One Dimensional Continuum
Falicov-Kimball Model in the Strongly Correlated Limit

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Abstract

In this paper we study the thermodynamics of the one dimensional continuum analogue of the Falicov-Kimball model in the strongly correlated limit using a method developed by Salsburg, Zwanzig and Kirkwood for the Takahashi gas. In the ground state it is found that the $f$ electrons form a cluster. The effect of including a Takahashi repulsion between $f$ particles is also studied where it is found that as the repulsion is increased the ground state $f$ electron configuration changes discontinuously from the clustered configuration to a homogeneous or equal spaced configuration analogous to the checkerboard configuration which arises in the lattice Falicov-Kimball model.
1 Introduction

The Falicov-Kimball model [1] was initially proposed as a simple model for the semiconductor-metal transition in SmB$_6$ and transition metal oxides. The model consists of two species of electrons—localised $f$ electrons and an itinerant band of $d$ electrons. The Hamiltonian is

$$\mathcal{H} = \sum_k \epsilon_k c_k^\dagger c_k + U \sum_i d_i^\dagger d_i f_i^\dagger f_i$$

(1.1)

where $f_i$ is the destruction operator for $f$ electrons on site $i$, $d_i$ is the destruction operator for the $d$-band Wannier state at site $i$ and $c_k$ is the destruction operator for the $d$ electron Bloch state with wave vector $k$ and kinetic energy $\epsilon_k$.

The only interaction then is an on-site interaction between $f$ and $d$ electrons. Of course the model could be extended to include longer range $f$-$d$ interactions, $f$-$f$ (lattice gas type) interactions and $d$-$d$ interactions. Spin could be introduced for the $d$ electrons with Hubbard-type interactions. In [2] and [3] the model was independently introduced as a model for crystallization and also viewed as a Hubbard model [4] where one of the spin species of electrons is immobile.

A great deal more is known about the Falicov-Kimball model than is known about the Hubbard model. In [1] the model was treated within a mean field framework. It was deduced that for large enough $U$ there is a first order phase transition which was interpreted as a semiconductor-metal transition.

In [2] it was established by means of operator inequalities that for the bipartite lattices with equal numbers of $f$ and $d$ electrons and a half-filled band, the ground state is ordered in any dimension, the $f$ electrons forming a checkerboard pattern. For $d \geq 2$ it was shown further that the crystalline order persists at finite temperature.

In [5] and [6] sharp upper and lower bounds are obtained for the ground state energy in the two dimensional case. For some special values of the parameters the bounds are shown to coalesce and so the exact ground state energy is derived. Some of the results of [2] and [3] are also independently reproduced. In [5] and [6] the thermodynamics of the model is investigated for large dimensionality $d$. An exact solution is obtained in the $d = \infty$ limit for the thermodynamic potential, the critical temperature, the order parameter and several correlation functions.

In [7] the ground state of the one dimensional model is studied by means of second order perturbation theory and exact numerical calculations for periodic configurations of the $f$ electrons. A restricted ground state phase diagram with a fractal structure is derived. In [8] the one dimensional model is studied for large negative $U$, the $f$ electrons being interpreted as nuclei. An exact formula for the leading order contribution (for large $|U|$) to the ground state energy is derived from which it is deduced that the system forms atoms ($d$-$f$ pairs) which have an effective repulsion between them if $|U|$ is sufficiently large.

In this paper we study the one dimensional continuum analogue of the Falicov-Kimball model in the strongly correlated limit. Although in terms of mathematical complexity this model is a long way removed from the lattice model with finite interaction strength in higher dimensions, there may be some generally applicable physics which can be deduced from this study. We obtain the exact thermodynamic potential via a method first used by Salsburg, Zwanzig and Kirkwood [11] for the Takahashi gas [12]. We discuss the ground state energy as well as a physical interpretation of the model in terms of the Takahashi gas. Finally, we discuss the effect of introducing a Takahashi type interaction between the $f$ particles.

2 Continuum Model and Exact Solution in One Dimension in the Limit of Strong Correlations

In the continuum analogue of the Falicov-Kimball model, we have a system of fermions ($d$ electrons) and stationary scatterers ($f$ electrons). If there are $M$ scatterers at positions $y_1, \ldots, y_M$
then the equation for the $d$ particle eigenfunction $\psi(x)$ is

$$
\left[ -\frac{1}{\pi^2} \nabla^2 + U \sum_{j=1}^{M} \delta(x - y_j) \right] \psi(x) = E \psi(x) \quad (2.1)
$$

where $E$ is the energy eigenvalue and we have scaled the fermion mass and Planck’s constant appropriately.

In the strongly correlated limit ($U = \infty$) the one dimensional continuum analogue of the Falicov-Kimball model reduces to a system containing a number of impenetrable barriers configured along the line. That is, if the length of the line is $V$ and there are $M$ f electrons at positions $0 < y_1 < y_2 < \ldots < y_M < V$ then the $d$ electrons experience impenetrable barriers at positions $y_0 \equiv 0, y_1, \ldots, y_M$, and $y_{M+1} \equiv V$ or infinitely high wells in the regions $(y_0, y_1), (y_1, y_2), \ldots, (y_M, y_{M+1})$.

