Integral representation of the Fermi distribution and its applications in electronic-structure calculations

S. Goedecker

Cornell Theory Center, Ithaca, New York 14853-3801

(Received 5 April 1993)

We show that the Fermi distribution can be represented by an infinite sum of contour integrals in the complex energy plane. The expansion converges very rapidly and a few terms are sufficient to obtain high accuracy.

I. INTRODUCTION

Many important quantities in electronic structure calculations are given as sums or integrals involving the Fermi distribution. These integrals usually cannot be solved analytically. Many methods have therefore been developed to evaluate these integrals approximately, the best known being the Sommerfeld expansion[1] and the Matsubara expansion.[2] Here we derive an integral representation which will turn out to be useful in the context of large-scale electronic-structure calculations, but will certainly also find other applications.

II. DERIVATION OF INTEGRAL REPRESENTATION

The Fermi distribution is given by

$$\frac{1}{1+e^{(\epsilon-\mu)/(kT)}} .$$

Let us first just differentiate and integrate the Fermi distribution with respect to μ,

$$\frac{1}{1+e^{(\epsilon-\mu)/(kT)}} = \int_{-\infty}^{\mu} \frac{\partial}{\partial y}\frac{1}{1+e^{y}}\Bigg|_{y=(\epsilon-\mu')/(kT)} \times \frac{-1}{kT}d\mu' .$$

The Taylor development of

$$1\Bigg/\left[\frac{\partial}{\partial y}\frac{-1}{1+e^{y}}\right]=2[1+\cosh(y)]$$

can easily be calculated and we get

$$\frac{1}{1+e^{(\epsilon-\mu)/(kT)}} = \frac{1}{2kT}\int_{-\infty}^{\mu}\frac{1}{2+\frac{1}{2!}\left[\frac{\epsilon-\mu'}{kT}\right]^{2}+\frac{1}{4!}\left[\frac{\epsilon-\mu'}{kT}\right]^{4}+\cdots}d\mu' . \tag{1}$$

Let us now truncate the infinite sum in the denominator to the (even) power n and let us denote the n zeros of the resulting nth-order polynomial which forms the denominator in Eq. (1) by $\alpha_\nu+i\beta_\nu$,

$$p(x)=2+\sum_{j=1}^{n/2}\frac{1}{(2j)!}x^{2j} .$$

Then a partial fraction decomposition can be found and we get

$$\frac{1}{1+e^{(\epsilon-\mu)/(kT)}}$$
$$=\int_{-\infty}^{\mu}\sum_{\nu=1}^{n}\frac{C_\nu}{(\epsilon-\mu')-kT(\alpha_\nu+i\beta_\nu)}d\mu' . \tag{2}$$

The expansion is extremely rapidly converging. In order to get a good overall approximation of

$$1\Bigg/\left[\frac{\partial}{\partial y}\frac{-1}{1+e^{y}}\right]=2[1+\cosh(y)] ,$$

the polynomial $p(y)$ has to be positive everywhere, to tend to ∞ for the argument tending to $\pm\infty$ and to coincide well with the exact function $2[1+\cosh(y)]$ near the

origin. All these requirements are fulfilled by the Taylor expansion. Table I gives the zeros, coefficients C_ν, and the maximal errors. The right-hand side of Eq. (2) can be seen as the sum of n line integrals of the Green's function $1/(\epsilon-z)$ in the complex plane, the path being n open lines which start at $\mu+kT(\alpha_\nu+i\beta_\nu)$ and go to $-\infty$. Since the Green's function is analytic away from the real axis, the result of the integration does not depend on the path.

Let us now look at these integrals more closely. Since

TABLE I. The coefficients α_ν, β_ν, and C_ν for $n=16$. The remaining 12 values can be determined by symmetry as described in the text. The error in approximating $1/\{(\partial/\partial y)[1/(1+e^{y})]\}$ is less than 1×10^{-6}. A MATHEMATICA program, which can be obtained by request from the author, was used for the calculation.

