Strongly Interacting Spinless Fermions in D=1 and 2 Dimensions: A Perturbative-Variational Approach

Miguel A. Martín-Delgado† and Germán Sierra‡

†Departamento de Física Teórica I
Universidad Complutense 28040-Madrid, Spain
‡Instituto de Matemáticas y Física Fundamental
CSIC, 28006-Madrid, Spain

Abstract

We propose a perturbative-variational approach to interacting fermion systems on 1D and 2D lattices at half-filling. We address relevant issues such as the existence of Long Range Order, quantum phase transitions and the evaluation of ground state energy. In 1D our method is capable of unveiling the existence of a critical point in the coupling constant at $(t/U)_c = 0.7483$ as in fact occurs in the exact solution at a value of 0.5. In our approach this phase transition is described as an example of Bifurcation Phenomena in the variational computation of the ground state energy. In 2D the van Hove singularity plays an essential role in changing the asymptotic behaviour of the system for large values of $t/U$. In particular, the staggered magnetization for large $t/U$ does not display the Hartree-Fock law $(t/U)e^{-2\sqrt{t/U}}$ but instead we find the law $(t/U)e^{-\frac{2}{3}t/U}$. Moreover, the system does not exhibit bifurcation phenomena and thus we do not find a critical point separating a CDW state from a fermion “liquid" state.

PACS numbers: 05.20.-y, 02.90.+p, 75.10.-6

*e-mail: mardel@fis.ucm.es (m.a.m-d), sierra@cc.csic.es (g.s.)
1 Introduction

The study of strongly correlated fermion systems apart from its theoretical interest has important practical applications ranging from high-$T_c$ superconductivity to quasi-one dimensional systems. It is usually emphasized the difficulties in handling models describing correlated electrons, such as the Hubbard model. This fact has led to various types of approximations schemes, which can be roughly classified as perturbative, variational, renormalization group techniques and numerical. The difficulty of the task suggests perhaps that one should combine various techniques in order to come as close as possible to the exact solution, which is probably impossible to unveil except in one dimension where there are models which happen to be integrable.

The aim of this paper is to combine perturbative and variational techniques in the study of strongly correlated fermions. We want to apply to these systems the ideas developed in reference [1] which were applied to the problem of the Ising model in a transverse field.

Let us suppose that we are given a hamiltonian of the form $H(\lambda) = H_0 + \lambda H_1$, where $H_0$ has a nondegenerate ground state $\psi_0$ and $\lambda$ is a coupling constant. In reference [1] it was proposed to construct the ground state $\psi(\lambda)$ of $H(\lambda)$ as

$$\psi(\lambda) = \exp(\sum_{n=1}^{\infty} \lambda^n U_n) \psi_0$$

Solving perturbation theory in $\lambda$ to order $\nu$ implies the knowledge of the collection of operators $\{U_n\}_{n=1,\ldots,\nu}$. Each operator $U_n$ consist in fact of a sum of "irreducible" operators $V_I$,

$$U_n = \sum_I p_{n,I} V_I$$

Hence inserting (1.2) into (1.1) and interchanging the order of the sums one arrives to a "dual" description of the ground state

$$\psi(\lambda) = \exp(\sum_I \alpha_I(\lambda) V_I) \psi_0$$

where $\alpha_I(\lambda) = \sum_n \lambda^n p_{n,I}$.

This expression suggests an alternative approximation to the ground state $\psi(\lambda)$ which consists in choosing only a class of irreducible operators $V_I$ whose weights $\alpha_I$ are determined variationally. This was precisely the approach applied in [1] to the Ising model in a transverse field, and it is our purpose to apply it in this paper to a system of spinless fermions defined on a hypercubic lattice in $D$ dimensions. The hamiltonian for this system is given by:

$$H = -t \sum_{<i,j>} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_{<i,j>} U(n_i - \frac{1}{2})(n_j - \frac{1}{2})$$

where $c_i (c_i^\dagger)$ are fermion annihilation (creation) operators satisfying standard canonical anticommutation relations (CAR algebra), $n_i = c_i^\dagger c_i$ is the number operator, $t$ is the hopping parameter and $U > 0$ is a repulsive coupling constant mimicking the residual Coulomb interaction. The sum in (1.4) is extended over all the links of the lattice. The lattice we shall be dealing with is made up of $L$ sites in each spatial direction. This amounts to a total number of sites $N = L^D$ and it is taken to be even for simplicity. The hopping parameter is defined positive $t > 0$ and Periodic Boundary Conditions are assumed in each direction.

We shall be concerned with the study of the ground state of $H$ when the system is at half-filling, i.e., when the number of electrons $N_e$ is half the number $N$ of lattice sites $N_e = \langle \sum_i n_i \rangle = N/2$ (so that by expanding (1.4) it means that the chemical potential is fixed by $\mu = DU$), and secondly when
the system is in the strong coupling regime, i.e., $U > t$. This means in particular that our unperturbed Hamiltonian is

$$H_0 = \sum_{<i,j>} U(n_i - \frac{1}{2})(n_j - \frac{1}{2}) \tag{1.5}$$

For $U > 0$ and at half-filling there are two ground states of $H_0$ corresponding to the unperturbed charge density states $|CDW(e/o)\rangle$,

$$|CDW(e/o)\rangle = \prod_{i \in \Lambda_{e/o}} c_i^\dagger |0\rangle \tag{1.6}$$

where we have taken into account that the hypercubic lattice with $N$ even can be divided into two interpenetrating sublattices $\Lambda_e$ “even” and $\Lambda_o$ “odd” (or black and blank sites).

Even though $H_0$ has two different ground states we shall apply our technique to each of the CDW states (1.6). This eventually means that after switching on the hopping term in (1.4) each initial CDW evolve into different CDW-states $\psi_{e/o}$, characterized by different values of the staggered magnetization $m_{st}$,

$$m_{st} = \frac{2}{N} < \sum_i (-1)^i n_i > \tag{1.7}$$

where $(-1)^i = 1(-1)$ for $i \in \Lambda_e(\Lambda_o)$. For the initial CDW states take on the values $m_{st}(even/odd) = (+1/ -1)$.

An interesting question arises as to whether $m_{st}$ vanishes for a critical value of $(t/U)_c$ different from infinity. Equivalently this amounts to the existence or not of Long Range Order (LRO) in the fermion system at zero temperature. It is clear that if $t/U = \infty$ the ground state of (1.4) is a Fermi-sea of free particles which has no preferred distribution in the space which in turn implies vanishing staggered magnetization $m_{st} = 0$. In 1-dimension the model (1.4) can be solved exactly \cite{3} and one obtains as the critical point the value $(t/U)_c = 1/2$. As a matter of fact, the Hamiltonian (1.4) is equivalent to the anisotropic $XXZ$-Heisenberg Hamiltonian, namely,

$$H_{XXZ} = -\frac{1}{2} \sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z) \tag{1.8}$$

This mapping is carried out by the standard Wigner-Jordan transformation and thus the relation between the anisotropy parameter $\Delta$ and those appearing in (1.4) is given by,

$$\Delta = -\frac{1}{2(t/U)} \tag{1.9}$$

The value $\Delta = -1$ (i.e. $(t/U)_c = 1/2$) corresponds precisely to the Isotropic Antiferromagnetic Heisenberg model in (1.8). The unperturbed $|CDW(e/o)\rangle$ states of the fermion model are mapped onto Néel states in the Heisenberg model. We must recall here that mean field theories or Hartree-Fock approximations to (1.4) always yield a non-vanishing staggered magnetization $m_{st}$ no matter how small is the coupling constant $U$ or the dimension of the lattice. This result is clearly wrong as we have already pointed out above for $D = 1$ and is explained on the basis that the HF method does not take properly into account the quantum fluctuations which are very strong in 1D. In reference \cite{2} this issue has been analyzed using RG-techniques showing that the existence of a solution of the gap equation for the CDW order parameter can be traced back to the fact that in perturbation theory one is disregarding some diagrams (those of BCS-type according to the terminology of reference \cite{3}), and when they are properly taken into account they balance the contributions from the diagrams which favor the CDW-instabilities. The outcome of this one-loop RG-calculation in $D = 1$ is a zero beta function $\beta(U) = 0$.
for the coupling constant $U$. This result is by all means only valid in the perturbative regime (i.e. $U/t$ small) and implies the existence of a non-trivial fixed point of the Renormalization Group which correspond to a Luttinger liquid. Application of the same technique to the case of higher dimensions $D > 1$ always encounters a CDW-instability.

In summary we have the following situations,

- $(t/U)_c = 1/2$ in $D = 1$. Exact.
- $(t/U)_c = \infty$ in Mean Field Theory, $\forall D$.
- $\beta(U) = 0$ in Renormalization Group Approach, $D = 1$.

We shall address in detail the issue of the critical value $(t/U)_c$ in the system of interacting fermions as well as other problems that emerge in connection to this one.

