν can be obtained as eigenvalues with, e.g. QR-rotations in a numerically stable way; using standard numerical libraries, $N = 40$ still yields accurate results, and enhanced precision calculations readily allow for larger N. However, $N = 30$ will be already sufficient for many applications as will be shown. In the following we stick to even N. For convenience, we also chose N and α so that no duplicate zeros z_ν are obtained. From the zeros we obtain the $2N$-zeros x_ν of $p_N(x;\alpha)$ as $\pm\sqrt{z_\nu}$. The zeros $x_{\nu;\alpha}$ do behave well, an example is plotted in Fig. 2(i).

Denoting

$$\gamma_\nu = \frac{e^\alpha}{4q'\left(x_\nu^2\right)x_\nu}, \tag{10}$$

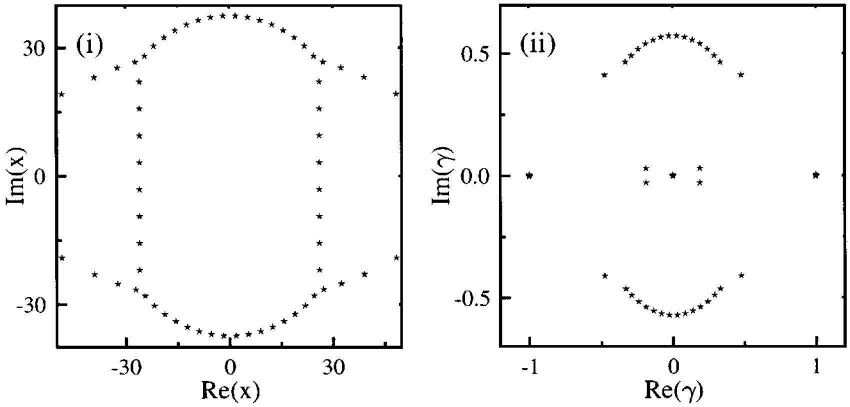

FIG. 2. Positions of the zeros x_ν (i) and the fractional coefficients γ_ν (ii) in the complex plane for the fractional expansion with $N = 32$ and $\alpha = 26$.

we now may write down the fractional decomposition

$$f_\alpha(x) \approx g_N(x;\alpha) = \sum_{\nu=1}^{2N} \frac{\gamma_\nu}{x - x_\nu}. \tag{11}$$

As shown in Fig. 2(ii), the coefficients γ_ν also behave well. The approximation Eq. (11) converges rapidly. Choosing, e.g. $N = 32$ and $\alpha = 26$, the error in approximating $f_\alpha(x)$ is less than 10^{-9} for all real x.

Clearly, for the reason of limited numerical precision, a Horner-like scheme should be used in order to evaluate the polynomial $q'(z) = \sum_{j=1}^{N} (jz^{j-1}/(2j)!)$ to avoid any explicit use of the factorial, i.e.,

$$q'(z) \\ = \frac{1}{2}\left(1 + \frac{z}{3*4}\left(2 + \frac{z}{5*6}\left(\cdots \frac{z}{(2N-2)(2N-3)}\left(N - 1 + \frac{zN}{(2N)(2N-1)}\right)\cdots\right)\right)\right).$$

We have considered the symmetric function f_α, since we may now exploit the *local symmetry* of $f_\alpha(x)$ about the points $x = \pm\alpha$, where $f_\alpha(x) = 0.5$. We can approximate successively the Fermi function as the sum of shifted functions $g_N(x;\alpha)$,

$$f(x) \approx g_N(x + \alpha;\alpha) + g_N(x + 3\alpha;\alpha) + \cdots + g_N(x + (2M - 1)\alpha;\alpha), \tag{12}$$

in the range $[-(2M-1)\alpha, \infty]$. This is visualized in Fig. 3 for $N = 32$ and $\alpha = 26$, using $MN = 96$ fractional terms [8]. For $x \to \infty$, the approximation Eq. (12) vanishes like x^{-2N}, compared to exponential decay of the Fermi function, resulting naturally in a good approximation. For negative x, the validity range of the approximation Eq. (12) may be increased by choosing a higher M, i.e., by successively adding shifted realizations of $g_N(x + (2m - 1)\alpha;\alpha)$. Principally, one could also use a single "basic function" ($M = 1$) in conjunction with a large value of α which necessitates, however, the use of enhanced precision for the calculation of the x_ν, as well as of the γ_ν; finally, this procedure will also be limited by the numerical accuracy of the eigenvalues of the matrix A, as well as of the

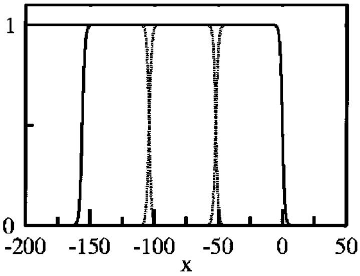

FIG. 3. Fermi function $f(x)$ and the fractional expansion with $M = 3$, $N = 32$, $\alpha = 26$. The dotted lines indicate the $M = 3$ shifted addents. The error in approximating $f(x)$ is less than 10^{-9} for $x \geq -135$.

accuracy of the the evaluation of the polynomial q' (see Ref. [9]). In contrast, the expansion Eq. (12) provides a systematic way to construct a step-like function over an arbitrarily large interval within fixed error bounds.