In this case the eigenvalue problem (2.1) is trivial, reducing to

$$
-\frac{1}{\pi^2} \psi''(x) = E \psi(x) \quad (2.2)
$$

$$
\psi(y_j) = 0 \quad \text{for} \quad j = 0, 1, \ldots, M + 1 \quad (2.3)
$$

$$
\psi(x) = 0 \quad \text{for} \quad x < 0 \quad \text{and} \quad x > V \quad (2.4)
$$

The single particle wavefunction for a state with wave number $k \geq 1$ in well $1 \leq j \leq M + 1$ is

$$
\psi_{jk}(x) = \begin{cases} 
\sqrt{\frac{2}{y_j - y_{j-1}}} \sin \left( \frac{\pi k (x - y_{j-1})}{y_j - y_{j-1}} \right) & y_{j-1} \leq x \leq y_j \\
0 & \text{otherwise} 
\end{cases} \quad (2.5)
$$

and the corresponding energy eigenvalue is

$$
E_{jk} = \frac{k^2}{(y_j - y_{j-1})^2} \quad (2.6)
$$

To calculate the thermodynamic potential for this model, we begin by defining a canonical partition function for the system with $M$ f electrons and $N$ d electrons viz

$$
Z_{MN} = \int Dy \prod_{j=1}^{M+1} \prod_{k=1}^{\infty} \sum_{n_{jk}=0,1} \exp(-\beta n_{jk} E_{jk}) \quad (2.7)
$$

where the primed sum is restricted to configurations with $N$ d particles ie

$$
\sum_{j=1}^{M+1} \sum_{k=1}^{\infty} n_{jk} = N \quad (2.8)
$$

and

$$
\int Dy = \int_0^V dy_M \int_0^{y_M} dy_{M-1} \ldots \int_0^{y_2} dy_1 \quad (2.9)
$$

The restriction on the sum can be removed by defining a grand canonical partition function

$$
\mathcal{Q}(V) = \sum_{N=1}^{\infty} z^N Z_{MN} \quad (2.10)
$$

$$
= \int Dy \prod_{j=1}^{M+1} \prod_{k=1}^{\infty} \left[ 1 + ze^{-\beta E_{jk}} \right] \quad (2.11)
$$

1. We assume fixed end boundary conditions.
where use has been made of (2.7).

Making the definition
\[
f(x) \equiv \prod_{k=1}^{\infty} \left[ 1 + ze^{-\beta k^2/z^2} \right] \tag{2.12}
\]
we have, using (2.6), (2.9), (2.11) and (2.12) that
\[
Q(V) = \int D_y \prod_{j=1}^{M+1} f(y_j - y_{j-1}) \tag{2.13}
\]
\[
= \int_0^V f(V - y_M) dy_M \int_0^{y_M} f(y_M - y_{M-1}) dy_{M-1} \tag{2.14}
\]
\[
= (f \ast \ldots \ast f)(V) \tag{2.15}
\]
where \(f \ast \ldots \ast f\) denotes the \((M+1)\)-fold Laplace convolution of \(f\).

We take the Laplace transform of \(Q\) with respect to \(V\) viz
\[
\mathcal{L}_Q(s) = \int_0^\infty e^{-sV} Q(V) dV \tag{2.16}
\]
\[
= \int_0^\infty e^{-sV} (f \ast \ldots \ast f)(V) \tag{2.17}
\]
\[
= [F(s)]^{M+1} \tag{2.18}
\]
where
\[
F(s) = \int_0^\infty f(x) e^{-sx} dx \tag{2.19}
\]
denotes the Laplace transform of \(f\) and we have made use of (2.15) and the Laplace convolution theorem.

Applying the Laplace inversion formula to (2.18) we then have
\[
Q(V) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} [F(s)]^{M+1} e^{sV} ds \tag{2.20}
\]
where the contour lies to the right of all singularities of \(F(s)\).

The singularity structure of \(F\) can be deduced from a different representation of \(f\) which we derive in appendix A viz
\[
f(x) = \frac{e^{\chi_f x}}{\sqrt{1 + z}} \prod_{k=1}^{\infty} \left| 1 - e^{2\pi(-v_k + iu_k)x} \right|^2 \tag{2.21}
\]
where
\[
\chi_f = \int_0^\infty \log \left( 1 + ze^{-\beta x^2} \right) dx \tag{2.22}
\]
denotes the thermodynamic potential for a system of free \(d\) particles,
\[
u_k = \sqrt{\frac{\mu + \sqrt{\mu^2 + (2k-1)^2\pi^2/\beta^2}}{2}} \tag{2.23}
\]
\[
u_k = \frac{(2k-1)\pi}{\sqrt{2\beta \mu + (2k-1)^2\pi^2/\beta^2}} \tag{2.24}
\]
The $u_k$ and $v_k$ form increasing sequences so $F(s)$ has simple poles at

\[
\begin{align*}
    s &= \chi_f \\
    s &= \chi_f - 2\pi (v_k \pm iu_k) \quad k = 1, 2, 3, \ldots \\
    s &= \chi_f - 4\pi v_k \quad k = 1, 2, 3, \ldots \\
    s &= \chi_f - 2\pi (v_k \pm iu_k + v_l \pm iu_l) \quad 1 \leq k < l \\
\end{align*}
\]

(2.25)

In (2.20) then, we must take $c > \chi_f$.