## 2 The Perturbative-Variational Ansatz for Interacting Fermions

According to the perturbative-variational (PV) method developed in reference [1] we must first determine the form of the set operators $\{U_n\}$ by inserting the exponential ansatz (1.1) in the Schrödinger equation for $H$. Then these operators serve us to construct variational wave functions by inserting them back in the exponential ansatz. The perturbative equations that determine the $U_n$ for the lowest order in perturbation theory obey the equations,

order $\lambda$: $([H_0, U_1] + H_1) \psi_0 = E^{(1)} \psi_0$ (2.10)

order $\lambda^2$: $([H_0, U_2] + [H_1, U_1] + 1/2([H_0, U_1], U_1)) \psi_0 = E^{(2)} \psi_0$ (2.11)

where $E^{(1)}$ and $E^{(2)}$ are the perturbative energies to first and second order.

A solution of equations (2.10) and (2.11) in the case where $H_0$ is given by equation (1.3) and $H_1$ is the hopping term of (1.4) is the following,

\[
U_1 = \frac{1}{2D-1} \sum_{<i,j>} T_{ij}
\]

\[
U_2 = \sum_{<i,j;k,l>} C_{ijkl} T_{ij} T_{kl}
\]

where $T_{ij} = c^\dagger_i c_j + c^\dagger_j c_i$ and $<i,j;k,l>$ is a path on the lattice from the point $i$ to the point $l$ without $i \neq j \neq k \neq l$ and $C_{ijkl}$ some constants which may depend on the shape of the path and on the dimension $D$, whose precise value is not important for our discussion. The perturbative energy up to second order is

\[
E = -\frac{NUD}{4} \left(1 + \frac{4}{2D-1}\left(\frac{t}{U}\right)^2\right)
\] (2.14)

Observe that $U_1$ is proportional to the kinetic term in the original hamiltonian $H$. The solution of these equations is by no means unique. We can add to $U_2$ an operator of the form $T_{il}$ with $i,l$ on the same sublattice. The action of such an operator on the state $|CDW\rangle$ is zero.

Now the second stage of the method, according to eqs. (1.1)-(1.3), consists in exponentiating the $U_n$ operators (2.12) and (2.13). The simplest ansatz takes into account only the $U_1$ operator yielding

\[
\psi_{e/o}^{(1)}(\alpha) = \exp\left(\frac{\alpha}{2} \sum_{<i,j>} (c^\dagger_i c_j + c^\dagger_j c_i)\right) |CDW\ (e/o)\rangle
\] (2.15)
whereas if we take into account the second order operator $U_2$ the ansatz will become

$$
\psi^{(2)}_{e/o}(\alpha) = \exp(\frac{\alpha}{2} \sum_{<ij>} T_{ij} + \frac{1}{2} \sum_{<ijkl>} \alpha_{ijkl}T_{ij}T_{kl})|CDW\ (e/o)>
$$

(2.16)

where $\alpha_{ijkl}$ will only depend on the shape of a 4-step non-backtracking path. In both cases the parameters $\alpha$'s are used to minimize the energy of the trial states, which fixes their dependence on the ratio $t/U$. For $t/U$ small we must have $\alpha \sim (t/U)^2$ and such that $\psi^{(1)}(\psi^{(2)})$ agrees to first (second) order with the exact ground state of $H$.

We notice that this is the essence of the PV method proposed in [1], namely, to use the results obtained to a given order in perturbation theory in order to establish a variational calculation which extends the validity of the perturbative results beyond perturbation theory.

In what follows we shall restrict ourselves to the analysis of the first order ansatz $\psi^{(1)}(\alpha)$ (hereafter called $\psi(\alpha)$).

As $t/U$ increases we expect also $\alpha$ to increase, after all the role of this hopping term in (1.4) is to disorder the CDW state, but that is precisely what the exponential operator in the ansatz (2.15) is doing on the CDW-states.

Eventually, as $t/U$ increases we may get $\alpha = \infty$ in which case, as is shown below, the state (2.15) becomes the Fermi-sea or ground state of $H_1$,

$$
\lim_{\alpha \to \pm \infty} \psi_{e/o}(\alpha) \sim |Fermi\ Sea> = \prod_{k \in Fermi\ Sea} c_k^\dagger |0>
$$

(2.17)

All the states $\psi(\alpha)$ with $\alpha$ finite have non-vanishing staggered magnetization and hence only for $\alpha = \infty$ we get a state with $m_{st} = 0$. This in turn implies that the value of $t/U$ at which $\alpha = \infty$ is nothing else but the critical value $(t/U)_c$. Therefore the rule to find in our approach the critical value $(t/U)_c$ is given by finding the minimum of the variational energy $E(\alpha; t/U)$ of the state $\psi(\alpha)$ for $t/U = const..$ This fixes $t/U$ as a function of $\alpha$, i.e., $t/U = F(\alpha)$. Then the critical value $(t/U)_c$ at which the staggered magnetization vanish is given by

$$(t/U)_c = \lim_{\alpha \to \infty} F(\alpha)
$$

(2.18)

If $(t/U)_c$ turns out to be non-zero then the ansatz (2.15) would be valid in the whole range $0 \leq t/U \leq (t/U)_c$ and beyond this the variational state remains the free Fermi sea (2.17). Hence to get more information we should study the model from the “other” side of coupling constant, as for example perturbation theory in $U$ or some other method.

To prove (2.17) notice that the ground state of the operator appearing in the exponential of (2.15) is, for either sign of $\alpha$, given by the Fermi sea at half-filling. Now if we let $\alpha$ go to $\infty$, and we introduce the resolution of the identity we project the state $\psi(\alpha)$ onto $|Fermi\ Sea>$. We note that a similar technique is used in the so called projected Monte Carlo method in order to filter out the ground state,

$$
\lim_{t \to \infty} e^{-tH}|\phi> \sim |G.S.\ of\ H> \sim |G.S.\ of\ H> |\phi>
$$

(2.19)

It is assumed that the trial state $|\phi>$ is not orthogonal to the true ground state of $H$.

For the ansatz (2.15) we do not have to resort to numerical computations to obtain the mean value of $H$ since this state is in fact a Hartree-Fock state of a restricted type.

To prove this we shall express the state (2.15) in momentum space. For that purpose we introduce the creation operator $c_{k}^\dagger$ and annihilation operator $c_{k}$ which are the Fourier transformed of $c_{i}$,

$$
c_{k}^\dagger = \frac{1}{\sqrt{N}} \sum_{i} e^{ik \cdot R_{i}} c_{i}^\dagger
$$

(2.20)
where \( k = \frac{2\pi}{L}(n_1, \ldots, n_D) \), with \( n_i = 0, 1, \ldots, L - 1 \) mod(\( L \)).

The CDW states (1.4) can then be expressed using (2.20) as,

\[
|\text{CDW}(e/o)\rangle = \frac{1}{\sqrt{2}} \prod_k (c^\dagger_{k} \pm c^\dagger_{k+Q})|0\rangle
\]

(2.21)

where \( Q = (\pi, \ldots, \pi) \) is the AF vector and \( \prod_k \) stands for the product over the reduced Brillouin zone, also called magnetic zone.

Taking into account that:

\[
- \sum_{<i,j>} \langle c^\dagger_i c_j + c^\dagger_j c_i \rangle = \sum_k \epsilon_k n_k
\]

(2.22)

\[
\epsilon_k = -2 \sum_a \cos(k_a)
\]

(2.23)

and \( n_k = c^\dagger_k c_k \), we can write the states (2.15) as

\[
\psi_{e/o}(\alpha) = \frac{1}{\sqrt{2}} \prod_k e^{-\frac{\alpha}{2}\epsilon_k} c^\dagger_k \left( c^\dagger_{k} \pm e^{-\frac{\alpha}{2}\epsilon_k+Q}c^\dagger_{k+Q} \right)|0\rangle
\]

(2.24)

From this expression we can immediately derive equation (2.17).

Concerning this result we would like to make some comments:

i) Equation (2.24) shows that the PV ansatz (2.15) is a Hartree-Fock state, i.e., it is a state of the form

\[
\psi_{HF} = \prod_k (u_k c^\dagger_k + v_k c^\dagger_{k+Q})|0\rangle
\]

(2.25)

with

\[
\begin{align*}
u_k &= \frac{1}{\sqrt{2}} e^{-\frac{\alpha}{2}\epsilon_k} \\
v_k &= \frac{1}{\sqrt{2}} e^{-\frac{\alpha}{2}\epsilon_k+Q}
\end{align*}
\]

(2.26)

ii) Since the functional dependence of \( u_k \) and \( v_k \) is fixed by equation (2.26), the PV state is a restricted Hartree-Fock state. This implies that the variational method applied to the PV state using \( \alpha \) as the unique variational parameter, needs not coincide with the variational method applied to an unrestricted HF state where all the parameters \( u_k, v_k \) are variational [6], [7].

