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Variational bounds for lattice fermion models: I. Spinless fermions

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Abstract. In this paper we assess the validity of mean-field theories for lattice fermion systems with attractive interactions by comparing variational upper bounds from two plausible mean-field approximations—a Van der Waals (independent particle) approximation and a pairing approximation of the BCS type—for the Helmholtz free energy of a spinless fermion model with attractive nearest-neighbour interactions. It is found that there is a crossover from the Van der Waals approximation giving the best bound to the pairing approximation giving the best bound as t, the hopping integral passes through a critical value t_c. This crossover phenomenon exists in all dimensions as well as for the limiting $d \to \infty$ model. We conclude that there can be no simple mean-field theory which is valid for fermion systems with attractive interactions.

1. Introduction

Fermion models with attractive interactions have been the subject of recent investigations of bipolaron systems [1–12] and high temperature superconductivity [13–16]. The RPA, pairing theories and other variational methods have been used to study such models but very little is known rigorously about the validity of the approximate theories. An exception is the BCS pairing theory which is known to hold rigorously [17] for the BCS reduced Hamiltonian under fairly general conditions on the attractive pair potential.

A model which has received considerable attention in recent times is the Hubbard model [18] which in its extended form has Hamiltonian

$$\mathcal{H} = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} - \sum_{ij\sigma\sigma'} U_{ij}^{\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \tag{1.1}$$

where $c_{k\sigma}^{\dagger}$ $(c_{k\sigma})$ is the creation (annhilation) operator for particles with hopping energy $\epsilon_{k\sigma}$ wavevector k and spin $\sigma = \uparrow$ or $\downarrow$, $n_{i\sigma}$ is the (occupation) number operator for particles with spin σ and position vector j and $U_{ij}^{\sigma\sigma'}$ is the coupling strength between particles with spin σ and σ' located on lattice sites i and j respectively.

On a hypercubic d-dimensional lattice of volume $V = L^d$ it is customary to allow only hopping between nearest-neighbour sites so that $\epsilon_{k\sigma}$ has the form

$$\epsilon_{k\sigma} = -2t_{\sigma}\epsilon\,(2\pi k_1/L, \ldots, 2\pi k_d/L) \tag{1.2}$$

with spin-dependent hopping integrals t_{σ} and

$$\epsilon\,(\theta_1, \ldots, \theta_d) = d^{-1/2}\,[\cos\theta_1 + \cdots + \cos\theta_d] \tag{1.3}$$

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with the $d^{-1/2}$ factor included to ensure the existence of a non-trivial density of states in the limit $d \to \infty$ [19].

In the interaction term of (1.1), $U_{ij}^{\sigma\sigma'}$ non-negative corresponds to attraction and for the usual Hubbard model $U_{ij}^{\sigma\sigma'}$ is negative when $i = j$ and σ, σ' are opposite spins and vanishes otherwise; that is the only interaction is on-site repulsion between particles of opposite spin. In reality, one would expect to have a mixture of short-range repulsion and longer-range attraction. In the present work, however, we will consider only purely attractive interactions so that Pauli exclusion provides the only effective repulsion between the particles.

Apart from some exact results in one dimension [20] very little is known rigorously about the Hubbard model. It is not even clear, for example, what might constitute a legitimate mean-field theory for the model although some progress has been made in this direction by Vollhardt [21] and others [22] who have obtained some limited rigorous results in high spatial dimension, where it is known that lattice spin models approach their well known mean-field theories [23].

Using the BCS model results [17] as a guide it might be tempting to conjecture that a pairing ansatz would yield an appropriate mean-field theory for models of the form (1.1) with attractive interactions. It will be noted, however, that in the case of zero hopping ($\epsilon_{k\sigma} = 0$) the model reduces to a classical two-component lattice gas. In this case we would expect a classical mean-field theory of the Van der Waals type to be more appropriate than a quantum mechanical pairing theory of BCS-type with perhaps some crossover between the two theories as the hopping is increased relative to the strength of the particle interactions.

Our purpose in this series of articles is to study the question of appropriate mean-field theories for lattice fermion models by obtaining variational bounds for the Helmholtz free energy for models of the form (1.1) using various independent and pairing forms for a trial density matrix.

In the present paper we consider a simple form of (1.1) where only one spin species of fermions is relevant and where hopping and attractive interactions take place on nearest-neighbour sites of a regular lattice. Our Hamiltonian is, therefore, taken to be

$$\mathcal{H} = \sum_k \epsilon_k c_k^\dagger c_k - d^{-1} \sum_{\langle ij \rangle} n_i n_j \tag{1.4}$$

where ϵ_k is given by (1.2) with $t_\sigma = t$ independent of spin and units are scaled to give an attraction between particles of strength d^{-1} which guarantees the existence of thermodynamic quantities in the limit $d \to \infty$.

Using Van der Waals, or independent particle and pairing forms for the trial density matrix we, in fact, find a crossover phenomenon of the type already mentioned. That is, there is a critical value t_c of the hopping integral t such that a Van der Waals theory gives a lower (higher) free energy compared with a BCS-type pairing theory for $t < t_c$ ($t > t_c$). Moreover, this crossover phenomenon holds for all dimensions d and also for the limiting $d \to \infty$ model.

This result suggests that there can be no simple mean-field theory for lattice fermion models which is valid for arbitrary combinations of hopping integrals and interaction strengths. This suggestion will be explored further in subsequent publications where we will consider the effects of spin dependence.

2. The variational principle

For a quantum mechanical system with Hamiltonian $\mathcal{H}$, the grand canonical partition function is given by

$$\mathcal{Q} = \operatorname{Tr} e^{-\beta(\mathcal{H}-\mu\mathcal{N})} \tag{2.1}$$

where $\beta = 1/kT$, with k Boltzmann's constant and T the absolute temperature, μ is the chemical potential and $\mathcal{N}$ is the number operator.

