NAGAOKA FERROMAGNETISM AS A TEST OF
SLAVE-FERMIK AND SLAVE-BOSON APPROACHES

DANIEL BOIES, F. A. JACKSON and A.-M. S. TREMBLAY
Département de Physique and Centre de Recherche en Physique du Solide
Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

Received 17 November 1994

The ferromagnetic to paramagnetic transition in the Nagaoka \((U = \infty)\) limit of the
Hubbard Hamiltonian is used to test the applicability of slave-boson and slave-fermion
(Schwinger boson) functional-integral approaches. Within the slave-fermion formalism
to one-loop order, the ferromagnetic phase is stable to spin-wave, gauge field, and
longitudinal fluctuations over a doping interval that is much too large compared with other
approaches. Furthermore, nonbipartite lattices such as \(hcp\) or \(fcc\) lattices are ferromag-
netic for \(t > 0\) over a wider doping interval than for \(t < 0\), in qualitative disagreement
with all other types of calculations. It is possible to remedy all these defects in order
to reach agreement, at least qualitatively, with previous studies. It suffices to take the
point of view that in the \(U = \infty\) limit it is best to represent the paramagnetic phase as
the mean-field solution of the \textit{slave-boson} representation, and the ferromagnetic phase as
the mean-field solution of the \textit{slave-fermion} representation. The transition between both
phases is taken to occur at the critical hole doping where the ground state energies are
equal. This seems to give the best possible comparison with other approaches, despite the
lack of a variational principle justifying comparisons of energies between slave-fermion
and slave-boson representations. On bipartite lattices, the critical hole density found
analytically by this procedure, \(\delta_c = 1/3\), is identical to the critical density obtained in
the Kotliar–Ruckenstein slave-boson approach. This value of \(\delta_c\) is also close to various
other estimates. Nevertheless, non-bipartite lattices with \(t > 0\) remain ferromagnetic
over a small but finite doping interval, in quantitative disagreement with some other
approaches.

1. Introduction

Approaches based on functional integrals have been developed in the last ten years
to deal analytically with strong electron correlations. These techniques allow simple
mean-field saddle point treatments that provide a useful starting point to discuss
phase diagrams. Although the various functional-integral representations used are
all in principle exact, in practice the mean-field starting points are mostly uncon-
trolled approximations. Loop expansion parameters, such as the inverse number of
fermion or boson flavors \((1/N)\), do give a minimum of mathematical rigor but are
often physically artificial and are not really small enough to justify the expansion.

PACS Nos.: 71.10.+x, 71.27.+a, 74.20.Hi, 75.10.Lp

1001
As an example of the ambiguity surrounding the use of such theories, let us consider the \( U = \infty \) Hubbard model, or equivalently the \( J = 0 \) limit of the \( t-J \) model. As discussed in the next section, there now seems to be general agreement that at zero temperature on bipartite lattices there should be a transition from a ferromagnetic to a paramagnetic state as one dopes with holes away from half-filling (the Nagaoka problem). One should then at least require that functional integral approaches reproduce this result. However, the two approaches used for the \( t-J \) model in general and for this problem in particular give contradictory results. The slave-fermion Schwinger-boson approach,\(^1,^2\) with \( N = 1 \) in a \( 1/N \) expansion, has a ferromagnetic saddle point which remains stable for all dopings, according to Ref. 2. On the contrary, the slave-boson approach,\(^3\) with \( N = 2 \) in a \( 1/N \) expansion,\(^4\) gives a stable paramagnetic saddle point over the same doping range. In fact, one can find in the literature authors who argue in favor of one or the other approach\(^5\) on the basis of various physical arguments or limiting cases. Given the success of the Schwinger-boson approach at half-filling,\(^6\) it is generally agreed\(^7\) that the slave-fermion parameterization is preferable close to half-filling even though there is no quantitative criterion to test its range of applicability. Furthermore, it is known that close to half-filling, the ground state energy obtained by slave-fermion approaches is lower than that obtained within the slave-boson framework, although this is never used as a quantitative criterion for preferring one or the other formulation because of the lack of a variational principle for these saddle-point mean-field theories.