The computation of the mean value of the hamiltonian \( H \) (1.4) on the state (2.24) is standard, we quote here the result and leave the details of the proof for the appendix A,

\[
E \equiv -\frac{1}{4} NDU e(t/U, \alpha)
\]

(2.27)

where \( e(t/U, \alpha) \) is the reduced energy

\[
e(t/U, \alpha) = 4 \frac{t}{U} I_1(\alpha) + I_0^2(\alpha) + I_1^2(\alpha)
\]

(2.28)

and \( I_0(\alpha), I_1(\alpha) \) are the following integrals,
\[ I_0(\alpha) = \int_{\Omega} \frac{d^D k}{(2\pi)^D} \frac{1}{\cosh(\alpha \epsilon_k)} \] (2.29)

\[ I_1(\alpha) = \frac{1}{2D} \int_{\Omega} \frac{d^D k}{(2\pi)^D} \epsilon_k \tanh(\alpha \epsilon_k) \] (2.30)

Here \( \Omega \) denotes the interior of the Brillouin zone \((-\pi \leq k_a \leq \pi)\).

Minimization of \( E \) with respect to \( \alpha \) yields

\[ \frac{t}{U} = -\frac{1}{2} \left( I_1 + \frac{I_0 I_0'}{I_1'} \right) \] (2.31)

where \( I_0' = dI_0/d\alpha \), etc. For a given value of \( t/U \) there may exist several values of \( \alpha \) satisfying (2.31). The desired value is selected by minimizing the energy \( E \). This equation will play the role for us of the standard gap equation of the HF method.

We can perform a consistency check of our formalism which consists in verifying that for small parameter \( \alpha \) it is linearly related to the effective coupling constant \( t/U \). This must be so because it means that we are very close to the ground state of \( H_0 \), the CDW state, and thus we are in the perturbative regime where both quantities are proportional, for that is the origin of the construction of the \( U_1 \) operator (2.12).

To prove this assertion we must evaluate the leading behaviour when \( \alpha \to 0 \) of the basic integrals \( I_0 \), \( I_1 \) in (2.29), (2.30). From these expressions we arrive at,

\[ I_0 \xrightarrow{\alpha \to 0} 1 \quad I_0' \xrightarrow{\alpha \to 0} -2D\alpha \] (2.32)

\[ I_1 \xrightarrow{\alpha \to 0} \alpha \quad I_1' \xrightarrow{\alpha \to 0} 1 \]

Inserting these small-\( \alpha \) behaviours in the defining relation (2.31) of \( t/U \) in terms of \( \alpha \) we find

\[ \frac{t}{U} \simeq \alpha (D - \frac{1}{2}) \] (2.33)

which is indeed the linear relation previously advanced in equation (2.12). This relationship is made explicit in Figure 2 where we have plotted the corresponding equation (2.33) for the cases \( D = 1 \) and 2 dimensions.

Once this check is done the big issue is to see whether we can extract nonperturbative results for the system of interacting fermions by going over large values of \( \alpha \) for which the perturbative relation (2.33) ceases to be true. In the forthcoming sections we investigate this issue in one and two dimensions.

### 3 Strongly Interacting Fermions in \( D = 1 \) and the Heisenberg Model

Let us consider the system of spinless fermions interacting by means of the hamiltonian \( H \) (1.4) in one dimensions. This is a very special case where exact formulas exist for the magnitudes of interest: ground state energy, magnetization or Long Range Order, density correlators, etc .... This allows us to confront our PV methods predictions with the exact test results. Moreover, this is a very demanding test ground for it is well-known that mean field theory treatments are usually doomed to failure because the strong quantum fluctuations occuring in one dimensions are not properly taken into account.

In one dimension the system undergoes a quantum phase transition at the critical value of the coupling constant \((t/U)_c = 1/2\). This is an essential singularity phase transition. For small values of \( t/U \) the system is in an ordered phase in coordinate space corresponding to a perturbation of the CDW
state. In this phase the staggered magnetization calculated by Baxter is non-vanishing. For large values of $t/U$ the system is in a disordered phase similar to a fermion “liquid” of Luttinger type.

Elucidating the existence of a finite critical value $(t/U)_c$ in this case with our method goes over the determination of the asymptotic behavior of integrals $I_0$, $I_1$ and its derivatives for $\alpha \to \infty$.

Let us outline how to compute the leading large-$\alpha$ behaviour of $I_0^{(D=1)}$ for it reveals the role played by the Fermi points in the physics of the system, and it is also useful to generalize the same technique to the more involved case of two dimensions discussed in next section.

For $\alpha \to \infty$ only the regions in the neighborhood of the points satisfying $\cos k = 0$, that is the Fermi points $k = \pi/2$ and $-\pi/2$, contribute significantly to the integral $I_0$ in equation (2.29) for $D = 1$. As matter of fact, both Fermi points contribute the same amount to the integral under consideration. Thus, it is convenient to introduce a cut-off $\Lambda$ to isolate the contribution around the point, say $k = \pi/2$:

$$I_0^{(D=1)} \sim 2 \int_{\pi/2-\Lambda}^{\pi/2+\Lambda} \frac{dk}{2\pi \cosh(2\alpha \cos k)}$$

Shifting variables $k = \pi/2 + \kappa$ with $\kappa$ small and thereby approximating $\cos k \simeq -\kappa$, we may write

$$I_0^{(D=1)} \sim \frac{2}{2\pi} \int_{-\Lambda}^{\Lambda} d\kappa \frac{1}{\cosh(2\alpha \kappa)}$$

Changing variables again $x = 2\alpha \kappa$ we can freely take the limit $\alpha \to \infty$ in the limits of integrations and arrive at

$$I_0^{(D=1)} \sim \frac{1}{2\pi \alpha} \int_{-\infty}^{\infty} \frac{dx}{\cosh x} = \frac{1}{2\alpha}$$

This result establishes that $I_0^{(D=1)}$ vanishes as a power of $\alpha$ with exponent $-1$ in the asymptotic region $\alpha \to \infty$. It is straightforward to extend this analysis to the other integrals $I_0'$, $I_1$ and $I_1'$ so that we summarize the results hereby:

$$I_0^{(D=1)} \sim \frac{1}{2\alpha}, \quad I_0^{(D=1)'} \sim -\frac{1}{2\alpha^2} \quad (3.34)$$

$$I_1^{(D=1)} \sim \frac{2}{\pi}, \quad I_1^{(D=1)'} \sim \frac{\pi}{24\alpha^3}$$

Now, in order to determine the critical value $(t/U)_c$, as prescribed in equation (2.18) we must insert the leading values (3.34) in the defining variational relation of $t/U$ (2.31). This immediately yields the critical value $(t/U)_c = \frac{\pi}{\alpha} \simeq 0.63662$ which is quite close to the exact value $(t/U)_c = 0.5$. However this quick derivation is not correct. The first indication that something peculiar is going on as explained above but it is not a monotonous increasing function. In fact, it exhibits a local maximum at $\alpha = 2.3307$. This in turn means that the relationship (2.31) is not invertible so that we cannot express $\alpha$ as a function of $t/U$ to be inserted in the energy equation and the remaining formulas.

Therefore, to determine the correct critical value $(t/U)_c$ we must proceed more carefully and in doing so we shall unveil the peculiarities of the PV method when applied to the special case of one dimensions. The correct procedure is exemplified in Figure 1 where we plot the reduced energy $e^{(D=1)}(\alpha; t/U)$ as a function of $\alpha$ for varying values of the coupling constant $t/U$ which is considered as a parameter. In this fashion we are correctly implementing the minimization program thereby assuring that we are picking up the absolute maximum of $e^{(D=1)}(\alpha; t/U)$ (recall that a maximum in the reduced energy correspond to a minimum of the ground state energy $E$ (2.27)), not just the local maximum. This local maximum contribution was the one we were only considering previously when the critical value $2/\pi$ was naively obtained.
For small values of $t/U$, say 0.2 (see Figure 1a), the function $e^{(D=1)}(\alpha; t/U)$ exhibits an absolute maximum for a finite value of $\alpha$ and an absolute minimum for $\alpha \to \infty$.

When $t/U$ is increased, say 0.4 (see Figure 1b), the relative height between the maximum and the minimum is reduced.

Eventually, for say $t/U \sim 0.735$ (see Figure 1c), a local minimum shows up nearby the absolute maximum and the minimum at $\alpha \to \infty$ becomes a local maximum. Yet, the first maximum dominates over the new maximum at infinity and it is thereby picked up in our minimization procedure.

We are able to compute the exact value taken by $e^{(D=1)}(\alpha; t/U)$ in the $\infty$, as a function of $t/U$. In fact, substituting the asymptotic behaviours \[8.34\] in $e^{(D=1)}(\alpha; t/U)$ we get,

$$e^{(D=1)}(\infty; t/U) = \frac{8}{\pi} \frac{t}{U} + \left(\frac{2}{\pi}\right)^2$$  

(3.35)

This is an increasing function of $t/U$ and eventually this local maximum will overcome the thus far absolute maximum occurring at a finite $\alpha$. When this fact happens, we are obtaining the true value of the critical point $(t/U)_c$.

As the coupling constant $t/U$ keeps being raised, two things happen: the local minimum moves towards the yet absolute maximum and the relative height of the maximum is reduced. The critical point occurs when the height of the local maximum at $\alpha$ infinity equals that of the maximum occurring at finite $\alpha$. This happens for the following value

$$(t/U)_c = 0.748375 \quad (\alpha_c = 1.80032)$$  

(3.36)

From this value of $t/U$ the maximum at infinity becomes the absolute maximum henceforth.