The thermodynamic potential is defined by

$$\chi = \lim_{V\to\infty} V^{-1} \log \mathcal{Q} \tag{2.2}$$

where the equation

$$n = \lim_{V\to\infty} \langle\mathcal{N}\rangle / V \tag{2.3}$$

provides a relationship between the (average) particle density n and the chemical potential where $\langle\ \rangle$ denotes the thermodynamic average defined by

$$\langle\mathcal{A}\rangle = \mathcal{Q}^{-1} \operatorname{Tr} \mathcal{A} e^{-\beta(\mathcal{H}-\mu\mathcal{N})}. \tag{2.4}$$

With μ and χ considered as functions of n and T the Helmholtz free energy is given by

$$\psi = \mu - \chi/n\beta. \tag{2.5}$$

A variational upper bound can generally be obtained by writing $\mathcal{H}$ in the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \tag{2.6}$$

with $\mathcal{H}_0$, the reference Hamiltonian, chosen so that the reference grand canonical partition function

$$\mathcal{Q}_0 = \operatorname{Tr} e^{-\beta(\mathcal{H}_0-\mu\mathcal{N})} \tag{2.7}$$

can be calculated easily but is also representative of the basic physics of the system.

With $\mathcal{Q}$ replaced by $\mathcal{Q}_0$ in (2.1) one obtains the reference thermodynamic potential χ_0 and the corresponding reference free energy

$$\psi_0 = \mu - \chi_0/n\beta \tag{2.8}$$

where in the equation (2.3) for n, the thermodynamic average is taken with respect to the reference system, i.e. $\mathcal{Q}$ and $\mathcal{H}$ in (2.4) replaced respectively by $\mathcal{Q}_0$ and $\mathcal{H}_0$.

A well known variational principle [24] then states that

$$\psi \leqslant \psi_0 + \lim_{V\to\infty} \langle\mathcal{H}_1\rangle_0 / nV \tag{2.9}$$

where $\langle\mathcal{H}_1\rangle_0$ denotes the average of $\mathcal{H}_1$ with respect to the reference system.

In the following sections of this paper we will compute the variational upper bound on the right-hand side of (2.9) for the model Hamiltonian (1.4) using two particular choices for the reference Hamiltonian $\mathcal{H}_0$.

3. Independent particle bound

The most obvious choice for $\mathcal{H}_0$ in the variational principle (2.9) is the kinetic energy part of $\mathcal{H}$, i.e. for the spinless fermion model (1.4),

$$\mathcal{H}_0 = \sum_k \epsilon_k c_k^\dagger c_k. \tag{3.1}$$

In this case we refer to the right-hand side of (2.9) as the trivial mean-field bound and denote it by ψ_{tr}. An elementary calculation yields

$$\psi_{\text{tr}} = \mu - \frac{f_0}{\beta n} - n - \frac{g_1^2}{n} \tag{3.2}$$

with the comparison density equation (2.3) for the reference system given by

$$n = 1 - f_1 \tag{3.3}$$

where

$$f_0 = \frac{1}{\pi^d} \int_{[0,\pi]^d} \log\left[1 + z e^{2\beta t \epsilon(\theta)}\right] \mathcal{D}\theta \tag{3.4}$$

$$f_i = \frac{1}{\pi^d} \int_{[0,\pi]^d} \frac{\mathcal{D}\theta}{\left(1 + z e^{2\beta t \epsilon(\theta)}\right)^i} \qquad i = 1, 2, 3, \ldots \tag{3.5}$$

$$g_i = \frac{1}{\pi^d} \int_{[0,\pi]^d} \frac{\epsilon(\theta)}{\left(1 + z e^{2\beta t \epsilon(\theta)}\right)^i} \mathcal{D}\theta \qquad i = 1, 2, 3, \ldots \tag{3.6}$$

and

$$\mathcal{D}\theta = \mathrm{d}\theta_1 \ldots \mathrm{d}\theta_d. \tag{3.7}$$

The trivial bound (3.2) can, in principle, be improved by noting that the exact free energy ψ, considered as a function of the specific volume $v = 1/n$, must be C^1, monotonic decreasing and concave [25]. It is clear that ψ_{tr} is C^1 but it need not be monotonic decreasing or concave. In any event we have

$$\psi \leqslant \text{CE}\{\psi_{\text{tr}}\} \equiv \psi_{\text{VW}} \tag{3.8}$$

where CE denotes the concave envelope, i.e. as a function of v, the greatest C^1 monotone decreasing concave function which is bounded above by ψ_{tr}.

We denote the concave envelope of ψ_{tr} by ψ_{VW} to highlight the similarity with conventional Van der Waals (mean-field) theory. In fact, as we will see later, ψ_{VW} is identical to the lattice gas version of Van der Waals theory [25] when $t = 0$. The independent particle bound with a concave envelope construction is also equivalent to the Husimi theory [26].

In the sequel we will say that ψ_{tr} is *stable* if it is monotonic decreasing and concave in v. In such cases we will say that ψ_{VW} is *trivial* because

$$\psi_{\text{VW}} = \psi_{\text{tr}} \qquad \text{for all } v. \tag{3.9}$$

Otherwise ψ_{VW} is *non-trivial* for some values of v where $\psi_{VW} < \psi_{tr}$.