In this paper, we use the Nagaoka problem as a testing ground for slave-fermion and slave-boson representations.\(^8\) A brief view of the literature on the Nagaoka problem is necessary to convince the reader that there is indeed a ferromagnetic-paramagnetic transition at finite hole doping on certain lattices, a task which is performed in the next section. In Sec. 3, the general slave-fermion and slave-boson formalisms are recalled. In Sec. 4, we present our main result, namely that the proper point of view is to combine both slave-fermion and slave-boson approaches: the ferromagnetic state is the saddle-point solution in the slave-fermion representation, whereas the paramagnetic state corresponds to that of the slave-boson representation. Despite the lack of a variational principle, our comparisons with results from other approaches show that it is possible to take the density at which the ground state energies of both saddle points become equal as an estimate of the critical density at which the phases exchange stability. On bipartite lattices, this critical hole concentration is analytically found to be \( \delta_c = 1/3 \), a value independent of dimension. This is precisely the critical hole concentration for a first-order transition found\(^9\) in the \( U = \infty \) limit of the most general Kotliar–Ruckenstein\(^10\) slave-boson approach. In fact, using the slave fermion representation only, instead of both formulations concomitantly, leads to qualitatively wrong results. Indeed, to one loop order, the ferromagnetic phase is stable to spin-wave, constraint gauge field, and longitudinal fluctuations over a much wider range of doping than found by any other approaches. Furthermore, non-bipartite lattices, such as the \( hcp \) or \( fcc \) lattices, are ferromagnetic for \( t > 0 \) over a wider doping interval than for \( t < 0 \),
in qualitative disagreement with all other types of calculations. These one-loop calculations are discussed in the appendices. In the first appendix, we present a slightly different discussion of the usual question of gauge choice\textsuperscript{11} while in the second appendix we investigate, to one-loop order, the effect of fluctuations on the local stability of the ferromagnetic state. Within our approach, this show that there is no continuous transition to other types of magnetic order before equality of the energies suggests a change between ferromagnetic and paramagnetic states. The last appendix is devoted to an alternate formulation of the saddle-point approximation.

2. Brief Review of Results on the Stability of the Nagaoka Ferromagnet

One of the primary motivations for the introduction of the Hubbard model was the study of ferromagnetism. As the short range repulsion $U$ increases, one does find within Hartree–Fock theory a ferromagnetic phase, the so-called Stoner ferromagnet. The stability of this phase has been studied extensively.\textsuperscript{12} Ever since the work of Kanamori,\textsuperscript{13} however, it has been known that short-range $T$-matrix effects would make the transition more difficult by renormalizing the effective repulsion $U$ to a smaller value. Recent Monte Carlo simulations on the two-dimensional model support the view that indeed the ferromagnetic Stoner transition cannot occur.\textsuperscript{14} This conclusion also follows from other recent studies,\textsuperscript{15} including exact results in infinite dimension.\textsuperscript{16}

Given the perturbative nature of the calculations in the Stoner regime, one cannot rule out the possibility of a ferromagnetic transition for arbitrarily large $U$. Indeed, Nagaoka\textsuperscript{17} proved a theorem stipulating that, for one hole,\textsuperscript{18} the ground state in the $U = \infty$ limit is a fully saturated ferromagnet in the following cases (see next section for definition of $t$): for $t > 0$ and $t < 0$ on the sc and bcc (bipartite) lattices and for $t < 0$ on the fcc and hcp lattices. The theorem also states that the saturated ferromagnet is not the ground state for $t > 0$ on the fcc and hcp lattices. The physics of this ferromagnetism is not the competition between potential and kinetic energy as in the Stoner ferromagnet, but rather is a purely kinetic energy effect involving interference of paths. A simplified and generalized proof has recently been given by Tasaki.\textsuperscript{19,20} Unfortunately, Nagaoka’s theorem has no relevance in the thermodynamic limit, hence the question that naturally arises is whether or not the Nagaoka ferromagnet on the appropriate lattices has any stability for a finite hole concentration. This has been the subject of recent debate, especially in the two-dimensional case, as reviewed by Müller–Hartmann et al.\textsuperscript{21} Although we do not pretend to give an exhaustive review of the subject, we summarize some available results below.

The stability of the ferromagnetic phase has been most widely investigated on the two-dimensional square lattice. Most of the arguments against the thermodynamic stability of the Nagaoka state on this lattice come from numerical simulations on finite systems with two\textsuperscript{22} or more\textsuperscript{23} holes, or from a critique of earlier variational studies.\textsuperscript{24} However, one should note the extreme sensitivity to boundary
conditions\textsuperscript{25–29} of the simulations used to question the stability of the Nagaoka ferromagnet. Furthermore, other numerical studies\textsuperscript{35,30–32} do not exclude the possibility of a stable Nagaoka state.