It is worth pointing out that in our procedure for one dimension explained above we have been implicitly describing an example of what has come to be known Bifurcation Phenomena in several branches of Physics (We shall see in next section that such phenomenon is absent in two dimensions.)

As a matter of fact, this way of thinking is well suited for our problem as well as enlightening. Bifurcation phenomena typically occurs in a system subject to the action of a certain potential say $V(x; p)$ where $x$ can be a generalized coordinate describing the state of the system and $p$ an external parameter which is somehow varied. For a certain initial value of $p$, the potential $V$ exhibits two minima $x_{m1} < x_{m2}$ with $V(x_{m1}) < V(x_{m2})$ and the system locates at $x_{m1}$. As the external parameter $p$ is varied, the two minima start approaching each other till eventually they meet, $V(x_{m1}) = V(x_{m2})$. This in turn defines the critical value $p_c$. As $p$ is yet more increased, the two minima exchange their roles, $V(x_{m1}) > V(x_{m2})$, and the system locates at $x_{m2}$. Altogether, when $p$ is varied at one go over its full range of validity, the system undergoes a “phase transition” from the state at $x_{m1}$ to the state at $x_{m2}$. But this is precisely what we have been describing above in our method where $e^{(D=1)}(\alpha; t/U)$ plays the role of the potential function $V(x; p)$, $\alpha \sim x$ and $t/U \sim p$. Interestingly enough, the phase transition we are describing in this fashion is the quantum phase transition occurring in the spinless interacting fermion system from the CDW state to the Fermi sea state.

This result is quite different from what one obtains using mean field theory, where there is always a solution of the gap equation for $\Delta_{CDW}$ no matter how small is the coupling constant $U$. The physical explanation of this result is that any perturbation having momentum $\pi$ links the ground state, given by the Fermi sea at half-filling, to states of arbitrarily low energy in which a particle just below right (left) Fermi point is pushed above the left (right) Fermi point. In this way the Fermi sea at half-filling becomes unstable under this perturbation turning into a CDW state. Our result above in $D = 1$ is precisely the opposite. It shows that starting from the CDW-ground-state it becomes unstable for $t/U$ bigger than a critical value $(t/U)_c$. 


We can summarize our discussion in the following diagram,

\[
\begin{array}{ccc}
\text{Fermi Sea} & \xrightarrow{\text{Mean Field}} & \forall U, \forall D \\
\text{PV-Method} & D = 1, t/U > (t/U)_c \\
\text{CDW} & \xrightarrow{\text{CDW}} & \text{Fermi Sea}
\end{array}
\]

Of course the correct result is that the CDW state for \( t/U > 1/2 \) should become a Luttinger liquid, but it is clear that in our approach we have not introduced enough parameters to tell the difference between a free Fermi liquid and a Luttinger liquid.

The outcome of the procedure outlined in Figure 1 is to achieve the correct set of values \((t/U, \alpha)\) associated to the PV method. When this collection of values is plotted it looks like in Figure 2. Notice firstly that \( t/U \) as a function of \( \alpha \) is single-valued and secondly, that from a finite initial value \( \alpha_c = 1.80032 \) the critical value \((t/U)_c = 0.748375 \) is reached once and for all.

Let us now turn our attention to physical quantities and consider first the staggered magnetization \( m_{st} \) or equivalently the averaged fermion density depending on whether we choose the anisotropic Heisenberg viewpoint \((1.8)\) or the spinless fermion description \((1.4)\).

First of all, notice that the staggered magnetization \( m_{st} \) precisely coincides in our method with the basic integral \( I_0(\alpha) \) \((2.29)\)

\[ m_{st}(t/U) = I_0(t/U) \]  

(3.37)

In fact, by going to momentum space and using the results of Appendix A we find

\[ m_{st} = \frac{2}{N} \sum_i (-1)^i < n_i > = \frac{2}{N} \sum_k < c_k^\dagger c_{k+Q} > = \sum_k \frac{1}{\cosh(\alpha\epsilon_k)} \]

However, in order to extract the physics underlying this magnitude we must not plot \( I_0 \) as a function of \( \alpha \) but instead as a function of the coupling constant \( t/U \). After all, the parameter \( \alpha \) is somehow an artifact of our method which is related to the physical parameter \( t/U \) by the plot in Figure 2. Expressing \( \alpha \) as a function of \( t/U \) in \( I_0(\alpha) \) we obtain the plot of the magnetization \( m_{st} \) which we show in Figure 3. In this figure we also plot the exact magnetization as given by Baxter \((10)\). Several remarks are in order. Only for small values of \( t/U \) there is a good quantitative agreement between both methods. Beyond these values \( t/U \sim 0.2 \) there is major quantitative disagreement. Yet, our approximate method gives a reasonable qualitative behaviour in the sense that it predicts the existence of a critical value \((t/U)_c\) beyond which the magnetization totally vanishes. However the PV method (to lowest order) predict an otherwise absent finite jump in the magnetization at the critical value.

In all, the physical meaning of the magnetization graphics is that we can predict with our method the absence of LRO for small \( t/U \) at zero temperature for the system of spinless interacting fermions.

Now we move on to consider another relevant physical quantity such as the ground state energy \((2.27)\) as a function of \( t/U \). In Figure 4 we plot the reduced energy \((2.28)\) as obtained by the PV method against the exact result given by several authors \((11), (12)\). The agreement is considerably much better than with the magnetization. In fact there is a very good quantitative agreement not only for small \( t/U \) but for the whole physical range till \( t/U = 0.5 \). The major difference though is the prediction of a bigger \((t/U)_c\) than the exact result.

As a precise quantitative check of our values we have collected our PV result for the reduced energy in the Isotropic Heisenberg Antiferromagnet \((t/U = 1/2)\) in Table 1 along with the exact result \((4)\) and several other methods. The result is a good estimation of the ground state energy.

Furthermore, we are also able to compute exactly within our approximate method any multi-density correlators. For instance, the density-density correlator \(< (n_i - 1/2)(n_{i+1} - 1/2) > \) computed in
Appendix A has the interpretation of the Short Range Order in the Heisenberg model for it is equivalent to the spin-spin correlator $< S_i^z S_{i+1}^z >$. In Appendix A we show how to compute it as a function of $t/U$. We do not show the plot of this quantity against the exact value but only remark that there is a good quantitative and qualitative agreement between them.

Finally, we close the analysis of the $D = 1$ dimension case by pointing out that the reduced energy $e(t/U)$ exhibits a finite jump in its derivative at the critical value $(t/U)_c = 0.748375$. The constant value of the derivative at the right hand side of the critical point comes from the linear contribution in equation (3.35) of the absolute maximum at $\alpha \to \infty$ previously discussed. The meaning of this fact is that our PV method predicts a first order quantum phase transition for the fermion system.
4 Strongly Interacting Fermions in \( D = 2 \) Dimensions

After studying the pros and cons of our PV approach to one-dimensional interacting fermions, we address the much more unknown case of \( D = 2 \) spinless fermions. This case is particularly interesting in physical applications such as high-\( T_c \) superconductivity.

First of all, we should quote a major difference occurring with the \( D = 2 \) fermions: there is no connection with the Heisenberg model in 2 dimensions (as far as the present knowledge is concerned). That is to say, the Wigner-Jordan mapping transforming (1.4) onto (1.8) ceases to work in higher dimensions. Correspondingly, all of our conclusions will be only valid for the fermion system but not for the spin system.

The system of 2D interacting spinless fermions is worse understood in comparison with the 2D Anisotropic Heisenberg model. The issue of LRO has been elucidated for the spin system in references \cite{13}, \cite{14} using the reflection property in connection with the Peierls argument. It turns out that in 2 dimensions there exists LRO for low temperature \( T \) and small enough anisotropic parameter. The main obstacle in extending similar results to spinless fermions relies on the fact that no type of reflection positivity property is known to hold for fermions. Recently, though, what has been possible to prove the most is the existence of LRO for low but finite temperature and small coupling constant \( t/U \) \cite{15}.

There is not exact proof of this statement at zero temperature, although it is believed that LRO persists for \( t/U \ll 1 \). In fact, numerical methods such as Quantum Montecarlo fails to provide a definite answer at zero temperature \cite{16}.

With this considerations in mind the study of exact properties for two-dimensional fermions at \( T = 0 \) remains an open problem and we undertake this study with our PV method developed in previous sections.

We follow a parallel analysis as described in one dimensions. The first key observation is that when plotting the function \( t/U = t/U(\alpha) \) as given in equation (2.31) NO local maximum shows up as is the case in \( D = 1 \). In fact, Figure 2 shows this dependence which turns out to be monotonically increasing. This property guarantees that the function is invertible so that we can trade the \( \alpha \) parameter in our PV results for the more physical parameter \( t/U \).