To determine the values of t and T for which ψ_{tr} is stable we calculate its derivatives with respect to v in appendix A. It is useful to define a function

$$F_d(y) = \frac{1}{y}\left\{ \int_0^\infty x J_0^d\left(\frac{x}{\sqrt{d}}\right) \operatorname{cosech}\frac{\pi x}{y}\,dx + \frac{d}{y}\int_0^\infty J_0^{d-1}\left(\frac{x}{\sqrt{d}}\right) J_1\left(\frac{x}{\sqrt{d}}\right) \operatorname{cosech}\frac{\pi x}{y}\,dx \times \int_0^\infty x^2 J_0^{d-1}\left(\frac{x}{\sqrt{d}}\right) J_1\left(\frac{x}{\sqrt{d}}\right) \operatorname{cosech}\frac{\pi x}{y}\,dx \times \left[\int_0^\infty x J_0^d\left(\frac{x}{\sqrt{d}}\right) \operatorname{cosech}\frac{\pi x}{y}\,dx\right]^{-1} \right\}. \tag{3.10}$$

We show that ψ_{tr} is stable for all temperatures if

$$t \geqslant F_d(\infty) \tag{3.11}$$

$$= \frac{1}{\pi}\int_0^\infty J_0^d\left(\frac{x}{\sqrt{d}}\right) dx + \frac{\sqrt{d}}{\pi}\int_0^\infty J_0^{d-1}\left(\frac{x}{\sqrt{d}}\right) J_1\left(\frac{x}{\sqrt{d}}\right) dx. \tag{3.12}$$

If $0 \leqslant t \leqslant F_d(\infty)$ then there exists a critical temperature T_c defined by

$$t = F_d\,(2t/kT_c) \tag{3.13}$$

above which ψ_{tr} is stable. For $0 \leqslant T \leqslant T_c$, ψ_{tr} is not stable, having two points of inflection.

In such cases ψ_{VW} is obtained from a double tangent construction as shown in figure 1.

$$\psi_{VW} = \begin{cases} \psi_{tr} & \text{for } v \leqslant v_l \\ \psi_l + \dfrac{\psi_g - \psi_l}{v_g - v_l}(v - v_l) & \text{for } v_l < v < v_g \\ \psi_{tr} & \text{for } v \geqslant v_g \end{cases} \tag{3.14}$$

where $\psi_l = \psi_{tr}(v_l)$ and $\psi_g = \psi_{tr}(v_g)$ with v_l and v_g interpreted as the liquid and gas specific volumes respectively. The region $v_l < v < v_g$ in which ψ_{VW} is non-trivial is interpreted as the coexistence region and writing $n_g = v_g^{-1}$ and $n_l = v_l^{-1}$, we have

$$n_l = 1 - n_g \tag{3.15}$$

and

$$t = G(n_g) \tag{3.16}$$

where

$$G(n) = \frac{4t}{\mu}\left[n - 1/2 + \frac{g_1\,(g_1 - g_2)}{f_1 - f_2}\right]. \tag{3.17}$$

The *order parameter* $2 - v_l$ is maximal at $T = 0$ and vanishes as $T \to T_c^-$.

Finally we note from (3.2) and (3.3) that when there is no hopping term ($t = 0$)

$$\beta\psi_{tr} = \log n + n^{-1}(1 - n)\log(1 - n) - \beta n. \tag{3.18}$$

In this case $kT_c = 1/2$ and (3.16) reduces to the familiar mean-field equation

$$n_g - \tfrac{1}{2} = \tfrac{1}{2}\tanh\beta\left(n_g - \tfrac{1}{2}\right). \tag{3.19}$$

The ground-state energy estimate in this case is easily calculated to be

$$\psi_{VW} = -1 \qquad \text{for all } v \text{ at } T = 0. \tag{3.20}$$

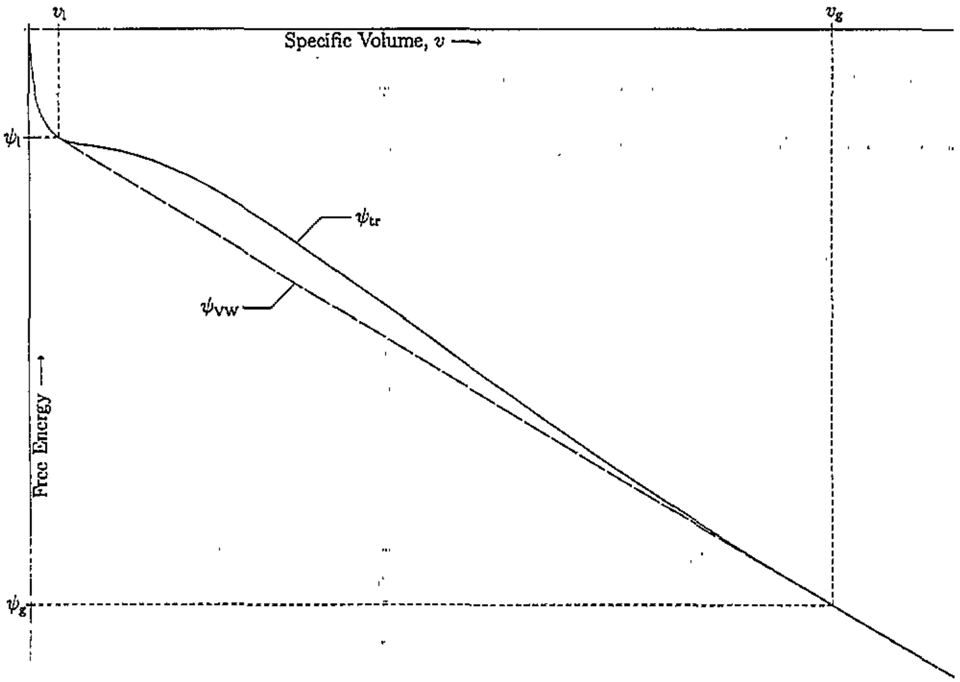

Figure 1. Double tangent construction for the trivial mean-field free energy, ψ_{tr}.