Now the thermodynamic potential $\chi$ is given by

\[
\chi \equiv \lim_{V \to \infty} \frac{\log Q(V)}{V}
\]

(2.26)

where in taking the limit, the well density

\[
m \equiv \frac{M + 1}{V}
\]

(2.27)

is held constant. We evaluate the right hand side of (2.20) for large $V$ and $M$ by the method of steepest descents. We write

\[
Q(V) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \exp [VH(s)] ds \quad c > \chi_f
\]

(2.28)

where

\[
H(s) \equiv s + m \log F(s)
\]

(2.29)

and so, assuming that $H(s)$ has a single stationary point $s_0$ in the half plane $\Re s > \chi_f$ we have

\[
\chi = H(s_0)
\]

(2.30)

From the pole structure of $F$ (2.25) and the fact that $\chi$ is real, we deduce that $s_0$ lies on the real axis, the schematic form of $H(s)$ being given as in Fig. 1. That is, $H(s)$ has a branch point at $s = \chi_f$ and $H(s) \sim s$ as $s \to \infty$. $s_0$ is therefore a local minimum of $H(s)$ on the real axis viz

\[
\chi = \min_{s > \chi_f} H(s)
\]

(2.31)

The steepest descents method was first employed by Salsburg, Zwanzig and Kirkwood [1] in their calculation of equilibrium properties of the Takahashi gas [2] which, as we shall in section 4, has some similarities with the present model.

The thermodynamics of the model can be determined from $\chi$. For instance, the fugacity can be rendered as a function of the temperature, the $d$ electron density $n \equiv N/V$ and the $f$ electron (well) density $m$ by inverting the relation

\[
n = \frac{\partial \chi}{\partial z}
\]

(2.32)

The Helmholtz free energy is then given by

\[
\psi = \mu - \frac{\chi}{n\beta}
\]

(2.33)

In general, $s_0$ cannot be calculated analytically. In the limit $\beta \to \infty$ however, the function $H(s)$ simplifies and the ground state energy can be derived.
3 Ground State Energy

The ground state energy (per d electron) is given by

$$\varepsilon_G = \mu - \frac{p_G}{n} \quad (3.1)$$

where

$$p_G \equiv \lim_{\beta \to \infty} \frac{\chi}{\beta} \quad (3.2)$$

denotes the ground state pressure and in (3.1) \( \mu \) is determined as a function of the d electron density by inverting the limiting form of (2.32) viz

$$n = \frac{\partial p_G}{\partial \mu} \quad (3.3)$$

To find \( p_G \) we require the limiting form of \( H(s)/\beta \). Now, using (2.22) we have

$$\chi_f = \int_0^\infty \log \left( 1 + e^{\beta(\mu - x^2)} \right) dx$$

$$\sim \beta \int_0^{\sqrt{\mu}} (\mu - x^2) \, dx$$

$$= \frac{2}{3} \beta \mu^{3/2} \quad (3.4)$$

Writing \( s = \beta \mu^{3/2} t \) then, we use (2.19) and (2.12) to get

$$F(s) = \int_0^\infty \prod_{k=1}^\infty \{ 1 + \exp \left[ \beta \mu \left( 1 - k^2/\mu x^2 \right) \right] \} \exp \left[ -\beta \mu t \sqrt{x} \right] \, dx$$

$$= \frac{1}{\sqrt{\mu}} \int_0^\infty \prod_{k=1}^\infty \{ 1 + \exp \left[ \beta \mu \left( 1 - k^2/x^2 \right) \right] \} \exp \left[ -\beta \mu t x \right] \, dx$$

$$\sim \frac{1}{\sqrt{\mu}} \int_0^\infty \prod_{k=1}^{\lfloor x \rfloor} \exp \left[ \beta \mu \left( 1 - k^2/x^2 \right) \right] \exp \left[ -\beta \mu t x \right] \, dx$$

$$= \frac{1}{\sqrt{\mu}} \int_0^\infty e^{\beta \mu g(x,t)} \, dx$$

(3.7)

(3.8)

(3.9)

(3.10)

where

$$g(x,t) \equiv \lfloor x \rfloor - \frac{\lfloor x \rfloor \left( \lfloor x \rfloor + 1/2 \right) \left( \lfloor x \rfloor + 1 \right)}{3x^2} - tx \quad (3.11)$$

and we have used the identity

$$\sum_{k=1}^K k^2 = K(K+1/2)(K+1) \frac{3}{3} \quad (3.12)$$

Clearly \( g(x,t) \sim (2/3 - t)x \) as \( x \to \infty \) and hence the integral (3.10) converges if \( t > 2/3 \) as we would expect from (3.6) and the requirement that \( s > \chi_f \).