Moreover, this conclusion is further backed by a similar analysis as in Figure 1 for the reduced energy \( e(\alpha; t/U) \) for increasing values of \( t/U \). We have performed such analysis with the result that there is no Bifurcation Phenomena present in \( D = 2 \) spinless fermions. In other words, the function \( e(\alpha; t/U) \) always (\( \forall (t/U) \)) has a maximum at finite \( \alpha \), which in turn is the absolute maximum for the whole range of \( \alpha \). The value \( e(\infty; t/U) \) at infinity never overcomes that maximum neither a local minimum appears in the vicinity of that maximum.

Thus, the minimization procedure of the PV method is entirely governed by the maximum at finite \( \alpha \) and the analysis is thereby simplified in \( D = 2 \) dimensions.

The second key observation present in Figure 2 is that there is not a finite critical value \( (t/U)_c \) of the coupling constant towards which \( \alpha \) tends asymptotically at infinity. Quite the contrary, \( t/U \) always grows as a function of \( \alpha \). In fact, we can compute the behaviour of \( (t/U)(\alpha) \) in the asymptotic regime \( \alpha \to \infty \) for the \( D = 2 \) case. To this purpose, we need to find that behaviour for the integrals \( I_0(\alpha) \), \( I'_0(\alpha) \), \( I_1(\alpha) \) and \( I'_1(\alpha) \) and then insert them in (2.31).

We have left out the calculation of the leading order behaviour of those basic integrals for the Appendix B. We hereby present the final results,

\[
I_0^{(D=2)}(\alpha) \sim \frac{\ln \alpha}{2\pi \alpha} \quad \frac{dI_0^{(D=2)}}{d\alpha}(\alpha) \sim -\frac{\ln \alpha}{2\pi \alpha^2} \quad (4.38)
\]

In doing this calculation it is essential to deal with the van Hove singularities (saddle point singularities) appearing at the corners \( A(\pi,0) \) and \( B(0,\pi) \) of the Fermi Surface (FS) for two-dimensional fermions.
as in Figure 5. Analogously as in $D = 1$ dimensions, only the region of the Brillouin zone near the FS contribute significantly to the integrals when $\alpha \to \infty$. Much care is needed to isolate this asymptotic behaviour as we have to distinguish the contribution of the van Hove points from the rest of the FS points which we call regular points (see Figure 5). In fact, in the intermediate step, there is a highly non-trivial cancellation of cut-off singularities between van Hove and regular-points contribution. Moreover, we have performed numerical analysis of these integrals in the asymptotic region $t/U \to \infty$ and we find numerical agreement with the results expressed in equation (4.38).

The main feature of equations (4.38) is the presence of the logarithmic terms which were absent in $D = 1$ dimensions (3.34). This is ultimately the signal of the van Hove singularity and the reason why $t/U$ grows indefinitely: substituting equation (4.38) in $t/U$ (2.31) we get

$$t/U \sim -\frac{2}{\pi^2} + \frac{3}{\pi^2} \ln \alpha$$

which explains the logarithmic growth of $t/U$ present in Figure 2.

Therefore, our method applied to $D = 2$ spinless fermions does not predict the existence of a quantum phase transition from the CDW state where we started out to a new phase, say a disordered fermion “liquid” state, as was the case in $D = 1$ dimensions.

The analysis of physical properties such as magnetization and ground state energy goes in parallel to the $D = 1$ case of section 3. We show our results in Figures 3 and 4. The main feature of these plots is the absence of a critical point $(t/U)_c$ which makes the magnetization decrease to zero at infinity and the reduced energy to grow to infinity on the contrary. In fact, from (4.39) the asymptotic relation between $\alpha$ and $t/U$ is

$$\alpha \sim e^{\pi^2 t/U}$$

Upon substitution of (4.40) in the magnetization (3.37) we obtain,

$$m_{st} \sim (t/U)e^{-\frac{2}{\pi^2} t/U}, \quad t/U \to \infty$$

It is interesting to compare the result (4.41) with those predicted by a Hartree-Fock method [17], which in 1,2 and 3 dimensions are given by

$$m_{st} \sim \frac{t}{U} e^{-2\pi t/U} \quad (D = 1, 3)$$

$$m_{st} \sim \frac{t}{U} e^{-2\pi \sqrt{t/U}} \quad (D = 2)$$

The square root behaviour in the exponential is due to a combined effect of the nesting of the $D = 2$ Fermi surface at half-filling and the van Hove singularity of the density of states. Hence, the HF result gives a stronger tendency to a CDW state in $D = 2$ as compared to $D = 1$ or 3. On the contrary, the PV method when extrapolated to the $U$ weak coupling regime, gives a behaviour similar to that of $D = 1, 3$ HF, the only difference being in the factor $\pi^2$ instead of $2\pi$. It is an interesting question to discriminate which of the two behaviours, namely the square root law $\sqrt{t/U}$ or the linear $\frac{t}{U}$ law in the exponent controls the gap in $D = 2$ dimensions at half-filling. We want to stress that formula (4.41) is obtained from an extrapolation of the PV state $\psi(\alpha)$ from the perturbative region of the ansatz ($t/U \ll 1$) to the non-perturbative ($t/U \gg 1$) by means of the variational method. We find indirect support for this method when taking the $t/U \to \infty$ in the PV formulas for we find that the physics of the system is governed by the momenta very close to the Fermi surface, and the Fermi surface is a concept which makes sense for a Fermi sea located at $t/U \to \infty$ in the coupling constant.

In reference [17] a numerical analysis has been done for the 2D Hubbard model showing that the $e^{-2\pi t/U}$ is not inconsistent with the numerical results.
Let us notice that in the above discussion we are comparing asymptotic behaviours concerning the staggered magnetization. Another similar analysis could be done as far as the gap $\Delta_{CDW}$ is concerned. In the HF method both quantities are easily related by $\Delta_{CDW} = U m_{st}$, but in our PV method that relationship is not that easy to obtain for one has to go through the computation of the gap by doing an extension of the PV ansatz to the first excited state of the system. We shall not dwell here upon this and other extensions which will be reported elsewhere.

5 Final Considerations

In section 2 and appendix A we have shown that the trial state $\psi^{(1)}$ based on the lowest order PV method is equivalent to a Hartree-Fock state of a restricted type. An straightforward generalization of the ansatz (2.15) is given by

$$\psi_{UHF} = \exp\left(\frac{1}{2} \sum_{<i,j>} c_i^\dagger A_{ij} c_j\right)|CDW>$$

(5.43)

where $A_{ij}$ is an hermitian matrix (i.e. $A_{ij}^* = A_{ji}$). If the matrix $A_{ij}$ is an hermitian matrix only depending on the difference $\vec{R}_i - \vec{R}_j$, then it can be shown that $\psi_{UHF}$ is an unrestricted HF state of the form (2.23) where the parameters $u_k$ and $v_k$ take generic values depending on the eigenvalues of the matrix $A$.

Carrying out the PV method to highest orders in the coupling constant $t/U$ we find operators as the ones in the exponent of (5.43), along with operators with a more complicated structure. This fact may already be seen from the expression of the operator $U_2$ (2.13). First of all, $U_2$ is a sum of operators involving 4-fermion terms, which implies that the corresponding state $\psi^{(2)}$ (2.16) is not a HF-state. In fact, working with this type of states is not simple at all. The interesting feature of $\psi^{(2)}$ is that it contains correlation effects which are absent in the HF-state $\psi^{(1)}$ (A similar phenomena happens for the Ising model in a transverse field ITF where the analogue of the $\psi^{(1)}$ state is also a mean field state, while the second order ansatz $\psi^{(2)}$ is not mean field and it incorporates correlations).

From a more physical point of view the effects of the operators $U_n$ or $V_I$ is that when they act on the unperturbed ground state, say $|CDW(even)>$, they change locally the even-CDW vacuum into an odd-CDW vacuum. From the form of the $U_2$ operator we see that the irreducible operators $V_I$ can be labelled by clusters of dimers, i.e., products of bilinear operators $T_{ij} = c_i^\dagger c_j + c_j^\dagger c_i$ with the links $<i,j>$ belonging to some cluster. The linear clusters are reminescents of the string operators considered in references [18], [19], but we should in principle consider all possible clusters in order to construct the exact solution via the exponential ansatz. This is probably beyond our present possibilities so that one has to restrict the class of operators to build an amenable ansatz. If these constructions were possible, the parameters $\alpha_I$ would give us information about the size of the CDW-patches in the true ground state. Work in this direction will be reported elsewhere.

In this paper we have chosen a variational technique in order to compute the parameters $\alpha_I$ of the exponential ansatz. There is however an alternative way to compute this parameters which is called the Fokker-Planck method [20]. This method tries to generalize to quantum lattice hamiltonians the well-known fact that in quantum mechanics, given a wave function of exponential form $\psi(x) = e^{-s(x)}$ one can find a hamiltonian $H_{FP}$, called Fokker-Planck hamiltonian, for which $\psi(x)$ is an exact ground state.

In the case of the ITF model, the Potts model and others the FP-method can be easily generalized for states of the form (1.3) due to the fact that the operators $V_I$ commute among themselves (in a sense they play the role of the x-coordinate in the quantum mechanical case.) Then, given the ansatz (1.3) one can find the corresponding FP-hamiltonian and can in turn compare with the original hamiltonian. From this comparison one finds the $\alpha'_I$s in terms of the coupling constants in $H$. 