4. A pairing bound

To develop a pairing bound (2.9) for the free energy we begin by writing the interaction term in (1.4) in terms of momentum space creation and annihilation operators i.e.

$$\mathcal{V} = -d^{-1} \sum_{\langle ij \rangle} n_i n_j \tag{4.1}$$

$$= -V^{-1} \sum_{klm} v_{l-k} c_k^{\dagger} c_l c_m^{\dagger} c_{k-l+m} \tag{4.2}$$

where

$$v_k = d^{-1} \sum_{j=1}^{d} \exp\left(2\pi i k_j / L\right). \tag{4.3}$$

We then write

$$\mathcal{V} = \mathcal{V}_n + \mathcal{V}_p + \mathcal{V}_c \tag{4.4}$$

where

$$\mathcal{V}_n = -V^{-1} \sum_{km} n_k n_m - V^{-1} \sum_{kl} v_{l-k} n_k (1 - n_l) \tag{4.5}$$

$$\mathcal{V}_p = -\sum_{kl}{}' J_{kl} b_k^{\dagger} b_l \tag{4.6}$$

$$\mathcal{V}_c = \mathcal{V} - \mathcal{V}_n - \mathcal{V}_p \tag{4.7}$$

where $n_k = c_k^\dagger c_k$ is the number operator for particles with wavevector k, $b_k = c_{-k}c_k$ is the annihilation operator for a d-wave (spinless) pair with momentum $2\pi k/L$, the primed sum is over vectors k with $0 \leqslant k_1 \leqslant L/2$ and

$$J_{kl} = \frac{4}{dV}\sum_{j=1}^{d} \sin\frac{2\pi k_j}{L} \sin\frac{2\pi l_j}{L}. \tag{4.8}$$

$\mathcal{V}_n$ arises from the $k = l$ and $l = m$ terms in (4.2) (those terms which can be written in terms of the n_k), $\mathcal{V}_\mathrm{p}$ consists of the pairing ($k = -m$) terms in (4.2) and $\mathcal{V}_\mathrm{c}$ consists of other correlations (terms in which $k \neq l, -m$ and $l \neq m$ in addition to an O(1) contribution from the $k = l = \pm m$ terms).

We apply the decoupling procedure of BZT [27] to $\mathcal{V}_\mathrm{p}$ and write

$$\mathcal{H}_1 = -\sum_{kl}{}' J_{kl}\left(b_k^\dagger - \phi_k^*\right)(b_l - \phi_l) + \mathcal{V}_n + \mathcal{V}_\mathrm{c} \tag{4.9}$$

where $\{\phi_k\}$ is a set of decoupling parameters. Using (2.6) and (4.9) we then arrive at

$$\mathcal{H}_0 = \sum_k \epsilon_k c_k^\dagger c_k + 2i\sum_k \alpha_k\left(\Delta b_k^\dagger - \Delta^* b_k\right) + V|\Delta|^2 \tag{4.10}$$

where

$$\alpha_k = \alpha\left(2\pi k_1/L, \ldots, 2\pi k_d/L\right) \tag{4.11}$$

$$\alpha\left(\theta_1, \ldots, \theta_d\right) = \frac{1}{\sqrt{d}}\left[\sin\theta_1 + \cdots + \sin\theta_d\right] \tag{4.12}$$

and

$$\Delta = \frac{2i}{d}\sum_l{}' \alpha_l \phi_l \tag{4.13}$$

is the gap parameter. We denote the upper bound (2.9) (which depends only on Δ) by $\psi(\Delta)$ in this case.

Since the reference Hamiltonian (4.10) is quadratic in the Fermi operators, it may be diagonalized by a Bogoliubov–Valatin transformation [27] and $\psi(\Delta)$ is readily evaluated. The final expression for $\psi(\Delta)$ is

$$\begin{aligned}\psi(\Delta) = \frac{\mu}{n}(n - 1/2) - \frac{|\Delta|^2}{n}\left[\frac{\beta}{2(2\pi)^d}\int_{[0,2\pi]^d} (\alpha(\theta))^2 h(\beta E(\theta))\mathcal{D}\theta - 1\right]^2 \\ - n - \frac{\log 2}{n\beta} - \frac{1}{(2\pi)^d n\beta}\int_{[0,2\pi]^d} \log\cosh\frac{\beta E(\theta)}{2}\,\mathcal{D}\theta \\ + \frac{1}{n}\left[\frac{\beta t}{2(2\pi)^d}\int_{[0,2\pi]^d} \epsilon(\theta)(\mu + 2t\epsilon(\theta))h(\beta E(\theta))\mathcal{D}\theta\right]^2\end{aligned} \tag{4.14}$$

where

$$h(x) = \frac{2}{x}\tanh\frac{x}{2} \tag{4.15}$$

$$E(\theta) = \sqrt{(\mu + 2t\epsilon(\theta))^2 + (\Delta\alpha(\theta))^2}. \tag{4.16}$$

The comparison density equation (2.3) for the reference system is

$$n = \frac{1}{2} + \frac{\beta}{4(2\pi)^d} \int_{[0,2\pi]^d} (\mu + 2t\epsilon(\theta))h(\beta E(\theta))\mathcal{D}\theta. \tag{4.17}$$

We note that $\psi(\Delta)$ depends only on $|\Delta|$ so we are lead to define the optimal upper bound

$$\psi \leqslant \psi_{\mathrm{p}} \equiv \min_{\Delta \geqslant 0} \psi(\Delta). \tag{4.18}$$

For given t and n there exists a critical temperature T_{c} above which ψ_{p} is *trivial* in that it reduces to ψ_{tr}. That is, for $T \geqslant T_{\mathrm{c}}$, $\psi(\Delta)$ is monotonic increasing for $\Delta \geqslant 0$ so that the minimum ψ_{p} occurs at $\Delta = 0$ whence from (3.1) and (4.10) we have $\psi_{\mathrm{p}} = \psi_{\mathrm{tr}}$. For $0 \leqslant T < T_{\mathrm{c}}$, $\psi(\Delta)$ is not monotonic for $\Delta \geqslant 0$, decreasing to a minimum for some $\Delta > 0$ before increasing so ψ_{p} is *non-trivial* in that $\psi_{\mathrm{p}} < \psi_{\mathrm{tr}}$. In such cases the condition determining the value of Δ which minimizes $\psi(\Delta)$ is

$$\psi'(\Delta) = 0. \tag{4.19}$$

Clearly then, T_{c} is determined by

$$\psi''(0) = 0 \qquad \text{at } T = T_{\mathrm{c}}. \tag{4.20}$$

For the rest of this section we will restrict our attention to some special cases.

