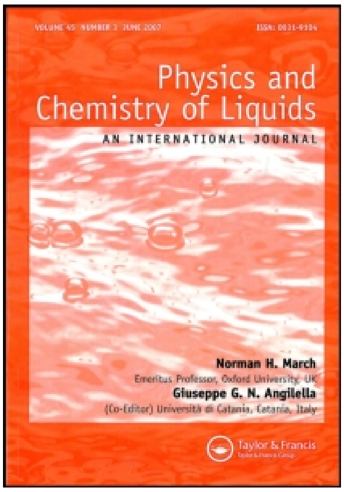

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SLATER SUM FOR A THREE-DIMENSIONAL INHOMOGENEOUS FERMI FLUID WITH ONE-DIMENSIONAL HARMONIC CONFINEMENT

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In early work, Bardeen [1] proposed a model whereby a three-dimensional Fermi fluid is confined to a half-space by a planar infinite barrier in the xy plane. Brown, Brown and March [2] subsequently worked out the Slater sum $S(z, \beta)$, $\beta = 1/k_B T$, for this same model of partial confinement. The present work considers $S(z, \beta)$ for additional harmonic confinement in the z direction. When the harmonic force constant is switched off the Slater sum calculated by Brown, Brown and March is recovered. The off-diagonal Slater sum, namely the canonical density matrix, is treated which in turn yields the Feynman propagator for this model when the reciprocal temperature β is replaced by the pure imaginary time.

Keywords: Inhomogeneous Fermi fluid; Slater sum; Propagator

In an early paper concerned with surface physics, Bardeen [1] introduced a model whereby a three-dimensional Fermi gas is confined to a half-space by a planar infinite barrier at $z = 0$ in the (xy)-plane. Subsequently, Brown, Brown and March [2] calculated the so-called Slater sum $S(\mathbf{r}, \beta)$ for this model, defined from the Bardeen wave

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functions $\psi_i(\mathbf{r})$ and corresponding energy levels ε_i as

$$S(\mathbf{r},\beta) = \sum_{\text{all } i} \psi_i(\mathbf{r})^* \psi_i(\mathbf{r}) \exp(-\beta\varepsilon_i) : \beta = 1/k_B T \tag{1}$$

where k_B denotes Boltzmann's constant while T is the absolute temperature. In fact, the procedure of Ref. [2] was to solve the Bloch equation for the canonical density matrix $C(\mathbf{r},\mathbf{r}',\beta)$, which has the Slater sum as its diagonal element. The result for $S(\mathbf{r},\beta)$ obtained by Brown, Brown and March [2], see also Moore and March [3], will be denoted by $S_{0B}(z,\beta)$, where B stands for (infinite) barrier and, anticipating additional one-dimensional confinement along the z-axis the subscript zero indicates the 'switching off' of such confining forces. The result of Ref. [2] was simply

$$S_{0B}(\mathbf{r},\beta) = \frac{1}{(2\pi\beta)^{3/2}}[1 - \exp(-2z^2/\beta)]. \tag{2}$$

This tends to the well known (classical) partition function density $1/(2\pi\beta)^{3/2}$ far from the infinite barrier at $z=0$.

Here, we propose to study one-dimensional confinement along the z-axis additional to the Bardeen infinite barrier, motivation for such a study being the very recent discussion, within the framework of approximate variational studies of a one-dimensional Schrödinger equation, by Fessatidis, Mancini and Prie [4] of an electron subjected to an infinite barrier B plus a confining homogeneous electric field of arbitrary strength. However, that model for the calculation of the Slater sum still presents difficulties for analytical study. We shall therefore show with a simpler, harmonic confinement potential energy

$$V(z) = \frac{1}{2}kz^2 \equiv \frac{1}{2}\omega^2 z^2 \tag{3}$$

along the z-axis, that the Slater sum, $S_{\omega B}(\mathbf{r},\beta)$, now obviously characterized by both the infinite barrier and the harmonic force constant k in Eq. (3) can be calculated in closed form.

Let us start from the known form of the canonical density matrix $C(\mathbf{r},\mathbf{r}',\beta)$:

$$C(\mathbf{r},\mathbf{r}',\beta) = \sum_i \psi_i(\mathbf{r})^* \psi_i(\mathbf{r}') \exp(-\beta\varepsilon_i) \tag{4}$$

calculated for a three-dimensional Fermi gas in the one-dimensional oscillator potential (3). The result is [5]

$$C(\mathbf{r},\mathbf{r}',\beta)=\frac{1}{2\pi\beta}\exp\left(-\frac{|\mathbf{x}-\mathbf{x}'|^2}{2\beta}\right)C_\omega(z,z',\beta) \tag{5}$$

where the classical angular frequency $\omega = k^{1/2}$ with particle mass taken as unity as in Eq. (3). In Eq. (5) $\mathbf{x}$ denotes a two-dimensional vector in the (xy) plane while C_z has the explicit form

$$C_\omega(z,z',\beta)=\left[\frac{\omega}{2\pi\sinh(\beta\omega)}\right]^{1/2}\exp\left\{-\frac{\omega}{4}\tanh\left(\frac{\beta\omega}{2}\right)(z+z')^2 -\frac{\omega}{4}\coth\left(\frac{\beta\omega}{2}\right)(z-z')^2\right\}. \tag{6}$$