13
It is an interesting question to see whether the FP-method can be extended to problems with fermions. The first problem that we encounter is that the operators $V_I$ no longer commute among themselves (see Appendix C). The advantage of the FP-approach is that one can introduce and do calculations with a large number of parameters $\alpha_I$ which serve to introduce much of the expected physics in the ansatz.

To summarize, we have employed a Perturbative-Variational (PV) method to study strongly interacting fermions at half-filling and zero temperature. To lowest order in PV we have stressed the similarities and differences with the mean field theory or Hartree-Fock method. To higher order in PV they clearly differ. In 1D our method is capable of unveiling the existence of a critical point in the coupling constant at $(t/U)_c = 0.7483$ as in fact occurs in the exact solution at a value of 0.5. In our approach this phase transition is described as an example of Bifurcation Phenomena in the ground state energy. In 2D the van Hove singularity plays an essential role in changing the asymptotic behaviour of the system for large values of $t/U$. In particular, the staggered magnetization for large $t/U$ does not display the Hartree-Fock law $(t/U)e^{-2\pi\sqrt{t/U}}$ but instead we find the law $(t/U)e^{-\pi^2/3t/U}$. Moreover, the system does not exhibit bifurcation phenomena and thus we do not find a critical point separating a CDW state from a fermion “liquid” state.

Many of the ideas and techniques that we propose in this paper can in principle be applied to the Hubbard model in the strong coupling regime $(U > t)$, which is believed to be one of the most prominent candidates for a microscopic description of the high-$T_c$ superconductors.

Acknowledgements

Work partially supported in part by CICYT under contracts AEN93-0776 (M.A.M.-D.) and PB92-1092 (G.S.).

We want to thank J.G. Esteve, F. Jimenez and M.A. Garcia-Bach for useful discussions.

It is a pleasure to thank A. Gonzalez for sharing with us his access to the Alpha computer Ciruelo to make some of the numerical computations in this work.
A The PV Formulas for Interacting Fermions

In section 2 we have briefly explained the fundamentals of the perturbative-variational method and at the end of it we have set up the basic equations (2.27)-(2.31) which encode the essence of our method as applied to the system of interacting fermions. In this appendix we give the highlights and some details of the computations leading to those equations.

The Hamiltonian (1.4) which is the subject of this study is split into two pieces,

\[ H = H_0 + H_1 \]  

(A.1)

\[ H_0 = U \sum_{\langle i,j \rangle} (n_i - \frac{1}{2})(n_j - \frac{1}{2}) \]  

(A.2)

\[ H_1 = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) = t \sum_k \epsilon_k n_k \]  

(A.3)

The norm of the variational state

\[ \psi(\alpha) = \exp\left(\alpha \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i)\right)|0> \]  

(A.4)

plays a major role in the calculation of all the averaged quantities and correlators of the theory. We shall denote this norm by \( Z \) for it recalls the partition function of an associated statistical model. To see this, let us compute its value.

\[ Z = \langle \psi(\alpha)|\psi(\alpha)\rangle = \langle CDW|\exp(-\alpha \sum_k \epsilon_k n_k)|CDW> \]  

(A.5)

To compute this partition function we note that the variational state (A.4) can be given the following representation in momentum space,

\[ |\psi> = \prod_k (u_k c_k^\dagger + v_k c_{k+Q}^\dagger)|0> \]  

(A.6)

\[ u_k = e^{-\frac{\alpha}{2}\epsilon_k} \]  

\[ v_k = e^{\frac{\alpha}{2}\epsilon_k} = e^{\frac{\alpha Q}{\sqrt{2}}} \]  

(A.7)

This representation allows us a readily derivation of the norm in terms of the functions \( u_k, v_k \) namely, \( Z = \prod_k (u_k^2 + v_k^2) = \prod_k \cosh(\alpha \epsilon_k) \), and we have made extensive use of the identity \( \epsilon_k = -\epsilon_{k+Q} \). In order to perform the continuum limit it is convenient to introduce the free energy \( f_N \) of the associated statistical model by means of the identity

\[ Z = \langle \psi(\alpha)|\psi(\alpha)\rangle \equiv \exp(Nf_N(\alpha)) \]  

(A.8)

Then, from the previous considerations we arrive at the final expression for the free energy.

\[ \exp(Nf_N(\alpha)) = \exp\left(\frac{1}{2} \sum_k \ln(\cosh(\alpha \epsilon_k))\right) \]  

(A.9)

\[ f(\alpha) \equiv \lim_{N \to \infty} f_N(\alpha) = \frac{1}{2} \int_{\Omega} \frac{d^Dk}{(2\pi)^D} \ln \cosh(\alpha \epsilon_k) \]  

(A.10)

Interestingly enough, equation (A.10) represents the free energy of a system of free fermions placed on a \( D \)-dimensional lattice as we already advanced.
The expectation value of the $H_1$ part of the hamiltonian is easy to evaluate in terms of the associated free energy

\[
\frac{\partial Z}{\partial \alpha} = - \langle \psi(\alpha) | \sum_k \epsilon_k n_k | \psi(\alpha) \rangle \quad \text{(A.11)}
\]

\[
\langle H_1 \rangle = - t \frac{\partial}{\partial \alpha} (\ln Z(\alpha)) \quad \text{(A.12)}
\]

with the following result already expressed in the continuum limit,

\[
\langle H_1 \rangle = - t N \frac{1}{2} \int_{\Omega} \frac{d^D k}{(2\pi)^D} \epsilon_k \tanh(\alpha \epsilon_k) \quad \text{(A.13)}
\]

This much for the mean value of $H_1$ in the exponential ansatz. As for the $H_0$ part of the hamiltonian, we need the expectation value $\langle \sum_{\langle i,j \rangle} n_i n_j \rangle$ which represents the correlation function of two density operators. Transforming the density operator to momentum space

\[
n_i = \frac{1}{N} \sum_{k_1, k_2} e^{-i(k_1 - k_2) R_i} c_{k_1}^\dagger c_{k_2} \quad \text{(A.14)}
\]

the afore mentioned density-density operator reads,

\[
\sum_{\langle i,j \rangle} n_i n_j = \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} \delta_{k_1+k_2,k_3+k_4} \sum_{a=1}^{D} e^{ik_a^{13}} c_{k_1}^\dagger c_{k_3} c_{k_2}^\dagger c_{k_4} \quad \text{(A.15)}
\]

where $k_a^{13} \equiv k_{a,1} - k_{a,3}$. At this stage it is apparent that the way to compute this correlator is Wick’s theorem. Thus the fermion correlator in $k$-space is

\[
\langle c_{k_1}^\dagger c_{k_2} \rangle = (\delta_{k_1-k_2,0} + \delta_{k_1-k_2,Q}) \frac{u_{k_1} u_{k_2}}{u_{k_1}^2 + u_{k_2}^2} \quad \text{(A.16)}
\]

where $u_k = v_{k+Q}$. Therefore the basic contractions are the following two,

\[
\langle n_k \rangle = \langle c_k^\dagger c_k \rangle = \frac{e^{-\alpha \epsilon_k}}{e^{\alpha \epsilon_k} + e^{-\alpha \epsilon_k}} \quad \text{(A.17)}
\]

\[
\langle c_k^\dagger c_{k+Q} \rangle = \frac{1}{e^{\alpha \epsilon_k} + e^{-\alpha \epsilon_k}} \quad \text{(A.18)}
\]

The contraction in equation (A.17) represents the average number of particles with momentum $k$ and we notice that it exhibits the standard Fermi-Dirac distribution form with the parameter $\alpha$ playing the role of the inverse temperature but recall that all our formalism is at zero temperature.