4.1. The half-filled band case ($n = 1/2$)

In this case (4.17) can be solved to obtain $\mu = 0$ so (4.14) and (4.16) reduce to

$$\begin{aligned} \psi(\Delta) = -\frac{1}{2} - 2\Delta^2 \left[\frac{\beta}{2(2\pi)^d} \int_{[0,2\pi]^d} (\alpha(\theta))^2 h(\beta E(\theta))\, \mathcal{D}\theta - 1\right]^2 - \frac{2\log 2}{\beta} \\ + \frac{1}{2}\left[\frac{\beta t}{(2\pi)^d} \int_{[0,2\pi]^d} (\epsilon(\theta))^2 h(\beta E(\theta))\, \mathcal{D}\theta\right]^2 \\ - \frac{2}{(2\pi)^d \beta} \int_{[0,2\pi]^d} \log\cosh \frac{\beta E(\theta)}{2} \mathcal{D}\theta \end{aligned} \tag{4.21}$$

and

$$E(\theta) = 2\sqrt{t^2(\epsilon(\theta))^2 + \Delta^2(\alpha(\theta))^2}. \tag{4.22}$$

By differentiating (4.21) it is easy to show that the condition (4.20) determining T_{c} can be written in the form (3.13) but with

$$F_d(y) = F_d^{(1)}(y) + \frac{F_d^{(2)}(y)\left(F_d^{(1)}(y) - F_d^{(2)}(y)\right)}{F_d^{(1)}(y)} \tag{4.23}$$

where

$$F_d^{(1)}(y) = \frac{y}{4(2\pi)^d} \int_{[0,2\pi]^d} (\alpha(\theta))^2 h(y\epsilon(\theta))\, \mathcal{D}\theta \tag{4.24}$$

$$F_d^{(2)}(y) = \frac{y}{4(2\pi)^d} \int_{[0,2\pi]^d} (\epsilon(\theta))^2 h(y\epsilon(\theta))\, \mathcal{D}\theta. \tag{4.25}$$

Using standard analysis we can rewrite (4.24) and (4.25) as one-dimensional integrals, i.e.

$$F_d^{(1)}(y) = \frac{\sqrt{d}}{\pi}\int_0^\infty J_0^{d-1}\left(\frac{x}{\sqrt{d}}\right) J_1\left(\frac{x}{\sqrt{d}}\right)\frac{1}{x}\tanh^{-1}\operatorname{sech}\frac{\pi x}{y}\,\mathrm{d}x$$

$$F_d^{(2)}(y) = \frac{\sqrt{d}}{\pi}\int_0^\infty J_0^{d-1}\left(\frac{x}{\sqrt{d}}\right) J_1\left(\frac{x}{\sqrt{d}}\right)\frac{\pi x}{y}\operatorname{cosech}\frac{\pi x}{y}\,\mathrm{d}x \tag{4.27}$$

and in the $d = \infty$ limit we have

$$F_\infty^{(1)}(y) = \frac{1}{2\pi}\int_0^\infty \tanh^{-1}\operatorname{sech}\frac{\pi x}{y}\mathrm{e}^{-x^2/4}\,\mathrm{d}x \tag{4.28}$$

$$F_\infty^{(2)}(y) = \frac{1}{2\pi}\int_0^\infty \frac{\pi x}{y}\operatorname{cosech}\frac{\pi x}{y}\mathrm{e}^{-x^2/4}\,\mathrm{d}x. \tag{4.29}$$

4.2. $t = 0$ case

In this case the critical temperature is given by

$$T_\mathrm{c} = \frac{2n-1}{4\tanh^{-1}(2n-1)} \tag{4.30}$$

and, in particular, $kT_\mathrm{c} = 1/4$ at half filling. The pairing free energy (4.18) is

$$\psi_\mathrm{p} = \frac{\mu}{n}\left(n-\frac{1}{2}\right) + \frac{\Delta^2}{n} + \frac{\log 2}{n\beta} - n - \frac{1}{(2\pi)^d n\beta}\int_{[0,2\pi]^d}\log\cosh\frac{\beta E(\theta)}{2}\mathcal{D}\theta \tag{4.31}$$

with (4.16) and (4.17) reducing to

$$E(\theta) = \sqrt{\mu^2 + 4\Delta^2(\alpha(\theta))^2} \tag{4.32}$$

$$n = \frac{1}{2} + \frac{\beta\mu}{4(2\pi)^d}\int_{[0,2\pi]^d} h(\beta E(\theta))\,\mathcal{D}\theta. \tag{4.33}$$

For $0 \leqslant T < T_\mathrm{c}$, the condition (4.19) determining Δ reduces to

$$1 = \frac{\beta}{2(2\pi)^d}\int_{[0,2\pi]^d}(\alpha(\theta))^2 h(\beta E(\theta))\,\mathcal{D}\theta. \tag{4.34}$$

It will be noted that (4.34) is only a slightly disguised form of the familiar energy gap equation in BCS theory.

