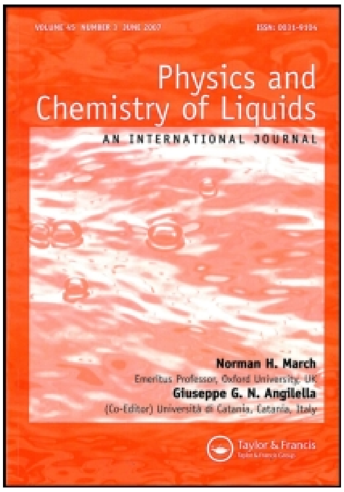

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LETTER

Slater sum for an inhomogeneous liquid of Fermions generated by a sech^2x potential in one dimension

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In one dimension, the Slater sum $S(x,\beta)$, which is the diagonal element of the canonical density matrix, satisfies a known partial differential equation characterised by a one-body potential $V(x)$. Here, for the case of a sech$^2 x$ potential in one dimension, it is stressed that $S(x,\beta)$ is explicitly related to the limit $S_0(\beta)$ as $V(x)\to 0$ and to $V(x)$ itself. This is the same input information as in the Thomas–Fermi result. The relevance to density functional theory is emphasised.

Keywords: inhomogeneous Fermi liquid; Thomas–Fermi limit; exact slater sum

In a recent article [1], we have been concerned with extracting a one-dimensional potential $V(x)$ from the Slater sum $S(x,\beta)$. In wave function terms, this quantity is defined by

$$S(x,\beta)=\sum_{\text{all } i}\psi_i^*(x)\psi_i(x)\exp(-\beta\varepsilon_i), \tag{1}$$

with β the inverse of the thermal energy $k_{\mathrm{B}}T: \beta=(k_{\mathrm{B}}T)^{-1}$. Here, the wave functions $\psi_i(x)$, together with the corresponding eigenvalues ε_i, are generated by the one-body Schrödinger equation

$$H\psi_i(x)=\varepsilon_i\psi_i(x), \tag{2}$$

where the Hamiltonian H, in units such that $\hbar^2=m=1$, is given by

$$H=-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x). \tag{3}$$

Going back to the early work of March and Murray [2], it is known that $S(x,\beta)$ satisfies the partial differential equation

$$\frac{1}{8}\frac{\partial^3 S(x,\beta)}{\partial x^3}-\frac{\partial^2 S(x,\beta)}{\partial x\partial\beta}-V(x)\frac{\partial S(x,\beta)}{\partial x}-\frac{1}{2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}S(x,\beta)=0. \tag{4}$$

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It is relevant for what follows on the $\mathrm{sech}^2 x$ potential, to note that the Thomas–Fermi (TF) approximation, valid for $V(x)$ varying slowly with x, yields

$$S_{\mathrm{TF}}(x,\beta) = S_0(\beta)\exp\big(-\beta V(x)\big), \tag{5}$$

where $S_0(\beta)$ is the free Fermion limit $V(x) \to 0$, given by

$$S_0(\beta) = (2\pi\beta)^{-1/2}. \tag{6}$$

While Equation (5) has a limited range of validity for $V(x)$ almost constant in space, the purpose of the present Letter is to emphasise that the same input information characterising $S_{\mathrm{TF}}(x,\beta)$ in Equation (5) determines $S(x,\beta)$ for the $\mathrm{sech}^2 x$ potential focussed on below.

Specifically, we take the potential $V(x)$ to be defined by

$$V(x) = -\gamma^2\,\mathrm{sech}^2(\gamma x), \tag{7}$$

which is known to generate a single bound state with energy given by $\varepsilon_0 = -\gamma^2/2$. The normalised bound-state wave function $\psi(x)$ is known to be [3,4]

$$\psi(x) = \sqrt{\frac{\gamma}{2}}\,\mathrm{sech}\,(\gamma x), \tag{8}$$

and hence the contribution, $S_{\mathrm{b}}(x,\beta)$ say, made to the Slater sum (1) is given by

$$S_{\mathrm{b}}(x,\beta) = \frac{\gamma}{2}\mathrm{sech}^2(\gamma x)\exp\big(\beta\gamma^2/2\big) = -\frac{1}{2\gamma}\exp\big(\beta\gamma^2/2\big)\,V(x), \tag{9}$$