The arguments for the stability of the Nagaoka ferromagnetic come from a variety of approaches. While a number of exact results\textsuperscript{30,33} have gone beyond the one-hole limit without reaching the thermodynamic limit, recent studies\textsuperscript{34} do show that for certain lattices with massive degeneracies, the Nagaoka mechanism can be proven to work at finite density. A number of approximate approaches also indicate the existence of a finite critical hold density (or doping) $\delta_c$, especially in two dimensions. For example, consider variational arguments: for the square lattice Shastry et al.\textsuperscript{35} have found an upper bound $\delta_c = 0.49$ for the stability of the Nagaoka phase. Variational Monte Carlo studies\textsuperscript{36} using Gutzwiller-type wavefunctions yield $\delta_c \approx 0.38$. Variational wavefunctions going beyond the simplest Gutzwiller ones lead Basile and Elser\textsuperscript{37} to $\delta_c = 0.41$ and Linden and Edwards\textsuperscript{38} to $\delta_c = 0.29$. More recent variational and small cluster work by Müller-Hartmann et al.\textsuperscript{21} on this same lattice leads to a critical density which is finite, even if lower ($\delta_c \approx 0.22$). Gutzwiller-type wavefunctions have, however, been criticized especially for two-dimensional systems because they do not account for the large incoherent part in the single-particle spectral weight.\textsuperscript{39} This critique is counterbalanced by other approaches which also point towards the stability of the Nagaoka state: mean-field theory,\textsuperscript{40} slave-bosons\textsuperscript{41} and three different forms of perturbation theory\textsuperscript{42–44} all find a stable Nagaoka ferromagnet over a finite range of doping. High temperature series expansions indicate the same result, $\delta_c = 3/11$ even though they are not completely conclusive.\textsuperscript{45} The smallest value of $\delta_c$ obtained so far is\textsuperscript{44} $\delta_c = 0.17$ and one of the perturbative studies\textsuperscript{43} finds $\delta_c = 1/3$ on a bipartite lattice as in the present work. This same critical density was also found by Möller et al.\textsuperscript{9} using the rotationally invariant version\textsuperscript{46} of the full Kotliar–Ruckenstein\textsuperscript{10} slave-boson approach. In the latter work, the paramagnetic to ferromagnetic transition is first order, as in a very early perturbative study by Ioffe and Larkin.\textsuperscript{42}

In higher dimensions and for non-bipartite lattices there are fewer studies.\textsuperscript{21} The extension to higher dimensions of the single spin flip Gutzwiller wave function yields a vanishing critical density in infinite dimension.\textsuperscript{47} For purposes of comparisons with our results, the critical dopings found for various lattices by Shastry et al.\textsuperscript{35} and by Müller–Hartmann et al.\textsuperscript{21} appear in Table 1. These two groups are the ones which considered the largest number of cases. Their results compare well with those of other authors. Many other results have been obtained, especially for the square lattice, so that more precise values of $\delta_c$ can be found in the references quoted in the above paragraphs.

### 3. Slave-Fermion and Slave-Boson Functional-Integral Representation

In the infinite $U$ limit, the Hubbard Hamiltonian may be written as

$$ H = - \sum_{ij, \sigma} t_{ij}(1 - n_{i, -\sigma}) c^\dagger_{ij} c_{ji}(1 - n_{j, -\sigma}), $$

(1)
Table 1. Critical hole concentration $\delta_c$ (starting from half-filling) at which the Nagaoka ferromagnet becomes unstable. In Shastry et al. a single-spin-flip variational wave function is used. Müller-Hartmann et al. use the same variational wave function. For the square lattice, however, their best estimate from other approaches is given. As discussed in the text, many other estimates exist for the value of $\delta_c$ on this lattice. In the column labeled "present work" we give the value of $\delta_c$ where the paramagnetic and the ferromagnetic phases have equal ground-state energies. We take this as an indication that this is where the transition between ferromagnetic and paramagnetic phase occurs. If only slave-fermions were used, the last column would represent the value of doping at which a continuous instability of the ferromagnetic phase would occur. Question marks indicate results unavailable from the quoted reference.