In the $T = 0$ limit the above reduce to

$$\psi_\mathrm{p} = \frac{\mu}{n}\left(n-\frac{1}{2}\right) + \frac{\Delta^2}{n} - n - \frac{1}{2(2\pi)^d n}\int_{[0,2\pi]^d} E(\theta)\,\mathcal{D}\theta \tag{4.35}$$

$$1 = \frac{1}{(2\pi)^d}\int_{[0,2\pi]^d}\frac{\mathcal{D}\theta}{E(\theta)} \tag{4.36}$$

$$n = \frac{1}{2} + \frac{\mu}{(2\pi)^d}\int_{[0,2\pi]^d}\frac{(\alpha(\theta))^2}{E(\theta)}\mathcal{D}\theta. \tag{4.37}$$

At half filling we have $\mu = 0$ and (4.36) can be solved to obtain $\Delta = I(d)/\pi$ where

$$I(d) = \sqrt{d}\int_0^\infty J_0^{d-1}\left(\frac{x}{\sqrt{d}}\right) J_1\left(\frac{x}{\sqrt{d}}\right)\frac{dx}{x}. \tag{4.38}$$

In this case (4.35) gives

$$\psi_p = -\frac{1}{2} - \frac{2(I(d))^2}{\pi^2}. \tag{4.39}$$

For instance, we have

$$\psi_p = \begin{cases} -\frac{1}{2} - \frac{2}{\pi^2} & \approx -0.70264 \qquad d = 1 \\ -\frac{1}{2} - \frac{16}{\pi^4} & \approx -0.66426 \qquad d = 2 \\ -\frac{1}{2} - \frac{1}{2\pi} & \approx -0.65915 \qquad d = \infty\,. \end{cases} \tag{4.40}$$

5. Comparison of pairing and independent particle bounds

5.1. The case $t = 0$

From (3.19) and (4.30) we note that the non-trivial region for the Van der Waals approximation properly contains the non-trivial region for the pairing approximation in the sense that the critical temperature in the pairing approximation is strictly less than the critical temperature in the Van der Waals approximation for all densities. Furthermore, $\psi_{tr} < \psi_p$ in the region where the Van der Waals approximation is non-trivial, the two approximations being equivalent when they are both trivial. In other words when $t = 0$ the Van der Waals approximation is always superior to the pairing approximation which is hardly surprising when one notes that the $t = 0$ model is purely classical. In other words one could hardly expect an artificial quantum decoupling scheme to provide a better mean-field theory than Van der Waals for a purely classical system.

The difference in the two approximation schemes is highlighted in the $T = 0$ case at half filling where the pairing ground-state energy estimates (4.40) are larger than the Van der Waals ground-state energy estimate (3.20) which, in turn, coincides with the exact ground-state energy

$$\psi = -1 \qquad \text{for all } v \text{ at } T = 0 \tag{5.1}$$

obtained for N particles on a d-dimensional hypercubic lattice when the particles form dN pairs of nearest-neighbour occupied sites.

At finite temperature the Van der Waals approximation becomes exact in the limit $d \to \infty$ [23] but in this limit the pairing estimate ψ_p still exceeds ψ_{VW}.

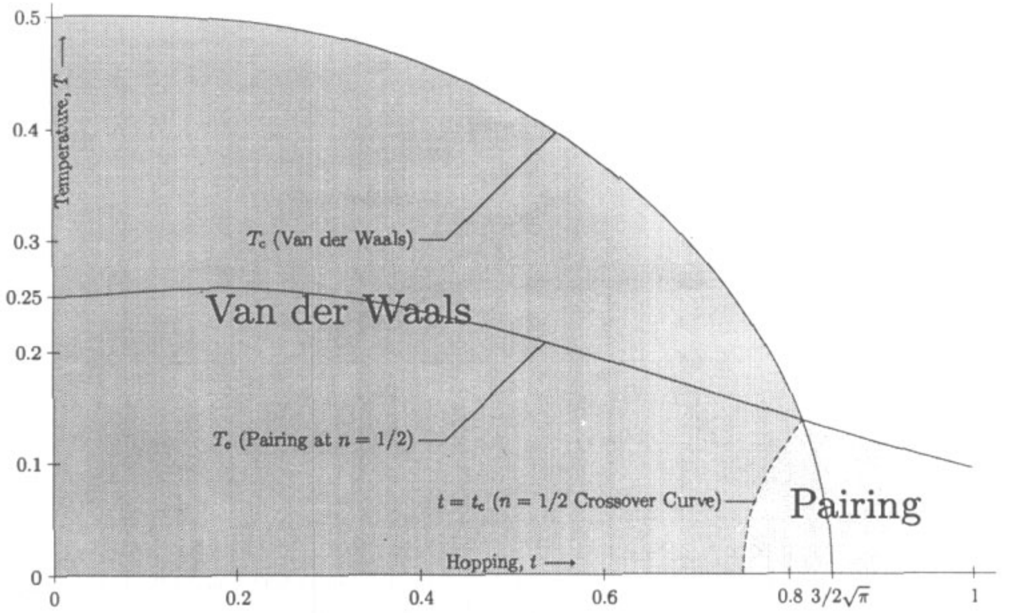

Figure 2. The Van der Waals and $n = 1/2$ pairing critical temperatures as functions of t for the infinite-dimensional spinless fermion model. Also depicted is the $n = 1/2$ crossover curve t_c. The Van der Waals approximation gives a better result for the $n = 1/2$ Helmholtz free energy in the dark shaded region. The pairing approximation gives a better result in the light shaded region. In the unshaded region both approximations are trivial.

5.2. *The case $t > 0$*

As noted in the introduction there is a crossover point $t = t_c$ such that $\psi_{VW} < \psi_p$ for $0 \leqslant t < t_c$ and $\psi_p < \psi_{VW}$ below criticality for $t > t_c$.

This crossover phenomenon is illustrated in figure 2 where we compare the Van der Waals critical temperature with the $n = 1/2$ pairing critical temperature for the $d = \infty$ case. Results for $d \geqslant 3$ are very similar. The crossover curve t_c is also shown.