A lengthy but straightforward calculation yields

\[
\frac{1}{N} \sum_{\langle i,j \rangle} \langle n_i n_j \rangle = \frac{1}{4} - \frac{D}{4} I_0^2 - \sum_{a=1}^{D} \frac{1}{4} I_a^2 \quad \text{(A.19)}
\]

where

\[
I_0(\alpha) = \frac{1}{N} \sum_k \frac{1}{\cosh(\alpha \epsilon_k)} \int_{\Omega} \frac{d^D k}{(2\pi)^D} \frac{1}{\cosh(\alpha \epsilon_k)} \quad \text{(A.20)}
\]

\[
I_a(\alpha) = \frac{2}{N} \sum_k \frac{\cos(k_a)}{1 + e^{-2\alpha \epsilon_k}} \quad \text{(A.21)}
\]
As a result the density-density correlation function turns out to be
\[
\frac{1}{N} \sum_{\langle i,j \rangle} < (n_i - \frac{1}{2})(n_j - \frac{1}{2}) > = -\frac{D}{4}(I_0^2 + I_1^2) \quad (A.22)
\]

Finally, the expectation value we were searching for is
\[
< H_0 > = U \sum_{\langle i,j \rangle} < (n_i - \frac{1}{2})(n_j - \frac{1}{2}) > = -\frac{UD}{4}(I_0^2 + I_1^2) \quad (A.23)
\]

Recalling that
\[
< H_1 > = -tN \frac{\partial f}{\partial \alpha} \quad (A.24)
\]

altogether the average energy is
\[
< H > = E = -tN \frac{\partial f}{\partial \alpha} - \frac{UDN}{4}(I_0^2 + I_1^2) \quad (A.25)
\]

Using the identity \( \frac{\partial f}{\partial \alpha} = DI_1(\alpha) \) the average energy is
\[
E = -tNDI_1 - \frac{UDN}{4}(I_0^2 + I_1^2) \quad (A.26)
\]

For the sake of simplicity it is convenient to introduce the reduced energy as follows
\[
e \equiv -\frac{4E}{UND} = 4 \frac{t}{U} I_1 + I_0^2 + I_1^2 \quad (A.27)
\]

The minimization condition \( \frac{\partial e}{\partial \alpha} = 0 \) for the reduced energy is equivalent to that of the energy \( E \) except for the fact that a minimum of \( E \) corresponds to a maximum of \( e \). Furthermore, we have
\[
e(t = 0) = 1 \iff E(t = 0) = -\frac{NUD}{4} \quad (A.28)
\]
B  The Asymptotic Formulas for Interacting Fermions in $D = 2$ Dimensions

In section 4 we have addressed the issue on the existence of a critical value $(t/U)_c$ for which a quantum phase transition exists in two spatial dimensions. To achieve this goal in our PV approximation scheme we need to evaluate the $\alpha \to \infty$ asymptotic behaviour of the basic integrals $I_0, I_1$ in (2.29), (2.30). This was easily done in $D = 1$ dimensions in section 3 but it becomes much more cumbersome in $D = 2$ dimensions and we present in this appendix the main details of this calculation.

Let us consider the integral $I_0$ in two dimensions as the paradigm of asymptotic evaluation:

$$I_0(\alpha) = \int_0^{2\pi} \int_0^{2\pi} \frac{1}{(2\pi)^2 \cosh(2\alpha(\cos k_1 + \cos k_2))} dk_1 dk_2$$

In the limit $\alpha \to \infty$ only the points in the neighbourhood of the region

$$\cos k_1 + \cos k_2 \equiv 0$$

contribute by a significant amount to the integral (B.1). But these points (B.1) form precisely the Fermi Surface (F.S.) of the system at half-filling. This surface is drawn in Figure 5. It is a square inscribed in the Brillouin zone with corners at the points $A(\pm \pi, 0), B(0, \pm \pi)$.

In order to isolate this contribution from the Fermi Surface we must distinguish two types of points on that curve.

**B1. Regular Points Contribution to $I_0$**

We call a regular point of the F.S. to any point such as $P_r$ in Figure 5 which is not a corner. Thus we have 4 sides of regular points each of which equally contributes to $I_0$. We restrict our attention to one side of the square, say the up-right one.

The contribution of the regular points come from a rectangle centered at the corresponding F.S. portion of infinitesimal width $2\Lambda$ (see Figure 5). We must also isolate the contribution of the corner points $A$ and $B$ so that we introduce another infinitesimal quantity $\epsilon$ such that the length of the rectangle is $\sqrt{2\pi} - 2\epsilon$.

From Figure 5 it is apparent that both infinitesima are not independent. In fact,

$$\Lambda = \epsilon$$

(B.3)

They are equal but we keep both for the sake of keeping track clearly where everything comes from.

Given a regular point on the F.S., we can parametrize any point in the relevant rectangular region of Figure 5 by two parameters $k_0, \kappa$ as

$$\begin{cases} 
  k_1 = k_0 + \kappa \\
  k_2 = \pi - k_0 + \kappa 
\end{cases}$$

(B.4)

where $k_0$ measures the position on the F.S. and $\kappa$ measures the distance from the F.S., that is ,

$$\begin{cases} 
  k_0 \in (\epsilon, \pi - \epsilon) \\
  \kappa \in (-\Lambda, \Lambda) 
\end{cases}$$

(B.5)
Thus, on each fringe the energy function $\cos k_1 + \cos k_2$ contributes like $-2 \sin k_0 \sin \kappa$. Substituting this into $I_0$ we have,

$$
\frac{2}{(2\pi)^2} \int_{-\epsilon}^{\pi-\epsilon} dk_0 \int_{-\Lambda}^{\Lambda} \frac{1}{\cosh(4\alpha \sin k_0 \sin \kappa)}
$$

As $\Lambda \ll 1$ we can approximate $\sin \kappa \simeq \kappa$. Changing variables to $x = (4\alpha \sin k_0) \kappa$ it is possible to perform the $\alpha \to \infty$ limit on the boundaries of integration in $\kappa$ to obtain

$$
\frac{2}{(2\pi)^2} \int_{-\epsilon}^{\pi-\epsilon} dk_0 \frac{1}{4\alpha \sin k_0} \int_{-\infty}^{\infty} dx \frac{1}{\cosh x}
$$

These integrals are known and collecting the factor 4 from the same number of fringes we arrive at the leading behaviour for $I_0^{(D=2)}$ coming from the regular points (R.P.),

$$
I_0^{(D=2)}_{\text{R.P.}} \sim -\frac{1}{\pi \alpha} \ln \epsilon \quad (B.6)
$$

We arrive at a $1/\alpha$ behaviour but we must be cautious with it for it comes with a $\ln \epsilon$ term which means that it is singular as $\epsilon \to 0$. This means that equation (B.6) is not the full story about $I_0$ and the contribution from the singular points $A$ and $B$ should contain a singular term which cancels out (B.6). We now check that this is in fact the case.

**B2. Singular Points Contribution (Van Hove Singularity) to $I_0$**

We have left out for the last moment the contribution from the corner points $A(\pm \pi, 0)$ and $B(0, \pm \pi)$. This amounts to the integration over the dashed region in Figure 5. Due to the identifications of the Brillouin zone boundaries, we can collect the 4 dashed regions into 2 dashed squares centered at $A(\pi, 0)$ and $B(0, \pi)$ by gluing them together.

As a matter of fact, both dashed squares contribute the same amount to $I_0$ so that we concentrate only on the evaluation of one of them, say $A(\pi, 0)$. Let us denote by $vH_A$ this dashed square around A. We can parametrize any point in $vH_A$ by $\kappa_1, \kappa_2$ as

$$
\begin{align*}
\kappa_1 &= \pi + \kappa_1 \\
\kappa_2 &= \kappa_2
\end{align*}
$$

Thus, on this dashed square the energy function $\cos k_1 + \cos k_2$ contributes like

$$
\cos k_1 + \cos k_2 \sim \frac{1}{2}(\kappa_1^2 - \kappa_2^2) \quad (B.8)
$$

Notice that this is a tipically van Hove-like singularity behaviour revealing the saddle-point nature of the singular points A and B. Inserting (B.8) in $I_0$ we get

$$
\frac{1}{(2\pi)^2} \int_{vH_A} d\kappa_1 d\kappa_2 \frac{1}{\cosh(\alpha(\kappa_1^2 - \kappa_2^2))}
$$

Now it is convenient to transform to light-cone coordinates $\kappa_\pm$,

$$
\begin{align*}
\kappa_1 &= \frac{1}{\sqrt{2}}(\kappa_+ + \kappa_-) \\
\kappa_2 &= \frac{1}{\sqrt{2}}(\kappa_+ - \kappa_-)
\end{align*}
$$

19
and thus we arrive at

\[
\frac{4}{(2\pi)^2} \int_0^\epsilon \int_0^\epsilon d\kappa_+d\kappa_- \frac{1}{\cosh(2\alpha \kappa_+\kappa_-)}
\]

Moreover, this integral can be evaluated by changing to variables \((u, v)\) as,

\[
\begin{cases}
  u = \kappa_+ \kappa_- \\
  v = \kappa_+ / \kappa_-
\end{cases}
\]

Eventually, after some algebra we obtain the following contribution from the van Hove point A:

\[
\frac{1}{2\pi \alpha} \ln \epsilon - \frac{1}{2(2\pi)^2} \int_0^\epsilon du \frac{\ln u}{\cosh(2\alpha u)}
\]

Notice that the \(\ln \epsilon\) contribution in (B.11) when multiplied by 2 singular points yields the desired cancelation of the singular behaviour obtained in (B.6) from the regular points.

In all, we are left with a finite contribution that can be extracted from (B.11). Therefore, the leading order behaviour of \(I_0(\alpha)\) as \(\alpha \to \infty\) is given by

\[
I_0^{(D=2)}(\alpha) \to \frac{\ln \alpha}{2\pi \alpha}
\]

The remarkable fact about this asymptotic behaviour is the presence of the \(\ln \alpha\) term in addition to the \(1/\alpha\) term already found in \(D = 1\) dimensions. This in turn is the distinctive characteristic feature of the \(D = 2\) dimensional problem.