<table>
<thead>
<tr>
<th>Lattice type</th>
<th>Shastry et al.</th>
<th>Müller-Hartmann et al.</th>
<th>Present work</th>
<th>Present work</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(Continuous)</td>
<td></td>
</tr>
<tr>
<td>Bipartite</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Square</td>
<td>0.49</td>
<td>0.22</td>
<td>1/3</td>
<td>0.7</td>
</tr>
<tr>
<td>Simple cubic</td>
<td>0.32</td>
<td>0.32</td>
<td>1/3</td>
<td>0.69</td>
</tr>
<tr>
<td>bcc</td>
<td>0.32</td>
<td>0.32</td>
<td>1/3</td>
<td>0.75</td>
</tr>
<tr>
<td>Hypercubic</td>
<td>?</td>
<td>$1 / \sqrt{2d \log(d)}$</td>
<td>1/3</td>
<td>?</td>
</tr>
<tr>
<td>Nonbipartite $t &lt; 0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Triangular</td>
<td>1</td>
<td>?</td>
<td>0.43</td>
<td>0.53</td>
</tr>
<tr>
<td>fcc</td>
<td>0.62</td>
<td>1</td>
<td>0.41</td>
<td>0.57</td>
</tr>
<tr>
<td>hcp</td>
<td>?</td>
<td>$\approx 1$</td>
<td>0.41</td>
<td>0.57</td>
</tr>
<tr>
<td>Nonbipartite $t &gt; 0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Triangular</td>
<td>0</td>
<td>?</td>
<td>0.19</td>
<td>0.74</td>
</tr>
<tr>
<td>fcc</td>
<td>0</td>
<td>$\approx 0$</td>
<td>0.22</td>
<td>+ 0.78</td>
</tr>
<tr>
<td>hcp</td>
<td>?</td>
<td>$\approx 0$</td>
<td>0.22</td>
<td>0.78</td>
</tr>
</tbody>
</table>

where $t_{ij}$ is a symmetric matrix whose elements are zero except in the case of nearest-neighbor sites where they are equal to the hopping integral $t$. The occupation number $n_{i,\sigma}$ for electrons of spin $\sigma$ on site $i$ is given, as usual, in terms of creation-annihilation operators by $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$. This three-body Hamiltonian describes the dynamics of holes in the spin background. It is the kinetic energy part of the $t-J$ model. The non-holonomic constraint of no double occupancy can be turned into an holonomic constraint by using either the slave-fermion Schwinger-boson representation, or the slave-boson one. We recall both approaches in turn.

The slave-fermion Schwinger-boson representation exploits the fact that in the singly-occupied subspace, the following replacement preserves the commutation relations

$$ (1 - n_{i,-\sigma}) c_{i,\sigma}^{\dagger} \rightarrow b_{i,\sigma}^{\dagger} f_i. \tag{2} $$

Here, $f_i$ are spinless fermions physically representing the hole degrees of freedom, and $b_{i,\sigma}$ are Schwinger bosons that carry the spin degrees of freedom. The
Hamiltonian (1) then takes the form
\[ H = \sum_{ij, \alpha} t_{ij} f_i^+ b_{i\alpha}^+ b_{j\alpha} f_j. \] (3)

In the physical subspace, there is only one slave-fermion or Schwinger boson per site. In other words, the following constraint has to be satisfied
\[ f_i^+ f_i + \sum_\sigma b_{i\sigma}^+ b_{i\sigma} = 1 \quad (\forall i). \] (4)

Following the standard procedure, the grand partition function \( Z \) in the grandcanonical ensemble can then be written as a functional integral in the coherent-state representation
\[ Z(T, h, \mu, N_s) = \int D\lambda D\Psi^* D\Psi \prod_\sigma D\Phi^* \Phi e^{-S[\Psi, \Phi, \lambda]} \] (5)

with the action \( S = \int_0^\beta d\tau L_{\text{SF}}(\tau) \) and the Lagrangian
\[
L_{\text{SF}}(\tau) = \sum_{ij} \Psi_i^* \left\{ (\partial_\tau - \mu - \lambda_i) \delta_{ij} + t_{ij} \sum_\sigma \Phi_i^* \Phi_j^* \right\} \Psi_i \\
+ \sum_{i\sigma} \Phi_i^* (\partial_\tau - \sigma h - \lambda_i) \Phi_i + \sum_i \lambda_i. \] (6)

The field variables \( \Psi_i \) are Grassmann numbers corresponding to the spinless fermions while the field variables \( \Phi_i \) are complex numbers corresponding to the Schwinger bosons. There is also one purely imaginary field variable \( \lambda_i \) per site coming from the Dirac representation of the delta function which enforces the constraint (4) at each site. An infinitesimal magnetic field \( h \) has also been introduced to break the rotational symmetry. The chemical potential \( \mu \) is adjusted such that the number of spinless fermions per site is \( \delta \). The number of lattice sites will be denoted by \( N_s \).

In the calculation of fluctuations, zero-frequency modes appear when one does not take into account gauge degrees of freedom. This necessitates a detailed discussion, deferred to Appendix A.