$\alpha_\nu+i\beta_\nu$	$C_\nu=A_\nu+iB_\nu$
$8.18322+i8.03979$	$-2.49379\times10^{-4}+i8.50867\times10^{-5}$
$3.73917+i8.19603$	$-1.29208\times10^{-2}+i2.65765\times10^{-3}$
$1.02555+i7.76630$	$-6.48392\times10^{-2}-i8.23174\times10^{-2}$
$5.20155\times10^{-4}+i3.14159$	$-961.323-i3.65247\times10^{-6}$

     <u>48</u>   17 573

$p(x)$ is real and symmetric, the zeros come in quartets (or pairs if the real part is zero), i.e., if $\alpha+i\beta$ is a zero, $\alpha-i\beta$, $-\alpha+i\beta$, and $-\alpha-i\beta$ are also zeros. Let us now assume that they come in quartets. The case when they come in pairs could be discussed in an analogous way. The symmetry is reflected in the coefficients C. Writing the coefficient C_ν belonging to $\alpha_\nu+i\beta_\nu$ as $C(\alpha+i\beta)$ we

have

$$C(-\alpha-i\beta)=-C(\alpha+i\beta) \; ,$$

$$C(\alpha-i\beta)=C^*(\alpha+i\beta) \; .$$

Writing the coefficients C_ν as $A_\nu+iB_\nu$, Eq. (2) can be rewritten as

$$\frac{1}{1+e^{(\epsilon-\mu)/(kT)}}=\sum_{\nu=1}^{n/4}\left[\int_{-\infty}^{\mu+T\alpha_\nu}\frac{A_\nu+iB_\nu}{(\epsilon-\mu')-ikT\beta_\nu}d\mu'+\int_{-\infty}^{\mu-T\alpha_\nu}\frac{-A_\nu+iB_\nu}{(\epsilon-\mu')-ikT\beta_\nu}d\mu'\right.$$
$$\left.+\int_{-\infty}^{\mu+T\alpha_\nu}\frac{A_\nu-iB_\nu}{(\epsilon-\mu')+ikT\beta_\nu}d\mu'+\int_{-\infty}^{\mu-T\alpha_\nu}\frac{-A_\nu-iB_\nu}{(\epsilon-\mu')+ikT\beta_\nu}d\mu'\right] \; .$$

By rearranging the different terms we obtain

$$\frac{1}{1+e^{(\epsilon-\mu)/(kT)}}=\sum_{\nu=1}^{n/4}\left[\int_{\Pi_\nu}\frac{2iB_\nu}{\epsilon-z}dz+\int_{\Lambda_\nu^+}\frac{A_\nu-iB_\nu}{\epsilon-z}dz\right.$$
$$\left.+\int_{\Lambda_\nu^-}\frac{A_\nu+iB_\nu}{\epsilon-z}dz\right] \; , \qquad (3)$$

where Π_ν is the path connecting $\mu+kT(-\alpha+i\beta)$ with $\mu+kT(-\alpha-i\beta)$ and $\Lambda_\nu^\pm$ is the path connecting $\mu+kT(-\alpha\pm i\beta)$ with $\mu+kT(\alpha\pm\beta)$ as shown in Fig. 1. If there are more than one set of zeros in the expansion, path Π can be chosen in such a way that it connects all the $\mu+kT(-\alpha\pm i\beta)$'s as shown in Fig. 1. The numerical effort for the finite temperature case is, therefore, not much higher than in the zero temperature limit since the total length of the path does not increase much. If the path integral is numerically approximated by a sum, it is easy to see that this corresponds to a Padé approximation of the Fermi distribution. Evidently, Eq. (3) can be generalized as an operator equation,

$$\frac{1}{1+e^{(H-\mu)/(kT)}}=\sum_{\nu=1}^{n/4}\left[\int_{\Pi_\nu}\frac{2iB_\nu}{H-z}dz+\int_{\Lambda_\nu^+}\frac{A_\nu-iB_\nu}{H-z}dz\right.$$
$$\left.+\int_{\Lambda_\nu^-}\frac{A_\nu+iB_\nu}{H-z}dz\right] \; , \qquad (4)$$

where H is the Hamiltonian.