The technique outlined above to isolate the leading contribution of \(I_0(\alpha)\) can also be applied to \(dI_0(\alpha)/d\alpha\) and \(dI_1(\alpha)/d\alpha\) (in fact \(I_1(\alpha)\) is easier to handle and does not requires that technique). In Table 2 we summarize the final results as well as the intermediate results showing explicitly that the cancelation of the singular \(\ln \epsilon\) terms also occurs for \(dI_0(\alpha)/d\alpha\) and \(dI_1(\alpha)/d\alpha\).
C  Fokker-Planck Hamiltonians for Fermions

In this appendix we want to describe in more detail the problems arising when trying to apply the FP-method of reference [20] to fermions. The question we want to answer is whether one can construct a hamiltonian for which the ansatz \( \psi(\alpha) \) (2.15) becomes an exact eigenstate. Following [20] we should act with \( H_0 \) on the state (2.15) and using the anticommutation relations of the operators \( n_j - \frac{1}{2} \), \( c_j \) and \( c_j^\dagger \)

\[
H_0|\psi(\alpha)\rangle = -\frac{U}{4} \sum_{<i,j>} \exp(-\frac{\alpha}{2} \sum_{<i,k>,k\neq j} T_{ik} - \frac{\alpha}{2} \sum_{<j,k>,k\neq i} T_{jk} + \text{rest unchanged})|CDW\rangle
\]

If the operators \( \{T_{ij}\} \) commute among themselves we could take the term \( \frac{\alpha}{2} \sum_{<l,m>} T_{lm} \) to the right of the exponential recovering in that fashion the state \( \psi(\alpha) \). This is precisely what happens in the cases described in reference [20]. Here however the operators do not commute and this complicates matters. We can apply the Baker-Campbell-Hausdorf formula to the last exponential in (C.1). The commutator between the sum of the first and second sums with the third gives operators which acting on \( |CDW\rangle \) vanishes. Hence to order \( \alpha^2 \) equation (C.1) becomes

\[
H_0|\psi(\alpha)\rangle \simeq -\frac{U}{4} \sum_{<i,j>} \exp(-\alpha \sum_{<i,k>,k\neq j} T_{ik} - \alpha \sum_{<j,k>,k\neq i} T_{jk})|\psi(\alpha)\rangle
\]

So that one gets up to order \( \alpha^2 \):

\[
H_{FP}|\psi(\alpha)\rangle = 0 \quad (C.3)
\]

with

\[
H_{FP} = U \sum_{<i,j>} \{(n_i - \frac{1}{2})(n_j - \frac{1}{2}) + \exp(-\alpha \sum_{<i,k>,k\neq j} T_{ik} - \alpha \sum_{<j,k>,k\neq i} T_{jk})\} \quad (C.4)
\]

Expanding the exponential in powers of \( \alpha \) we observe that the terms linear in \( \alpha \) correspond precisely to \( U_1 \) with the correct relationship between \( \alpha \) and \( t/U \) (2.33). In fact, from these type of comparison is how one derive the \( \alpha \)-parameters as functions of the coupling constants. Now, to order \( \alpha^2 \) we also find the operators appearing in \( U_2 \), but there are some more operators which acting on \( |CDW\rangle \) give nothing. The solution of the PV-equations is by no means unique.

Higher order parameters in \( \alpha \) give some new terms but also others that are already contained in \( U_1 \) and \( U_2 \). This means in particular that the relation between \( t/U \) and \( \alpha \) is rather non-linear, \( t/U = g(\alpha) = (D - \frac{1}{2})\alpha + \ldots \). In order to improve the ansatz one should add to the exponential of the ansatz the unwanted operators that appear in the FP-hamiltonian (we mean those operators which do not appear in the original ansatz). This program has been successfully implemented for Ising-like models but it remains to be seen whether it can also be extended for fermions.
References

[1] J.G. Esteve and G. Sierra, Phys. Rev. B to be published.

[2] S. Shankar, Rev. Mod. Phys. 66, 129 (1994).

[3] C.N. Yang, Phys. Rev. Lett. 19, 1312 (1967).

[4] W. van der Linden, Phys. Rep. 220, 53 (1992).

[5] S. Rodriguez, Phys. Rev. 116, 1474 (1959).

[6] T.W. Ruijgrok and S. Rodriguez, Phys. Rev. 119, 596 (1960).

[7] T. Oguchi, Phys. Rev. Lett. 11, 266 (1963).

[8] M.A. Garcia-Bach, R. Valenti, S.A. Alexander and D.J. Klein, Int. J. Quantum Chem. 12 273, (1977). Croatica Chemica Acta 64, (1991) 415.

[9] L. Hulthen, Arkiv. Mat. Astron. Fysik. A 26, 1 (1938).

[10] R.J. Baxter, Exactly Solved Models in Statistical Mechanics, Academic Press, London 1982.

[11] R. Orbach, Phys. Rev. 112, 309 (1958).

[12] L.R. Walker, Phys. Rev. 116, 1089 (1959).

[13] J. Frohlich, E.H. Lieb, Comm. Math. Phys. 60, 233 (1978).

[14] F.J. Dyson, E.H. Lieb, B. Simon, J. Stat. Phys. 18, 335 (1978).

[15] P. Lemberger, N. Macris, Lett. Math. Phys. 28, 295 (1993).

[16] J. Gubernatis, E. Scalapino, D.J. Sugar, W.D. Toussaint, Phys. Rev. B 32, 103 (1985).

[17] E. Hirsch, Phys. Rev. B31, 4403 (1985).

[18] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).

[19] B. Shraiman, E. Siggia, Phys. Rev. Lett. 60, 740 (1988).

[20] F. Jimenez and G. Sierra, CSIC preprint February 1995.
Table captions

**Table 1** : Reduced ground state energy $e(t/U = 1/2)$ values for the isotropic case as compared to several methods in D=1 dimensions.

**Table 2** : Asymptotic leading order behaviour for the basic integrals in $D = 2$ dimensions showing the cancelation of the singular $\ln \epsilon$ terms between the contributions of the regular points on the Fermi Surface and the van Hove singularities.
Figure captions

Figures 1 a) - d) : Reduced energy $e(\alpha; t/U)$ in 1D eq. (2.28) for several values of the coupling constant $t/U$ showing the bifurcation phenomena responsible for the existence of a critical point $(t/U)_c$ in the PV approach.

Figure 2 : The coupling constant $t/U$ as a function of the PV parameter $\alpha$ for 1D (solid line) showing the existence of a critical point $(t/U)_c$ and 2D (grey line) showing the $\ln \alpha$ behaviour for large $\alpha$.

Figure 3 : Staggered magnetization versus the coupling constant $(t/U)$: exact 1D result (solid line), PV 1D result (strong solid line) and PV 2D result (grey line).

Figures 4 : Reduced energy versus the coupling constant $(t/U)$: exact 1D result (black line), PV 1D result (black-grey solid line) and PV 2D result (grey line).

Figure 5 : Brillouin zone for 2D fermions at half-filling showing the Fermi Surface formed of regular points $P_r$ and van Hove singular points $A(\pi,0)$ and $B(0,\pi)$. $\Lambda = \epsilon$ are the cut-offs.
| Method                                      | Reference | $e(t/U = 1/2)$ Isotropic case |
|--------------------------------------------|-----------|------------------------------|
| Neel                                       | [4]       | 1.6766                       |
| Free Fermi Sea                             | [3]       | 1.7232                       |
| Present PV solution                        | [3]       | 1.7292                       |
| Jordan-Wigner transformed UHF solution     | [3]       | 1.7580                       |
| RVB ansatz ($M = 3$)                       | [3]       | 1.7726                       |

Table 1: Reduced ground state energy $e(t/U = 1/2)$ values for the isotropic case as compared to several methods in D=1 dimensions.

| $D = 2$ Integrals | $\alpha \to \infty$ Behaviour | R. P. Contribution | Van Hove Contribution |
|-------------------|--------------------------------|--------------------|-----------------------|
| $I_0^{(D=2)}(\alpha)$ | $\frac{\ln \alpha}{2\pi \alpha^2}$ | $-\frac{1}{\pi \alpha} \ln \epsilon$ | $\frac{1}{\pi \alpha} \ln \epsilon + \frac{\ln \alpha}{2\pi \alpha^2}$ |
| $\frac{dI_0^{(D=2)}}{d\alpha}(\alpha)$ | $-\frac{\ln \alpha}{2\pi \alpha^2}$ | $\frac{1}{\pi \alpha^2} \ln \epsilon$ | $-\frac{1}{\pi \alpha^2} \ln \epsilon - \frac{\ln \alpha}{2\pi \alpha^2}$ |
| $I_1^{(D=2)}(\alpha)$ | $(\frac{2}{\pi})^2$ | | |
| $\frac{dI_1^{(D=2)}}{d\alpha}(\alpha)$ | $\frac{\ln \alpha}{24\pi \alpha^3}$ | $-\frac{1}{24\pi \alpha^3} \ln \epsilon$ | $\frac{1}{24\pi \alpha^3} \ln \epsilon + \frac{\ln \alpha}{24\alpha^3}$ |

Table 2: Asymptotic leading order behaviour for the basic integrals in $D = 2$ dimensions showing the cancelation of the singular $\ln \epsilon$ terms between the contributions of the regular points on the Fermi Surface and the van Hove singularities.