Finally, in figures 3 and 4 we have plotted the ground-state energy estimates for the half-filled band for $d = 1$ and $d = \infty$ respectively. In the $d = 1$ case we also plot the exact ground-state energy

$$\psi = \begin{cases} -1 & 0 \leqslant t \leqslant 1/2 \\ -1 - 4t\sqrt{1 - \dfrac{1}{4t^2}} \displaystyle\int_0^\infty \left[1 - \dfrac{\tanh\left[w \cos^{-1}(-1/2t)\right]}{\tanh \pi w}\right] \mathrm{d}w & t > 1/2 \end{cases} \tag{5.2}$$

which is obtainable by using the Wigner–Jordan transformation to transform $\mathcal{H}$ into an anisotropic spin-1/2 Heisenberg Hamiltonian [28] and then applying the exact results of Cloizeaux and Gaudin [29]. It is interesting to note that $\psi_{VW} = \psi$ for $0 \leqslant t \leqslant 1/2$ and $\psi_{VW} = \psi_p = \psi$ when $t = 1/2$. Details regarding the calculation of ψ_{VW} and ψ_p in the $d = \infty$ limit will be supplied on request.

As mentioned in the introduction, the crossover phenomenon, which persists in the limit $d \to \infty$, strongly suggests that we have a long way to go in finding an all encompassing mean-field theory for lattice fermion systems.

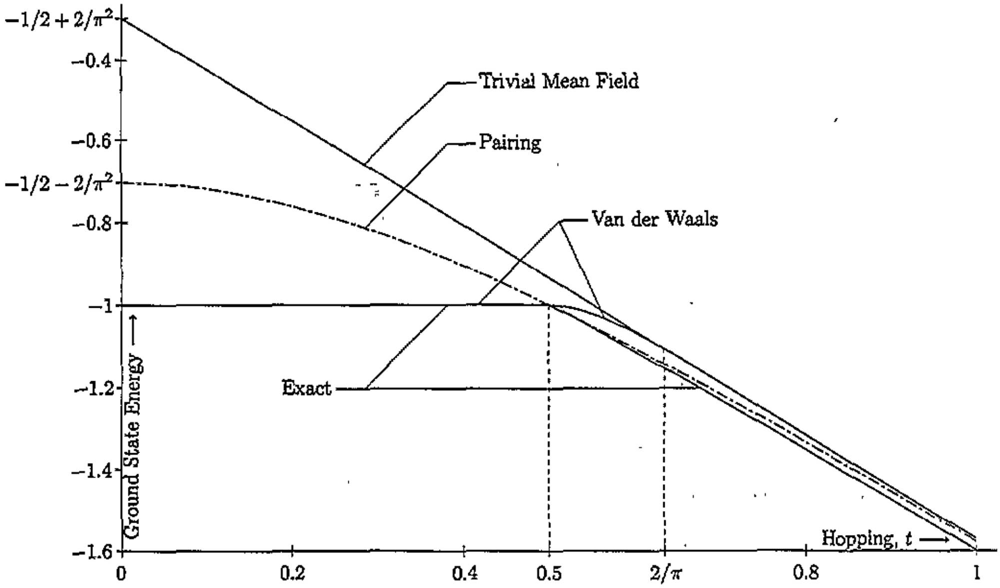

Figure 3. Ground-state energy estimates from the trivial mean-field, Van der Waals and pairing approximations for the one-dimensional spinless fermion model in the $n = 1/2$ case (half-filled band) as functions of t. Also included is the exact ground-state energy which is recovered by the Van der Waals approximation for $0 \leqslant t \leqslant 1/2$.

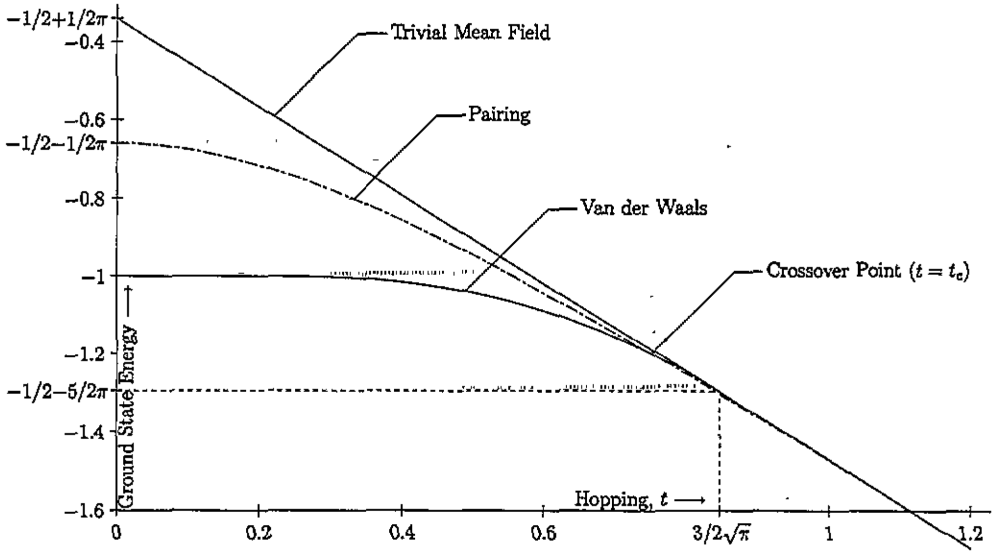

Figure 4. Ground-state energy estimates from the trivial mean-field, Van der Waals and pairing approximations for the infinite dimensional spinless fermion model in the $n = 1/2$ case (half-filled band) as functions of t.

5.3. The quasi-chemical equilibrium theory

As mentioned in section 3, the independent particle approximation with concave envelope construction is equivalent to the Husimi theory which, in the present formulation of the variational principle, amounts to taking

$$\mathcal{H}_1 = -V^{-1} \sum_{km} (n_k - \rho_k)(n_m - \rho_m) - V^{-1} \sum_{kl} v_{l-k} (n_k - \rho_k)(1 - (n_l - \rho_l)) + \mathcal{V}_p + \mathcal{V}_c. \tag{5.3}$$

That is, the term $\mathcal{V}_n$ in (4.4) is decoupled using the parameters $\{\rho_k\}$. When optimized over the ρ_k, the upper bound (2.9) equates to ψ_{VW}. In the pairing approximation, on the other hand, $\mathcal{V}_p$ is decoupled by the parameters $\{\phi_k\}$.