In the slave-boson representation, the spin degrees of freedom are carried by the fermions, and the hole degrees of freedom by spinless bosons. The equations corresponding to Eqs. (2)–(6) are
\[ (1 - n_{i, -\sigma}) c_{i\sigma}^+ \rightarrow b_i f_i^+; \] (7)
\[ H = -\sum_{ij, \sigma} t_{ij} f_i^+ b_{i\sigma}^+ b_{j\sigma} f_j; \] (8)
\[ b_i^+ b_i + \sum_\sigma f_i^+ f_i = 1 \quad (\forall i); \] (9)
\[
L_{SB}(\tau) = \sum_{(i,j), \sigma} \Psi_{i\sigma}^* \left\{ \left( \partial_\tau - \mu - e h - \lambda_i \right) \delta_{ij} - t_{ij} \Phi_i^\dagger \Phi_j \right\} \Psi_{i\sigma} \\
+ \sum_i \Phi_i^* (\partial_\tau - \lambda_i) \Phi_i + \sum_i \lambda_i.
\]

(10)

Note that we use the same symbol for fermions and bosons in both representations. The presence or absence of a spin index makes the notation unambiguous. However, different symbols must be used for the chemical potentials \( \mu \) and \( \bar{\mu} \) in the two representations since they are conjugate respectively to \( \delta \) and \( 1 - \delta \).

4. Saddle Point Solutions for the Paramagnetic and Ferromagnetic Phases

As usual in the mean-field approximation, boson variables take a macroscopic value (Bose condensation) and fluctuations in space and imaginary time are neglected. With this type of approach, the mean-field solution to the slave-fermion representation describes a ferromagnetic state, while the mean-field solution to the slave-boson representation has a paramagnetic character. We consider both cases in turn. The gauge choice has to be made before the saddle point solution but, for the time being, we can proceed in the most simple-minded manner: Appendix A shows why this works. Note that the mean-field solutions discussed in the present section can also be obtained from an alternate point of view where the dynamics of both fermions and bosons are treated on an equal footing. This approach, discussed in Appendix C, makes the Bose condensation mechanism more explicit.

4.1. Ferromagnetic phase (slave-fermions)

For the discussion of energies in Sec. 3, one must first choose a thermodynamic potential which depends on the appropriate intensive variables, namely \( T, h, \delta \). This thermodynamic potential is the magnetic analog of the free-energy density, \( g_{SF}(T, h, \delta) = G_{SF}(T, h, \delta, N_\delta)/N_\delta \), which can be obtained from the following Legendre transform

\[
g_{SF}(T, h, \delta) = -\frac{1}{\beta N_\delta} \ln Z_{SF}(T, h, \mu, N_\delta) + \mu \delta,
\]

(11a)

the value of \( \mu \) on the right-hand side being obtained as usual from

\[
\frac{\partial g_{SF}(T, h, \delta)}{\partial \mu} = 0.
\]

(11b)

Evaluating the slave-fermion grand partition function appearing in expression (11a) in the saddle-point approximation, the Schwinger bosons take the mean-field values

\[
\Phi_i^\sigma = \Phi_0^\sigma \delta_{q,0} \quad (\sigma = \pm 1) \quad \lambda_q = \lambda_0 \delta_{q,0}
\]

(12)
where \( q \equiv (q, \omega_n) \) and \( \Phi_0^\sigma \) is real (corresponding to a particular gauge choice, as discussed in Appendix A). The free-energy density is then obtained from the extremum of

\[
g_{\text{SF}}(T, h, \delta; \lambda_0, \Phi_0^\sigma) = -\frac{1}{\beta N_\sigma} \sum_k \ln \left( 1 + e^{-\beta(E(k)-\mu^*)} \right) - \sum_\sigma (\Phi_0^\sigma \lambda_0 + \sigma h \Phi_0^{-\sigma}) + \lambda_0 + \mu \delta \tag{13}
\]

with respect to \( \Phi_0^\sigma \) and \( \lambda_0 \). The renormalized dispersion relation \( E(k) \) is given by

\[
E(k) = \left( \sum_\sigma \Phi_0^\sigma \right) t(k) \tag{14}
\]

where, with unit lattice spacing

\[
t(k) \equiv 2t \sum_{\nu=1}^d \cos k_\nu. \tag{15}
\]

The quantity \( \mu^* \), defined by

\[
\mu^* \equiv \mu + \lambda_0, \tag{16}
\]

plays the role of the spinless-fermion chemical potential. Defining the Fermi-Dirac distribution function by \( f(E(k)) = (e^{\beta(E(k)-\mu^*)} + 1)^{-1} \), the saddle point (extremum) equations then take the form

\[
\frac{\partial g_{\text{SF}}(T, h, \delta; \lambda_0, \Phi_0^\sigma)}{\partial \lambda_0} = \sum_\sigma \Phi_0^\sigma - (1 - \delta) = 0, \tag{17}
\]

\[
\frac{\partial g_{\text{SF}}(T, h, \delta; \lambda_0, \Phi_0^\sigma)}{\partial \Phi_0^\sigma} = 2\Phi_0^\sigma \left( \frac{1}{N_\sigma} \sum_k f(E(k))t(k) - \lambda_0 - \sigma h \right) = 0; \quad (\sigma = \pm 1). \tag{18}
\]