Evaluating (3.10) by Laplace’s method we then have

$$F(s) \sim \exp \left[ \beta \mu \max_{x\geq0} g(x,t) \right]$$

(3.13)

whence from (2.29), (2.31) and (3.2) we obtain

$$p_G = \min_{t>2/3} h(t) \quad (3.14)$$
where

\[ h(t) \equiv \lim_{\beta \to \infty} \frac{H(\beta \mu^{3/2}t)}{\beta} \]  

(3.15)

\[ = \mu^{3/2}t + m \mu \max_{x \geq 0} g(x, t) \]  

(3.16)

\[ g(x, t) \] is sketched as a function of \( x \) for various values of \( t \) in figure 2. We see that \( \max_{x \geq 0} g(x, t) = g(0, t) = 0 \) for all \( t > 2/3 \). From (3.16) we therefore have

\[ h(t) = \mu^{3/2}t \]  

(3.17)

and so from (3.14) we have

\[ p_G = \frac{2}{3} \mu^{3/2} = \lim_{\beta \to \infty} \frac{\chi_t}{\beta} \equiv p_G^{(f)} \]  

(3.18)

That is, as \( \beta \to \infty \), \( s_0 \sim \chi_t + O(1) \), the large \( \beta \) form of \( H(s) \) being as indicated in Fig. 1.

\( p_G \) therefore equates to \( p_G^{(f)} \)—the ground state pressure for a free system of \( d \) electrons. Using (3.3) we get

\[ \mu = n^2 \]  

(3.19)

and hence the ground state energy is

\[ \varepsilon_G = \varepsilon_G^{(f)} \]  

(3.20)

where \( \varepsilon_G^{(f)} \) denotes the well known free fermion ground state energy

\[ \varepsilon_G^{(f)} = \frac{n^2}{3} \]  

(3.21)

The ground state is therefore a state where all of the \( f \) particles are clustered at the ends and all but one of the wells is unoccupied and of zero width, the \( d \) electrons occupying the large well.

In the following section we interpret this result by considering the analogy between the present model and the Takahashi gas.

4 Physical Interpretation and Inclusion of a Takahashi Interaction Between \( f \) Electrons

In order to physically interpret the above result we recall that, for a Takahashi gas [12], we have a system of \( M \) particles at positions \( 0 < y_1 < \ldots < y_M < V \) with a repulsive interaction

\[ \sum_{0 \leq i < j \leq M+1} \phi(y_j - y_{j-1}) \]  

(4.1)

where

\[ \phi(x) = \begin{cases} 
\infty & 0 \leq x \leq a \\
v(x) & a < x < 2a \\
0 & x \geq 2a 
\end{cases} \]  

(4.2)

and in (4.2) \( a > 0 \) is the hard core exclusion distance and \( v(x) > 0 \).

Because of the hard core exclusion, the interaction only acts between nearest neighbours and the partition function is

\[ Z_M = \int_0^V e^{-\beta \phi(V - y_M)} dy_M \int_0^{y_M} e^{-\beta \phi(y_M - y_{M-1})} dy_{M-1} \]

\[ \cdots \int_0^{y_2} e^{-\beta \phi(y_2 - y_1)} e^{-\beta \phi(y_1)} dy_1 \]  

(4.3)
As mentioned in section 2, Laplace convolution and the method of steepest descents have been employed to solve for the Helmholtz free energy of the Takahashi gas.

Taking (4.3) as a starting point, we could define a model partition function with longer range forces by relaxing the requirement that \( \phi(x) \) vanishes for \( x \geq 2a \). As pointed out however, such a partition function is unphysical in that only nearest neighbours interact and the specific two-body potential form (4.2) is required for (4.3) to be valid.

We note however that the grand canonical partition function from the present model (2.14) is of the form (4.3) if we identify \( \phi(x) \) with \( \log f(x) \). That is, the nearest neighbour potential between \( f \) electrons can be considered an effective interaction induced by the \( d \) electrons. As can be seen from (2.12), this interaction is temperature dependent, long ranged and attractive. This sheds some light on the clustering of the \( f \) particles observed in section (3). A further physical interpretation arising from an approximate evaluation of the thermodynamic potential is given in appendix B.

Intuitively, from the results mentioned in section 1 for the lattice Falicov-Kimball model we might expect that the ground state \( f \) electron configuration would be the analogue of the checkerboard configuration with the \( f \) particles homogeneously spaced along the line. In appendix C we derive the ground state energy from the equally spaced configuration

\[
\varepsilon^{(ES)}_G = \frac{m}{3n} \left( \left\lfloor \frac{n}{m} \right\rfloor + 1 \right) \left[ 3 \left( \left\lfloor \frac{n}{m} \right\rfloor + 1 \right) \left( \frac{n}{m} - \left\lfloor \frac{n}{m} \right\rfloor \right) + \frac{n}{m} \left( \left\lfloor \frac{n}{m} \right\rfloor + \frac{1}{2} \right) \right] \quad (4.4)
\]

We show explicitly that this lies above the exact ground state energy (3.21) which arises from the highly inhomogeneous \( f \) electron configuration mentioned in section 3.