the second step involving Equation (7). As shown in [4], the continuum (c) contribution to the Slater sum $S(x,\beta)$ is given by

$$S_{\mathrm{c}}(x,\beta) = S_0(\beta) - \frac{1}{2\gamma}\mathrm{erfc}(\sqrt{2\beta}\gamma/2)\exp\big(\beta\gamma^2/2\big)\,V(x), \tag{10}$$

the total Slater sum being

$$S(x,\beta) = S_{\mathrm{b}}(x,\beta) + S_{\mathrm{c}}(x,\beta). \tag{11}$$

The entire x-dependence of the total Slater sum for this potential is seen from Equations (9)–(11) to be contained in $V(x)$, somewhat analogous to the TF approximation quoted in Equation (5). $S_0(\beta)$ defined in Equation (6) enters both expressions (5) and (11), the latter via Equation (10). Of course, the remaining β-dependence, while elementary in the TF limit (5), is much richer for the $\mathrm{sech}^2(\gamma x)$ potential, via Equations (9)–(11).

Let us next return to the partial differential Equation (4) for the Slater sum $S(x,\beta)$. Then, the shape of $S(x,\beta)$ in Equations (9)–(11) for the $\mathrm{sech}^2(\gamma x)$ potential can be written in the compact form

$$S(x,\beta) = S_0(\beta) + V(x)h(\beta). \tag{12}$$

Substituting this form into Equation (4) it is readily shown that:

$$\frac{\mathrm{d}h(\beta)}{\mathrm{d}\beta} + \left(\frac{\frac{3}{2}V(x)V'(x) - \frac{1}{8}V'''(x)}{V'(x)}\right)h(\beta) = -\frac{1}{2}S_0(\beta). \tag{13}$$

But for $V(x)$ in Equation (7):

$$\frac{\frac{3}{2}V(x)V'(x) - \frac{1}{8}V'''(x)}{V'(x)} = -\frac{\gamma^2}{2}, \tag{14}$$

and we recover $h(\beta)$ as above in Equations (9)–(11). Any potential satisfying Equation (14) will evidently lead to the form (12) for the Slater sum. This is related to density functional theory (DFT), which works with a Fermion density $n(x, E)$ related to the Slater sum by inverse Laplace transform [2].

Finally, we return to the approximate TF result (5). We propose a generalisation of the form

$$S(x, \beta) = u(\beta)\exp[-V(x)\, g(\beta)]. \tag{15}$$

By substitution in (4), we show that the 'generalised TF form' gives the precise result for $S(x, \beta)$ for the harmonic oscillator potential

$$V(x) = \frac{1}{2}\omega^2 x^2. \tag{16}$$

We find specifically

$$g(\beta) = \frac{2}{\omega}\tanh\left(\frac{\omega}{2}(\beta - C_1)\right), \tag{17}$$

$$u(\beta) = \frac{C_2}{\sqrt{\sinh(\omega(\beta - C_1))}}, \tag{18}$$

where C_1 and C_2 are integration constants. When $C_1 = 0$ and $C_2 = \sqrt{\omega/2\pi}$, this coincides with the well-known result [1]:

$$S(x, \beta) = \left(\frac{1}{2\pi\beta}\right)^{1/2}\left(\frac{\beta\omega}{\sinh(\beta\omega)}\right)^{1/2}\exp\left[-\omega x^2 \tanh\left(\frac{\beta\omega}{2}\right)\right]. \tag{19}$$

Of course, this is less general than the result involving Equations (12) and (14), which work for the $\text{sech}^2(\gamma x)$ potential.

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References

[1] N.H. March and L.M. Nieto, Phys. Lett. A **373**, 1691 (2009).
[2] N.H. March and A.M. Murray, Phys. Rev. **120**, 830 (1960).
[3] E.W. Montroll, J. Math. Phys. **11**, 635 (1970).
[4] I.A. Howard, A. Minguzzi, N.H. March, and M.P. Tosi, J. Math. Phys. **45**, 2411 (2004).