As can be seen from the expression for the free-energy functional (13), \( \lambda_0 \) plays the role of the boson chemical potential. The equation for the slave-fermion chemical potential is obtained from (11b), namely

\[
\frac{\partial g_{\text{SF}}(T, h, \delta, \lambda_0, \Phi_0^\sigma)}{\partial \mu} = -\frac{1}{N_\sigma} \sum_k f(E(k)) + \delta = 0. \tag{19}
\]

The solution of these mean field equations manifestly breaks the rotational symmetry when \( h \to 0 \) since only one boson species can condense at a time. Explicitly, the magnetic order parameter behaves as

\[
\Phi_0^\sigma = (1 - \delta), \quad \Phi_0^{-\sigma} = 0 \quad (h \to 0^*). \tag{20}
\]
This saddle point was chosen because it describes a saturated ferromagnet, as can be seen from the Schwinger-boson expression for the magnetization \( m = \frac{1}{2} \sum_\sigma \sigma \Phi_0^2 \), which in the present context gives \( \lim_{\lambda \to 0^+} m(\lambda) \propto \sigma(1 - \delta) \). Thus, this solution represents a fully-polarized state.

The previous results were first obtained for the square lattice in the Hamiltonian representation.\(^2\) Even though there is in this case a solution to the gap equation over the whole doping range \( 0 \leq \delta \leq 1 \), ferromagnetism on the square lattice is actually unstable to phase separation before \( \delta \) reaches unity, a fact that, to our knowledge, had yet to be pointed out. One can check that the chemical potential following from Eq. (16) leads to a divergent compressibility of the spinless fermion liquid at a finite value \( \delta_c \) in both one and two dimensions. More explicitly, defining the inverse compressibility by

\[
\kappa^{-1} = |\delta|^2 \left( \frac{d\mu}{d\delta} \right) \equiv |\delta|^2 \left( \frac{1 + F_0^*}{N(\mu^*)} \right)
\]  

(21)

with \( N(E) \) the renormalized spinless-fermion (hole) density of states, we find the following expression for the Landau parameter \( F_0^* \)

\[
F_0^* = -\frac{2\mu^* N(\mu^*)}{1 - \delta}.
\]

(22)

The compressibility thus diverges when

\[
1 - \delta - 2\mu^* N(\mu^*) = 0.
\]

(23)

Even though our approach fails in one dimension, we quote the results since they can be obtained analytically. Specifically, the last equality takes the form

\[
1 - \delta + \frac{2}{\pi \tan(\pi \delta)} = 0.
\]

(24)

This leads to a critical hole of \( \delta_c \approx 0.66 \) (\( d = 1 \)). The corresponding value for the two dimensional square lattice is obtained numerically as \( \delta_c \approx 0.7 \) (\( d = 2 \)). The appearance of such a density-wave instability implies a phase separation of the spinless fermion liquid. This tendency of the holes to form a uniform density wave stems from the fact that the effective hole–hole interaction becomes attractive at \( \delta = 0.5 \). Indeed, as seen from expression (22), the Landau parameter \( F_0^* \) becomes negative at this value of \( \delta \) because the effective chemical potential \( \mu^* \) becomes positive for a half-filled spinless-fermion band

\[
F_0^* > 0, \quad 0 \leq \delta < 0.5
\]

\[
F_0^* < 0, \quad 0.5 < \delta \leq 1.
\]

However, it should be noted that nothing peculiar happens to the magnetic order parameter at the concentration \( \delta_c \) found above.
The above instability also reveals itself to next order in the loop expansion, that is when Gaussian fluctuations are taken into account. For all the lattices we studied, no new instability at finite wave vector occurs to this order, as discussed in Appendix B. The doping at which the ferromagnetic phase become unstable, to one-loop order, is the same as the one where the above compressibility instability occurs. This doping appears in the last column of Table 1. It is not only too large compared with other approaches, but also in qualitative disagreement with all other calculations for non-bipartite lattices. Indeed, we find that these lattices are stable for a wider range of dopings for \( t > 0 \) than for \( t < 0 \), in qualitative disagreement with all other types of calculations, including what can be inferred from the instabilities found by Nagaoka for one hole and \( t > 0 \). To find a physically correct result, one must go beyond the slave-fermion approach and consider also the slave-boson approach to allow an estimate of the energy of the paramagnetic phase and the possibility of an exchange of stability between the two phases.