It is natural then to investigate the effect of including a Takahashi term (4.2) (a short range repulsive potential between \( f \) particles) in the model. In this case the barriers cannot cluster together and the resulting model should more closely resemble the lattice model where the \( f \) electrons cannot cluster into a very small region.

With the Takahashi term included, the grand canonical partition function has the form (2.14) but with \( f \) now defined by

\[
f(x) \equiv \prod_{k=1}^{\infty} \left[ 1 + ze^{-\beta k^2/x^2} \right] e^{-\beta \phi(x)} \quad (4.5)
\]

The pole structure of \( F(s) \) does not change and the thermodynamic potential is still obtained from (2.31).

We restrict our attention to the Tonks case where \( v(x) \equiv 0 \) in order to calculate the effect that a repulsive \( f-f \) interaction has on the ground state. As the hard core exclusion distance \( a \) is increased from 0 to the extreme value \( 1/m \), the number of allowed barrier configurations is reduced until the only allowed configuration is the homogeneous configuration. The ground state energy \( \varepsilon_G \) should in turn increase monotonically from the free fermion value (3.21) to the equal spacing value (4.4). Alternatively, the ground state pressure \( p_G \) should decrease monotonically from the free fermion value (3.18) to the equal spacing value

\[
p^{(ES)}_G = m \mu \left( \frac{\sqrt{\mu}}{m} \right) - \frac{m^3}{3} \left( \left\lfloor \frac{\sqrt{\mu}}{m} \right\rfloor + 1/2 \right) \left( \left\lfloor \frac{\sqrt{\mu}}{m} \right\rfloor + 1 \right) \quad (4.6)
\]

which is derived in appendix C.

To derive the ground state pressure we repeat steps (3.7)-(3.10) with the modified form (4.5) viz

\[
F(s) = \int_0^\infty \prod_{k=1}^{\infty} \left\{ 1 + \exp \left[ \beta \mu \left( 1 - k^2/\mu x^2 \right) \right] \right\} \exp \left[ -\beta \mu t \sqrt{\mu} x \right] e^{-\beta \phi(x)} dx \quad (4.7)
\]

\[
= \int_a^\infty \prod_{k=1}^{\infty} \left\{ 1 + \exp \left[ \beta \mu \left( 1 - k^2/\mu x^2 \right) \right] \right\} \exp \left[ -\beta \mu t \sqrt{\mu} x \right] dx \quad (4.8)
\]
In this chapter we have studied the thermodynamics of a one-dimensional continuum analogue of the Falicov-Kimball model in the limit of strong correlation. As mentioned in the introduction, in terms of mathematical and physical complexity, this model is a long way removed from a lattice
model with finite strength interactions in higher dimensions. As shown in section 3, however, the exact solution does afford a neat physical interpretation and the addition of a repulsive $f-f$ interaction enriches the model leading to a ground state analogous to that observed in lattice models if the repulsion is sufficiently strong. Finally, we indicate some directions for further work.

The calculation of the ground state $f$ electron configuration and $d$ electron distribution in the case where the $f-f$ interaction is of the Tonks form could be taken further and made more precise. Also, a study of the ground state when $v(x)$ is non-zero may prove interesting because in this case the Takahashi repulsion will contribute directly to the ground state energy and not simply through the reduction of allowed $f$ configurations. It should be possible to generalise to the present model a method used by Salsburg, Zwanzig and Kirkwood in the calculation of correlation functions for the Takahashi gas [1]. The calculation of the $f-f$ correlation function, especially at zero temperature may be of some interest. It may be of interest to generalise the model to higher dimensions $d$ where the barriers are impenetrable $d-1$ dimensional hyperplanes. Finally, it might be interesting to investigate this model in the case where the $d$ particles have a different energy spectrum, different statistics, or both.

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Appendix

A. A Representation for $f$

In this appendix we derive the representation (2.21) for the function $f$. Now from (2.12) we have

$$\log f(x) = \frac{1}{2} \sum_{k=-\infty}^{\infty} \mathcal{F}(k/x) - \frac{1}{2} \log(1 + z) \quad (A.1)$$

where

$$\mathcal{F}(w) \equiv \log \left(1 + ze^{-\beta w^2} \right) \quad (A.2)$$

$\mathcal{F}(w)$ is absolutely integrable so the Poisson summation formula can be applied to (A.1) viz

$$\log f(x) = \frac{x}{2} \sum_{k=-\infty}^{\infty} \tilde{\mathcal{F}}(2\pi kx) - \frac{1}{2} \log(1 + z) \quad (A.3)$$

$$= x\chi_f + x \sum_{k=1}^{\infty} \tilde{\mathcal{F}}(2\pi kx) - \frac{1}{2} \log(1 + z) \quad (A.4)$$

where

$$\tilde{\mathcal{F}}(y) \equiv \int_{-\infty}^{\infty} \mathcal{F}(w) e^{iwy} dw \quad (A.5)$$

denotes the Fourier transform of $\mathcal{F}$ and we have noted using (2.22) that $\tilde{\mathcal{F}}(0) = 2\chi_f$.