The formula developed here can be of great usefulness every time we need to evaluate physical quantities requiring the Fermi distribution. Let us consider as an example the calculation of the charge density ρ in an independent electron approximation,

$$\rho(\mathbf{r})=2\sum_i\Psi_i(\mathbf{r})\frac{1}{1+e^{(\epsilon_i-\mu)/(kT)}}\Psi_i^*(\mathbf{r}) \; .$$

The factor of 2 in front comes from the fact that each orbital is occupied by two electrons. The charge density at finite temperature can be approximated with very high accuracy by a few terms in the sum

$$\rho(\mathbf{r})=\sum_{\nu=1}^{n/4}2\left[2iB_\nu\int_{\Pi_\nu}\left\langle\mathbf{r}\left|\frac{1}{H-z}\right|\mathbf{r}\right\rangle dz+(A_\nu-iB_\nu)\int_{\Lambda_\nu^+}\left\langle\mathbf{r}\left|\frac{1}{H-z}\right|\mathbf{r}\right\rangle dz+(A_\nu+iB_\nu)\int_{\Lambda_\nu^-}\left\langle\mathbf{r}\left|\frac{1}{H-z}\right|\mathbf{r}\right\rangle dz\right] \; . \qquad (5)$$

In the limit of zero temperature, the contribution of the Λ paths vanish, the Π path becomes a closed loop which intersects the real axis at the Fermi energy, and the sum $\sum_{\nu=1}^{n/4}4B_\nu$ tends to $1/\pi$ giving

$$\rho(\mathbf{r})=\sum_{i\,\mathrm{occ}}\Psi_i(\mathbf{r})\Psi_i^*(\mathbf{r})=\frac{i}{\pi}\oint\left\langle\mathbf{r}\left|\frac{1}{H-z}\right|\mathbf{r}\right\rangle dz \; . \qquad (6)$$

This result, namely, that the charge density at zero temperature can be written as a complex contour integral over the Green's function, has been known for a long time.[3]

Let us finally still give an intuitive interpretation of the integration along a Π path. Such an integral is equivalent to a real integral.
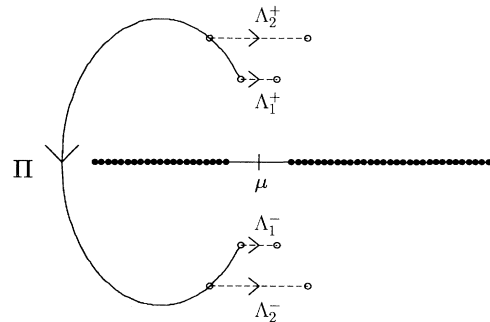

FIG. 1. The integration path in the complex energy plane. A nonvanishing density of states is denoted by dots in the real axis. The Π path is represented by the solid line, the Λ paths by the dashed line.

$$\int_{\Pi} \left\langle \mathbf{r} \left| \frac{1}{H-z} \right| \mathbf{r} \right\rangle dz$$

$$= \int_{-\infty}^{\mu - T\alpha} \left\langle \mathbf{r} \left| \frac{2i}{(H-\mu')^2 + (kT\beta)^2} \right| \mathbf{r} \right\rangle d\mu' \ .$$

This means that the local density of states is first convoluted with a Lorentzian and then a sum is taken over this smoothed density.

III. COMPARISON WITH MATSUBARA EXPANSION

The Matsubara expansion[2]

$$\frac{1}{1+e^y} \approx \frac{1}{2} - 2 \sum_{m=0}^{M} \frac{y}{y^2 + [(2m+1)\pi]^2} \tag{7}$$

is an expansion in rational functions which have poles at $\mu \pm im\pi kT$ for odd m. To obtain a moderate accuracy in an interval ΔE at least of the order of $M = \Delta E / kT$, terms have to be included in Eq. (7), which is usually unacceptably large. In the case of the expansion proposed in this paper, all the path integrals can be approximated by sums. Let us denote the total number of terms necessary to approximate the Fermi distribution in this way with a certain accuracy by N. To obtain the same accuracy with

Matsubara expansion, an M, which is orders of magnitude larger, is required. The Matsubara expansion is therefore not to be recommended for numerical applications.

IV. CONCLUSIONS

Contour integration techniques are a useful method in theoretical solid-state physics.[4] Even though people have already simulated the influence of finite temperature through an unclosed path, there has been no systematic theory behind these methods. The integral representation of the Fermi distribution, which we derived, is a powerful tool and allows a systematic calculation of finite temperature properties through contour integration techniques.

[1]N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia, 1976).
[2]G. D. Mahan, *Many Particle Physics* (Plenum, New York, 1981).
[3]V. Heine, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1955), Vol. 35, p. 3547.
[4]A. R. Williams, P. J. Feibelbaum, and N. D. Lang, Phys. Rev. D **26**, 5433 (1982).