The two approximation schemes can be combined into a single formalism, the quasi-chemical equilibrium theory [26] which extends the independent particle ansatz to include pairing correlations. That is, we write

$$\mathcal{H}_1 = -V^{-1} \sum_{km} (n_k - \rho_k)(n_m - \rho_m) - V^{-1} \sum_{kl} v_{l-k} (n_k - \rho_k)(1 - (n_l - \rho_l))$$
$$- \sum_{kl}{}' J_{kl} \left(b_k^\dagger - \phi_k^*\right)(b_l - \phi_l) + \mathcal{V}_c \tag{5.4}$$

decoupling both $\mathcal{V}_n$ and $\mathcal{V}_p$.

The quasi-chemical equilibrium theory, however, reduces to the better of the two approximations—pairing if $\psi_p < \psi_{VW}$ or Van der Waals if $\psi_{VW} \leqslant \psi_p$.

6. Summary and discussion

In this paper we have compared variational upper bounds from two plausible mean-field approximations—a Van der Waals (independent particle) approximation and a pairing approximation of the BCS type—for the Helmholtz free energy of a spinless fermion model with attractive nearest-neighbour interactions in an attempt to assess the validity of mean-field theories for lattice fermion systems with attractive interactions. It was found that the Van der Waals approximation yields a better free energy estimate for strong couplings and the pairing approximation yields a better result in the regime of weak attractions with a crossover occurring when t, the strength of the hopping (relative to the interaction strength), passes through a critical value t_c.

The crossover phenomenon was found to exist in all dimensions d and persists in the limit $d \to \infty$ where we might expect to find an exact mean-field theory. This result suggests that there can be no simple mean-field theory for fermion systems with attractive interactions in the limit $d \to \infty$.

In future publications we will explore the effects of spin dependence and competing interactions (short-range repulsion and longer-range attraction) on the nature and validity of mean-field theories for these models.

Acknowledgment

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Appendix. Critical temperature for the independent particle bound

In this appendix we determine the values of t and T for which ψ_{tr} is stable (monotonic decreasing and concave in v).

We define the pressure p_{tr} derived from ψ_{tr} by

$$p_{\mathrm{tr}} = -\partial\psi_{\mathrm{tr}}/\partial v. \tag{A.1}$$

A routine calculation using (3.2)–(3.6) yields

$$p_{\mathrm{tr}} = \frac{f_0}{\beta} - n^2 - g_1^2 - 2ng_1\frac{g_1 - g_2}{f_1 - f_2}. \tag{A.2}$$

Clearly ψ_{tr} is stable if and only if p_{tr} is positive and monotonic increasing. It is easily established that p_{tr} is positive and monotone if v is sufficiently small or large. It follows that ψ_{tr} is stable if and only if p_{tr} has no turning points.

On differentiating (A.2) it is found that p_{tr} has a turning point at $v = 1/n$ if and only if

$$t = \mathcal{F}(n) \tag{A.3}$$

where

$$\mathcal{F}(n) = 2\beta t\left[f_1 - f_2 - \frac{(g_1-g_2)^2}{f_1-f_2} - \frac{g_1\,(g_1 - 3g_2 + 2g_3)}{f_1 - f_2} - \frac{g_1\,(g_1-g_2)\,(f_1 - 3f_2 + 2f_3)}{(f_1-f_2)^2}\right] \tag{A.4}$$

Now $\mathcal{F}(1-n) = \mathcal{F}(n)$ so turning points occur in pairs spaced evenly about $n = 1/2$. $\mathcal{F}$ is positive, $\mathcal{F}(0) = 0$ and $\mathcal{F}(n)$ is monotone increasing in n on $[0, 1/2]$. It follows that p_{tr} is stable if and only if $t \geqslant \mathcal{F}(1/2)$. If $t < \mathcal{F}(1/2)$ then p_{tr} has two turning points and so ψ_{tr} has two points of inflection and is unstable.

We consider the function $\mathcal{F}(1/2)$. From (3.3) we note that

$$z = 1 \qquad \text{when } n = 1/2. \tag{A.5}$$

Also from (3.6) we have

$$g_1 - g_2 = 0 \qquad \text{when } z = 1 \tag{A.6}$$

so combining (A.4)–(A.6) we obtain

$$\mathcal{F}(1/2) = 2\beta t\left[f_1 - f_2 + \frac{2g_1\,(g_2 - g_3)}{f_1 - f_2}\right](z = 1). \tag{A.7}$$

We next apply standard methods to convert the d-dimensional integrals in (A.7) to one-dimensional integrals and obtain

$$\mathcal{F}(1/2) = F_d(2\beta t) \tag{A.8}$$

where F_d is given by (3.10). The expression (3.10) is easier to evaluate in high dimensions than the d-dimensional integrals in (A.7). For instance, in the $d = \infty$ case we have

$$F_\infty(y) = \frac{1}{y}\int_0^\infty x\left(1 + \frac{x^2}{4}\right)\mathrm{e}^{-x^2/4}\operatorname{cosech}\frac{\pi x}{y}\,\mathrm{d}x. \tag{A.9}$$

Now $F_d(0) = 0$ and F_d is monotonic increasing for positive argument with limit (3.12) $\left(F_1(\infty) = 2/\pi,\ F_\infty(\infty) = 3/2\sqrt{\pi}\right)$. It is clear from the stationarity condition (A.3), (A.8) and the properties of $\mathcal{F}$ and F_d that ψ_{tr} is stable for all temperatures if $t \geqslant F_d(\infty)$. If $0 \leqslant t < F_d(\infty)$ then there exists a critical temperature T_{c} determined from (3.13) such that ψ_{tr} is stable for $T \geqslant T_{\mathrm{c}}$ and unstable for $0 \leqslant T < T_{\mathrm{c}}$. In the cases where ψ_{tr} is unstable (A.3) possesses two solutions equally spaced about half-filling so p_{tr} has two turning points or ψ_{tr} has two inflections.

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