On integrating by parts we find that

$$\tilde{\mathcal{F}}(y) = -\frac{1}{iy} \int_{-\infty}^{\infty} \mathcal{F}'(w) e^{iwy} dw \quad (A.6)$$

Now

$$-\mathcal{F}'(w) = \frac{2\beta wze^{-\beta w^2}}{1 + ze^{-\beta w^2}} \quad (A.7)$$
so, above the real axis \(-F'(w)\) has simple poles at \(w = w_l^{\pm} = \pm u_l + iv_l\) \(l = 1, 2, 3, \ldots\) where \(u_l\) and \(v_l\) are the positive, real solutions of

\[
\beta \left( u_l^{\pm} \right)^2 = \beta \mu \pm (2l - 1)\pi i \quad (A.8)
\]

That is, the intersection of the two hyperboli

\[
u_l^2 - v_l^2 = \mu \quad (A.9)
\]

The explicit values of \(u_l\) and \(v_l\) are given by (2.23) and (2.24). The residue of \(-F'(w)e^{iw}\) at \(w = w_l^{\pm}\) is \(-e^{iw_l^{\pm}}y\). Assuming \(y > 0\), using (A.6) and closing the contour above the real axis we therefore have

\[
\tilde{F}(y) = -\frac{2\pi}{y} \sum_{l=1}^{\infty} \left( e^{iw_l^{+}y} + e^{iw_l^{-}y} \right) \quad (A.11)
\]

Combining (A.4) with (A.11) we arrive at

\[
\log f(x) = x\chi_f - \frac{1}{2} \log(1 + z) - \sum_{k=1}^{\infty} \frac{1}{k} \sum_{l=1}^{\infty} \left( e^{2\pi ikw_l^{+}x} + e^{2\pi ikw_l^{-}x} \right) \quad (A.12)
\]

Using the Taylor expansion

\[
\sum_{k=1}^{\infty} \frac{r^k}{k} = -\log(1 - r) \quad (A.13)
\]

we then have

\[
\log f(x) = x\chi_f - \frac{1}{2} \log(1 + z) + \sum_{k=1}^{\infty} \log \left( 1 - e^{2\pi ikw_l^{+}x} \right) \left( 1 - e^{2\pi ikw_l^{-}x} \right) \quad (A.14)
\]

from which the required representation (2.21) follows.

**B Approximate Low Temperature Calculation of the Thermodynamic Potential and Further Physical Interpretation**

In this appendix we give an approximate direct evaluation of the thermodynamic potential which should be reasonable at very low temperatures and which admits a neat physical interpretation.

Now using (2.21) and (2.19) we can write

\[
F(s) = \frac{1}{\sqrt{1 + z}} \left[ \frac{1}{s - \chi_f} + G(s) \right] \quad (B.1)
\]

where

\[
G(s) \equiv \int_{s-\chi_f}^{\infty} e^{-(s-\chi_f)x} \left[ \prod_{k=1}^{\infty} \left| 1 - e^{2\pi i(-v_k + iu_k)x} \right|^2 - 1 \right] dx \quad (B.2)
\]

is analytic for \(\Re s > 2\pi v_1\).

The right hand side of (2.20) is dominated by the pole at \(s = \chi_f\) for large \(M\). The terms arising from the other singularities of \(F\) are exponentially small. Using (B.1) we write

\[
(F(s))^{M+1}e^{\chi V} = \frac{e^{\chi V}}{(1 + z)^{M+1}} \sum_{j=0}^{M+1} \left( M + 1 \right) \left[ G(s) \right]^{M+1-j} \sum_{l=0}^{\infty} \frac{(s - \chi_f)^l V^l}{l!} \quad (B.3)
\]

\(^2\)It is easily seen that the integral on the closing contour approaches zero as long as the closing contour is chosen to bisect the poles so that the denominator of \(-F'(w)\) is bounded away from 0.
From (2.24) and (2.25) we see that the poles of $F(s)$ accumulate on the line $\Re s = \chi f$ as $\beta \to \infty$. We therefore make the approximation $G(s) \approx G(\chi f)$ and so from (B.3) we approximate the residue of $(F(s))^{M+1}e^{sV}$ at $s = \chi f$ by

$$
\frac{e^{\chi f V}}{(1 + z)^{M+1}} \sum_{j=1}^{M+1} \binom{M+1}{j} \frac{[G(\chi f)]^{M+1-j} V^{j-1}}{(j-1)!}
$$

(B.4)