We now note that while Eq. (5) with C_z given by Eq. (6) satisfies the Bloch equation

$$\hat{H}_\mathbf{r}C=-\frac{\partial C}{\partial\beta} \tag{7}$$

with the 'initial' condition

$$C(\omega;\mathbf{r},\mathbf{r}',\beta=0)=\delta(\mathbf{r}-\mathbf{r}') \tag{8}$$

we wish to introduce the Bardeen infinite barrier B. For this case, $C_{\omega B}(z,z',\beta)$ must clearly vanish when either z or z' is zero, because of the conditions the barrier imposes on the Bardeen wave functions in Eq. (4). However, the one-dimensional harmonic oscillator wave functions without the barrier, which are implicit in Eq. (6), can be divided into symmetric (s) and antisymmetric (a) about $z=0$. The anti-symmetric functions plainly satisfy the barrier boundary condition, and therefore we must project the 'antisymmetric' part out of Eq. (6).

Thus C_ω in Eq. (6) can be written as a sum of a symmetric and an antisymmetric part:

$$C_\omega = C^{(s)}+C^{(a)}. \tag{9}$$

Evidently, both $C^{(s)}$ and $C^{(a)}$ will still satisfy the Bloch equation (7) with $\hat{H}_\mathbf{r}$ containing the harmonic potential (3), and, with the introduction of a factor of 2, one can readily restore the delta function boundary condition (8) on the antisymmetric part $C^{(a)}$.

We note here the most direct route to the calculation of the Slater sum $S_{\omega B}(z, \beta)$ in the presence of the infinite barrier (B). To project out the antisymmetric part, we write

$$S_{\omega B}(z, \beta) = S_\omega(z, \beta) - C_\omega(z, -z, \beta) \tag{10}$$

and using Eq. (6) one finds almost immediately

$$S_{\omega B}(z, \beta) = \left\{ \frac{\omega}{2\pi \sinh(\beta\omega)} \right\}^{1/2} \left[\exp(-4Az^2) - \exp(-4Bz^2)\right] \tag{11}$$

where A and B are defined by

$$A(\beta, \omega) = \frac{\omega}{4} \tanh\left(\frac{\beta\omega}{2}\right) \tag{12}$$

and

$$B(\beta, \omega) = \frac{\omega}{4} \coth\left(\frac{\beta\omega}{2}\right). \tag{13}$$

Letting the force constant $k = \omega^2$ tend to zero, $A \to 0$ as $\beta k/8$ from Eq. (12) while B from Eq. (12) has the limit $1/2\beta$. Equation (11) then reduces to the infinite barrier Slater sum given in Eq. (2).

The off-diagonal generalization of Eq. (10) to the canonical density matrix associated with one-dimensional harmonic confinement plus the planar infinite barrier reads

$$C_{\omega,B}(z, z', \beta) = C_\omega(z, z', \beta) - C_\omega(z, -z', \beta) \tag{14}$$

and again using Eq. (6) one obtains

$$C_{\omega,B}(z, z', \beta) = \left\{ \frac{\omega}{2\pi \sinh(\beta\omega)} \right\}^{1/2} \{ \exp\left[-A(z - z')^2 - B(z + z')^2\right] - \exp\left[-A(z + z')^2 - B(z - z')^2\right]\} \tag{15}$$

which reduces to Eq. (11) on putting $z' = z$.

We think it is of some interest to present an alternative argument to the above for projecting out the antisymmetric part $C^{(a)}$. This alternative adopted below is to use a complex Fourier transform (FT). Implementing the FT technique to separate $C^{(s)}$ and $C^{(a)}$ in

Eq. (9), and using Eqs. (5) and (6) we need to evaluate the integral

$$I = \left\{\frac{\omega}{2\pi\sinh(\beta\omega)}\right\}^{1/2}\int_{-\infty}^{\infty}\exp\left\{-A(z+z')^2\right\}$$
$$\exp\left\{-B(z-z')^2\right\}\exp(-ipz')\,dz'. \tag{16}$$