### 4.2. Paramagnetic phase (slave-bosons)

The thermodynamic potential \( g_{SB}(T, h, \delta) = G_{SB}(T, h, \delta, N_s)/N_s \), in the slave-boson representation, is obtained from the Legendre transform

\[
g_{SB}(T, h, \delta) = -\frac{1}{\beta N_s} \ln Z_{SB}(T, h, \mu, N_s) + \mu(1 - \delta) \tag{25a}
\]

the value of \( \mu \) being chosen so that

\[
\frac{\partial g_{SB}(T, h, \delta)}{\partial \mu} = 0. \tag{25b}
\]

In the saddle-point approximation for the partition function, the bosons take the mean-field value

\[
\Phi_q = \Phi_0 \delta_q, 0 \quad (\sigma = \pm 1), \quad \lambda_q = \lambda_0 \delta_q, 0 \tag{26}
\]

where \( q \equiv (q, \omega_n) \) and \( \Phi_0 \) is real (corresponding to the radial gauge choice, as discussed in Appendix A). We use overbars to distinguish slave-boson from slave-fermion mean-fields. The free-energy density is then obtained from the minimization of

\[
g_{SB}(T, 0, \delta; \lambda_0, \Phi_0) = -\frac{2}{\beta N_s} \sum_{k} \ln(1 + e^{-\beta(E(k) - \mu)} - \bar{\Phi}_0^2 \lambda_0 + \lambda_0 + \mu(1 - \delta). \tag{27}
\]

The factor of two in front of the logarithm comes from the sum over spins. The magnetic field is taken to be zero from the start since the mean-field solution does not break rotational invariance. The renormalized dispersion \( E(k) \) is now given in this gauge by

\[
E(k) = -(\bar{\Phi}_0^2) t(k). \tag{28}
\]
Here, the quality $\bar{\mu}^*$ defined by
\[
\bar{\mu}^* \equiv \bar{\mu} + \bar{\lambda}_0
\] (29)
plays the role of the quasi-electron chemical potential instead of the hole chemical potential. The saddle point equations then read
\[
\frac{\partial g_{SB}(T, 0, \delta; \bar{\lambda}_0, \bar{\Phi}_0)}{\partial \bar{\lambda}_0} = -\bar{\Phi}_0^2 + \delta = 0,
\] (30)
\[
\frac{\partial g_{SB}(T, 0, \delta; \bar{\lambda}_0, \bar{\Phi}_0)}{\partial \bar{\Phi}_0} = 2\bar{\Phi}_0 \left( -\frac{2}{N_e} \sum_k f(E(k))t(k) - \bar{\lambda}_0 \right) = 0.
\] (31)
As seen from the expression for the free-energy functional (27), $\bar{\lambda}_0$ act as the boson chemical potential. The equation for the chemical potential is obtained from
\[
\frac{\partial g_{SB}(T, 0, \delta; \bar{\lambda}_0, \bar{\Phi}_0)}{\partial \bar{\mu}} = -\frac{2}{N_e} \sum_k f(E(k)) + (1 - \delta) = 0.
\] (32)
The solution of these mean field equations describes a paramagnetic state with a renormalized mass. Contrary to the ferromagnetic state, this state does not have a charge instability. Indeed, the electron compressibility is proportional to
\[
\frac{\partial \bar{\mu}}{\partial (1 - \delta)} = \frac{1}{2N(\bar{\mu}^*)},
\] (33)
which is always positive.

4.3. Transition between slave-fermion and slave-boson representations

In addition to possible second-order instabilities of the ferromagnetic state, we must take into account the possibility of a first-order transition. Such a transition can occur in Landau theories for a vector order parameter when the sixth order terms are taken into account. As mentioned in the introduction, we cannot strictly speaking use energy considerations as a criterion for a first-order phase transition because the slave-fermion and slave-boson mean-field theories are not based on a variational principle. Nevertheless, comparisons with the results from other approaches will allow us to check that free energies can serve as an indication of the critical hole density at which the phases exchange their stability. We will refrain from calling this a first-order transition, but we point out that in the case of bipartite lattices, the critical hole concentration which we will find analytically is precisely the same as the one where Möller et al. do find a first-order transition within a single slave-boson scheme, namely the rotationally invariant version of the Kotliar–Ruckenstein slave-bosons. In this section, we closely follow the approach used by Möller et al. The equality of free-energies takes the form
\[
g_{SF}(T, 0, \delta) = g_{SB}(T, 0, \delta).
\]
Working at zero temperature and substituting the optimization Eqs. (17)-(19) in the expression (13) for the slave-fermion energy in the ferromagnetic state, we find that this thermodynamic potential reduces to the ground-state energy

$$gSF(0, 0, \delta) = \frac{1}{N_s} \sum_k E(k) f_{\beta=\infty}(E(k)).$$  \hspace{1cm} (34)