In this approximation then the dominant contribution to the partition function is

$$
Q(V) \approx \frac{e^{\chi f V}}{V(1 + z)^{M+1}} \sum_{j=1}^{M+1} \binom{M+1}{j} \frac{[G(\chi f)]^{M+1-j} V^{j}}{(j-1)!}
$$

(B.5)

Making use of the identity

$$
\frac{1}{(j-1)!} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^s}{s^j} ds \quad c > 0
$$

(B.6)

we have

$$
\sum_{j=1}^{M+1} \binom{M+1}{j} \frac{[G(\chi f)]^{M+1-j} V^{j}}{(j-1)!}
$$

(B.7)

$$
= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds e^s \sum_{j=1}^{M+1} \binom{M+1}{j} [G(\chi f)]^{M+1-j} \left( \frac{V}{s} \right)^j
$$

(B.8)

$$
= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^s \left\{ \left[ \frac{V}{s} + G(\chi f) \right]^{M+1} - [G(\chi f)]^{M+1} \right\} ds
$$

$$
= \frac{V^{M+1}}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^s \left\{ \left[ 1 + \frac{G(\chi f) s}{V} \right]^{mV} - \left[ G(\chi f) s \right]^{mV} \right\} ds
$$

$$
\approx \frac{V^{M+1}}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \exp \left[ s (1 + mG(\chi f)) \right]
$$

$$
= \frac{V^{M+1}}{M!} \left[ 1 + mG(\chi f) \right]^M
$$

(B.9)

where we have used the standard limit

$$
\lim_{V \to \infty} \left[ 1 + \frac{a}{V} \right]^V = e^a
$$

(B.11)

Combining (B.5) and (B.10) we then have

$$
Q(V) \approx \frac{V^{M+1}}{M!} \frac{e^{\chi f V}}{(1 + z)^{M+1}} \left[ 1 + mG(\chi f) \right]^M
$$

(B.12)

Taking the thermodynamic limit ($V \to \infty$ with $m = (M+1)/V$ fixed) we obtain the approximate thermodynamic potential

$$
\chi \approx m - m \log m + \chi f + m \log \left[ \frac{1 + mG(\chi f)}{\sqrt{1 + z}} \right]
$$

(B.13)

The above expression has a simple interpretation. The first term is an entropy term arising from the barrier configurations. The second term is the free fermion term arising from states where all wells have zero width except one with width $V$. The last term arises from states where a macroscopic number of wells have non-zero width.
Finally, from (B.2) and (2.21) we have

$$G(\chi f) = \int_0^\infty \left[ \prod_{k=1}^\infty \left| 1 - e^{2\pi (-v_k + i\omega_k)x} \right|^2 - 1 \right] dx$$  \hspace{1cm} (B.14)$$

Using methods from section 3 it can be shown that the last term in (B.13) does not contribute to the ground state pressure and so we recover the result (3.20) within this approximation.

C  Ground State Energy and Pressure for the Homogeneous \(f\) Electron Configuration

In this appendix we calculate some ground state quantities for the homogeneous or equal spaced \(f\) configuration. That is, the position of the \(j\)th barrier is

$$y_j = j \frac{V}{M+1} = \frac{j}{m} \quad j = 1, \ldots, M$$  \hspace{1cm} (C.1)$$

In this case the \(M+1\) wells all have width 1/\(m\) and so the energies (2.8) reduce to

$$E_{jk} = m^2 k^2$$  \hspace{1cm} (C.2)$$

For \(N d\) electrons, the lowest energy is achieved by filling the lowest energy states of the wells with as close to equal filling as possible. We write

$$N = (q + r)(M + 1)$$  \hspace{1cm} (C.3)$$

where

$$q \equiv \left\lfloor \frac{N}{M + 1} \right\rfloor = \left\lfloor \frac{n}{m} \right\rfloor$$  \hspace{1cm} (C.4)$$

is the integral part of \(n/m\) and

$$r \equiv \frac{N}{M + 1} - \left\lfloor \frac{N}{M + 1} \right\rfloor = \frac{n}{m} - \left\lfloor \frac{n}{m} \right\rfloor \in [0, 1)$$  \hspace{1cm} (C.5)$$

The first \(q\) levels are filled in each well and the \((q+1)\)th level is filled in \((M+1)r\) of the wells. Using (C.2) then, the ground state energy per \(d\) particle is

$$\varepsilon_{G}^{(ES)} = \frac{1}{N} \left[ (M + 1) \sum_{k=1}^{q} m^2 k^2 + (M + 1)rm^2(q + 1)^2 \right]$$  \hspace{1cm} (C.6)$$

$$= \frac{m^3}{n} \left[ \frac{q(q + 1/2)(q + 1)}{3} + r(q + 1)^2 \right]$$  \hspace{1cm} (C.7)$$

where we have made use of (3.12). Using (C.4), (C.3) and a little manipulation, we then arrive at (4.4).