Physically I involves both direct and momentum space wave function $\psi_n(z)$ and $\hat{\psi}_n(p)$ respectively:

$$I = \sum_n \exp(-\beta\varepsilon_n)\psi_n(z)\hat{\psi}_n(p). \tag{17}$$

After regrouping the terms in the exponents in Eq. (16), I can be evaluated as

$$I = \left\{\frac{\omega}{2(A+B)\sinh(\beta\omega)}\right\}^{1/2}\exp\left\{-\frac{4ABz^2}{A+B}-\frac{p^2}{4(A+B)}\right\}$$
$$\left[\cos\left(\frac{A-B}{A+B}\right)pz + i\sin\left(\frac{A-B}{A+B}\right)pz\right]. \tag{18}$$

The most remarkable feature of Eq. (18) is the relative simplicity of the z dependence. Now, we require to Fourier invert the p variable to z' in the imaginary part of Eq. (18) in order to recover $C_{\omega B}$.

To conclude the harmonic confinement with infinite barrier, let us determine the position z_m of the spatial maximum for the Slater sum in Eq. (11). By differentiating with respect to z one gets

$$z_m = \sqrt{\frac{\ln(A/B)}{4(A-B)}}. \tag{19}$$

Figure 1 shows a plot of $\zeta = \sqrt{\omega}z_m$ against $\gamma = \beta\omega$ in units where $e = -1$, $\hbar = 1$, $m_e = 1$ and $4\pi\varepsilon_0 = 1$.

To conclude, we note the following points:

(i) the main result (15) of this Letter becomes the Feynman propagator for the infinite barrier plus harmonic confinement model when $\beta \to it$, the pure imaginary time;

(ii) it would be of interest for the future if one could 'switch on' to the C matrix (15) a linear potential Fz, as considered in Ref. [3]. One could write for the Slater sum

$$S_{F\omega B}(z,\beta) = S_{\omega B}(z,\beta)\exp[-\beta U(z,\beta)] \tag{20}$$

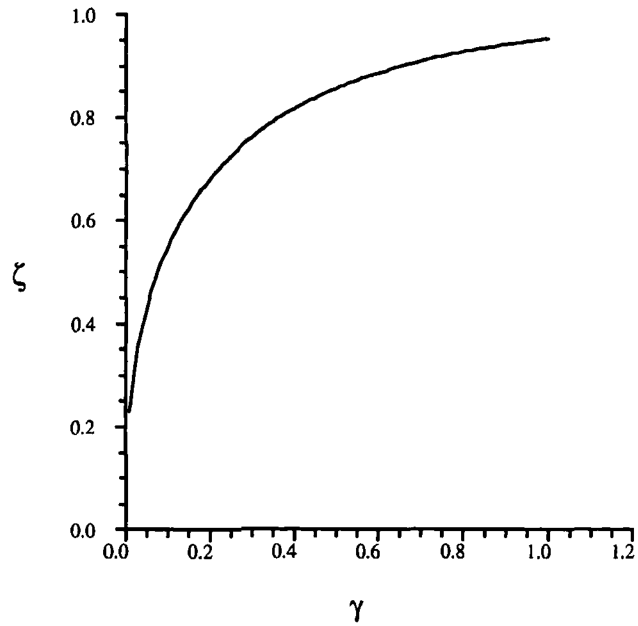

FIGURE 1 Shows in dimensionless form the variation of maximum (z_m) in Eq. (19). The dependent variable ζ plotted is defined as $\omega^{1/2}z_m$ while $\gamma=\beta\omega$. As $\gamma\rightarrow 0$, it is to be noted that $\zeta\rightarrow 0$ with an infinite slope.

where $U(z,\beta)$ is the effective potential associated with the 'perturbation' Fz. The simplest choice of $U(z,\beta)$ is to take it from the case of purely free electrons in a potential Fz, when it becomes [6]

$$U(z,\beta) = Fz + \frac{\beta^3 F^2}{24}. \tag{21}$$

In this regime the position of the spatial maximum of the Slater sum $S_{\omega B}(z,\beta)$ is shifted towards the barrier by a displacement Δz_m proportional to the field F. Admitting a linear response one can easily find the result

$$\Delta z_m = \beta F \frac{S_{\omega B}(z_m,\beta)}{S''_{\omega B}(z_m,\beta)} \tag{22}$$

where the second derivative is made with respect to z.

A more refined treatment would replace the 'local' term Fz by a non-local form derived from the perturbation theory of March and Murray [7], namely

$$U(z,\beta) = \int dz_1\, Fz_1 \int_0^{\beta} d\beta_1 C_{\omega,B}(z,z_1,\beta-\beta_1) \\ C_{\omega,B}(z_1,z,\beta_1) + O(F^2) \qquad (23)$$

but the detail proliferates when the form (6) is used in that framework so we shall not go into further detail. However, a future study of the symmetric linear potential $F|z|$ is called for as one could then use the techniques described above to project out the antisymmetrical part reflecting the infinite barrier.

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