We note, that the function $f_{(\xi\alpha)}(\xi x)$ (see Eq. (5)) represents for sufficiently large ξ a nearly perfect projector on the subspace $x \in [-\alpha, \alpha]$. The presented rational expansion may, therefore, also find applications in other fields than physics, especially when applied to operators.

3. APPLICATION TO OPERATORS

The main interest of the approximation Eq. (12) lies in its generalization as operator equation, replacing x by some Hamiltonian $\mathbf{H}$. Then, the Fermi density operator

$$\rho(kT) = 1 \bigg/ \left(1 + \exp\left(\frac{\mathbf{H} - \mu}{kT}\right)\right) \approx kT \sum_{\nu=1}^{2N} \sum_{m=1}^{M} \frac{\gamma_\nu}{\mathbf{H} - \mu + kT[(2m-1)\alpha - x_\nu]} \tag{13}$$

can be approximated efficiently with MN evaluations of the Green's function. One may, furthermore, benefit from the fact that the zeros x_ν, as well as the corresponding $\gamma_{\nu;\alpha}$, come in quartets $x_\nu, x_\nu^*, -x_\nu, -x_\nu^*$ if the z_ν are distinct.

When applied to operators $\mathbf{H}$, the effect of the approximation Eq. (13) is to cut off the contributions of states with eigenvalues smaller than $\epsilon_l = \mu - kT(2M-1)\alpha$ (see also Fig. 3). This has no consequences if the spectrum of H is lower bounded with no eigenvalues in this domain. There are certainly applications when this effect is wanted, e.g. when considering the contributions of subbands separately.

In the example of Fig. 3, $M = 3$ may be too small for applications involving real metals, since the eigenvalue spectrum is covered down to -3.5 eV only at room temperature, and a higher M may be needed. However, $M = 3$ and $N = 32$ already is well adapted for, e.g. two-dimensional electron gases in mesoscopic systems. Assuming a Fermi level of about 15 meV, the Fermi density operator can be approximated quite exactly at temperatures down to 1.5 K.

The following simple example demonstrates how the total charge density can be obtained without solving an eigenvalue problem. Consider the Hamiltonian

$$H = \sum_j \epsilon_j a_j^\dagger a_j - \sum_{j,k} t_{j,k}(a_j^\dagger a_k + H.c.),$$

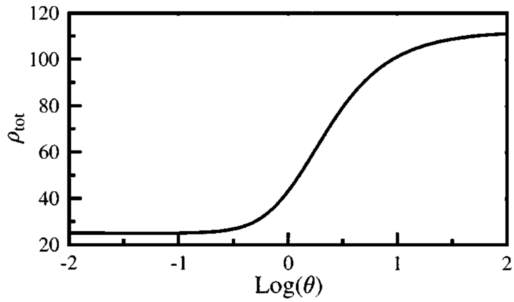

FIG. 4. Total charge $n_{\text{tot}} = \sum_{j=1}^{N_s} n_j$ as function of $\theta := kT/(\mu - \lambda_{\text{min}})$, where λ_{min} is the smallest eigenvalue (see text). The error in approximating n_{tot} using Eq. (13) with $N = 32$, $\alpha = 18$, and $M = 3$ is less than 10^{-6}.

where the on-site energies ϵ_j have been chosen from a uniform random distribution $\epsilon_j \in]3, 5[$, and the hopping amplitudes $t_{j,k}$ have been chosen as 1 for $j, k \equiv (j_x, j_y)^T$, $(k_x, k_y)^T$ being nearest neighbors in the two-dimensional plane. This Hamiltonian describes free spinless electrons in a discrete two-dimensional space in the presence of a random impurity potential. Hard wall boundary conditions have been assumed for a system with $N_s = 15 \times 15$ sites, allowing conveniently for direct diagonalization. The chemical potential has been fixed between the 25th and 26th smallest eigenvalue of H, $\mu = (\lambda_{25} + \lambda_{26})/2$; i.e., the system is in contact with a heat bath of constant chemical potential. We are interested in the total charge density as function of temperature T, especially in the limit of $T \to 0$.

In our case, the considered system is small enough to calculate the charge density n_j at site j exactly as

$$n_j = \sum_{i=1}^{N_s} \left|u_j^{(i)}\right|^2 f\left(\frac{\lambda_i - \mu}{kT}\right),$$

where the $u^{(i)}$ are the normalized eigenvectors, thus allowing for direct comparison.

We now approximate the Fermi density operator ρ according to Eq. (13). As noted in the Introduction, the charge density is given in this case by the diagonal elements of ρ. The results presented in Fig. 4 have been obtained using $MN = 96$ evaluations of the Green's function. It is seen that the charge density is indeed very well approximated in the domain where Eq. (12) approximates Eq. (3) as discussed previously. The total charge density at zero temperature (which is, of course, given by the number of states with energy smaller than the chemical potential, i.e., 25 in the present example), is practically identical to the total charge density at low temperatures.

4. CONCLUSIONS

A fractional approximation of the Fermi density operator has been proposed and the necessary concepts have been presented. This method becomes increasingly appropriate for higher temperatures where the numerical effort decreases. However, its range of convergence can be arbitrarily extended toward lower temperatures. It is expected to be useful especially for large-scale calculations at finite temperatures as, e.g. investigations of disordered systems, mesoscopic systems, and electronic structure calculations, in general.

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8. Since the x_ν and γ_ν come in complex-conjugate pairs, the numerical effort for evaluating Eq. (11) is reduced by a factor of two.
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