We next show explicitly that the exact ground state energy (3.20) (from the highly inhomogeneous configuration) lies below the ground state energy from the homogeneous configuration. Using (3.20), (B.21), (4.4), (C.4) and (C.5) we have

$$\varepsilon_{G}^{(ES)} = \frac{m^3}{3n}(q + 1) \left\{ 3(q + 1)r + q(q + 1/2) \right\}$$  \hspace{1cm} (C.8)$$

$$= \frac{m^3}{3n}(q + 1) \left\{ q^2 + (3r + 1/2)q + 3r \right\}$$  \hspace{1cm} (C.9)$$

$$= \frac{m^3}{3n}(q + 1) \left\{ \left( q + \frac{3r + 1/2}{2} \right)^2 + 3r - \frac{(3r + 1/2)^2}{4} \right\}$$  \hspace{1cm} (C.10)$$
\[ m^3 = 3n \left( q + 1 \right) \left\{ \left( q + r + \frac{r + 1}{2} \right)^2 + 3r - \frac{9r^2}{4} - \frac{3r}{4} - \frac{1}{16} \right\} \] (C.11)

\[ = m^3 \left( q + 1 \right) \left\{ (q + r)^2 + (r + 1)(q + r) + \left( \frac{r + 1}{2} \right)^2 + 3r \right. \\
\left. \quad - \frac{r(9r + 3)}{4} - \frac{1}{16} \right\} \] (C.12)

\[ \geq m^3 \left( q + 1 \right) \left\{ (q + r)^2 + \frac{1}{4} + 3r - \frac{12r}{4} - \frac{1}{16} \right\} \] (C.13)

\[ \geq \frac{m^3}{3n} (q + r)^3 \] (C.14)

\[ = \frac{n^2}{3} \] (C.15)

\[ = \varepsilon_G \] (C.16)

Thus, as required.

Finally, we calculate the ground state pressure from the homogeneous configuration in terms of \( m \) and \( \mu \). To do so we find the grand canonical partition function for the specific barrier configuration (C.1). The canonical partition function is

\[ Z_{MN}^{(ES)} = \sum_{j=1}^{M+1} \sum_{k=1}^{\infty} \sum_{n_{jk}} e^{-\beta E_{jk} n_{jk}} \] (C.18)

and, using (C.2), the associated grand canonical partition function is

\[ Q^{(ES)}(V) = \sum_{N=0}^{\infty} \sum_{M+1}^{\infty} \prod_{j=1}^{M+1} \prod_{k=1}^{\infty} \left( 1 + z e^{-\beta m^2 k^2} \right) \] (C.19)

\[ = \prod_{k=1}^{\infty} \left( 1 + z e^{-\beta m^2 k^2} \right)^{M+1} \] (C.20)

The thermodynamic potential is

\[ \chi^{(ES)}(V) = \lim_{V \to \infty} \frac{\log Q^{(ES)}}{V} \] (C.22)

\[ = m \sum_{k=1}^{\infty} \log \left( 1 + \exp \left[ \beta \mu \left( 1 - m^2 k^2 / \mu \right) \right] \right) \] (C.23)

\[ \sim m \beta \mu \sum_{k=1}^{\lfloor \sqrt{\mu}/m \rfloor} \left[ 1 - \frac{m^2 k^2}{\mu} \right] \] (C.24)

\[ \approx m \beta \mu \left\lfloor \sqrt{\mu}/m \right\rfloor \left( \frac{\sqrt{\mu}}{m} \right)^{1/2} \left( \left\lfloor \sqrt{\mu}/m \right\rfloor + 1 \right)^{1/2} \] (C.25)

so the ground state pressure \( p_G^{(ES)} \equiv \lim_{\beta \to \infty} \frac{\chi^{(ES)}}{\beta} \) is given by (4.6).
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List of Figures

1. The schematic form of $H(s)$ on the real axis (solid line) and the large $\beta$ form (dot-dashed line).
2. $g(x,t)$ as a function of $x$ for various values of $t$.
3. $h(t)$ as a function of $t$ for various values of the exclusion distance $a$ in the case where $\mu = 5$ and $m = 2$.
4. Ground state pressure $p_G$ (solid line) as a function of the exclusion distance $a$ in the case where $\mu = 5$ and $m = 2$. $p_G$ equates to $(1 - ma)p_G^{(f)}$ (dot-dashed line)—the ground state pressure from a free fermion system with restricted volume $V - Ma$—in the region $0 < a < \tilde{a}_c$. 
Figure 1: The schematic form of $H(s)$ on the real axis (solid line) and the large $\beta$ form (dot-dashed line).

Figure 2: $g(x, t)$ as a function of $x$ for various values of $t$.

Figure 3: $h(t)$ as a function of $t$ for various values of the exclusion distance $a$ in the case where $\mu = 5$ and $m = 2$.

Figure 4: Ground state pressure $p_G$ (solid line) as a function of the exclusion distance $a$ in the case where $\mu = 5$ and $m = 2$. $p_G$ equates to $(1 - ma)p_G^{(t)}$ (dot-dashed line)—the ground state pressure from a free fermion system with restricted volume $V - Ma$—in the region $0 < a < a_c$. 

16