Changing to an integration over energy $\epsilon$, this may be rewritten

$$gSF(0, 0, \delta) = (1 - \delta) \int_{\min(t(k))}^{\mu^*/(1-\delta)} d\epsilon N(\epsilon).$$  \hspace{1cm} (35)

Similarly, the paramagnetic state described by the slave-boson representation has a ground state energy given by

$$gSB(0, 0, \delta) = \frac{2}{N_s} \sum_k \tilde{E}(k) f_{\beta=\infty}(\tilde{E}(k)) = -2\delta \int_{-\mu^*/\delta}^{\max(t(k))} d\epsilon N(\epsilon).$$  \hspace{1cm} (36)

The ground state energies of the paramagnetic and ferromagnetic states are thus equal when the condition $gSB = gSF$ is satisfied for a given $\delta$. In the general case, we have checked this condition numerically. The results for the value of $\delta$ at which the transition occurs appear in the second to last column of Table I. Clearly, these values are in qualitative agreement with those obtained through other approaches. The only real disagreements are for bipartite lattices in infinite dimension and for non-bipartite lattices with $t > 0$ which we find to be stable over a finite doping range while Nagaoka's theorem suggests $\delta_c = 0$.

For bipartite lattices, such as the square and simple cubic lattice, the value $\delta_c = 1/3$ obtained in the work of Ref. 9 can be analytically confirmed. Indeed, for these lattices we have particle–hole symmetry so that $N(\epsilon) = N(-\epsilon)$ and $W \equiv \max(t(k)) = -\min(t(k))$. The condition for the transition then becomes

$$(1 - \delta) \int_{-W}^{\mu^*/(1-\delta)} d\epsilon N(\epsilon) = 2\delta \int_{-W}^{\mu^*/\delta} d\epsilon N(\epsilon).$$  \hspace{1cm} (37)

This condition is satisfied for $\delta = \delta_c \equiv 1/3$ since both the prefactors and the integration limits of the two integrals above become equal. The latter equality follows from the equations determining the chemical potential, (16) and (29), which are written as

$$\frac{1}{N_s} \sum_k f_{\beta=\infty}(E(k)) = \delta_c = \int_{-W}^{\mu^*/(1-\delta_c)} d\epsilon N(\epsilon) = 1/3$$  \hspace{1cm} (38)

and

$$\frac{2}{N_s} \sum_k f_{\beta=\infty}(\tilde{E}(k)) = 1 - \delta_c = 2 \int_{-\mu^*/\delta_c}^{W} d\epsilon N(\epsilon) = 2/3$$  \hspace{1cm} (39)
implying that at $\delta = \delta_c = 1/3$, we have the equality of the integration limits

$$\frac{\mu^*}{\delta_c} = \frac{\mu^*}{(1 - \delta_c)}.$$  \hspace{1cm} (40)

5. Discussion and Conclusions

Slave-fermion and slave-boson representations of the $U = \infty$ Hubbard model are both exact. However, saddle-point solutions are approximate, and in the literature one finds authors using either one or the other approach, some arguing on physical grounds that one of these approaches is better. In this paper, the comparisons with numerous results on the Nagaoka ferromagnetic to paramagnetic transition have been used as a benchmark to show that in fact to describe the possible phases of the model and to estimate their range of stability, ground state energy comparisons between both representations are a useful guide, despite the lack of a variational theorem. In the Nagaoka problem, the ferromagnetic state is more naturally represented by a slave-fermion saddle point whereas the paramagnetic state has a simple representation as a slave-boson saddle point. The slave-fermion ferromagnetic saddle-point by itself becomes unstable only through a continuous transition at a critical concentration given by the last column of Table 1. Comparisons with the results of other approaches in the second and third columns clearly show that this estimate of the stability of the ferromagnetic phase gives results which are both quantitatively and qualitatively wrong.

Taking instead the equality of ground state energies as an indication of an exchange of stability of the ferromagnetic and paramagnetic phases, we estimated the non-trivial dependence of the critical doping on lattice and, for non-bipartite lattices, on the sign of $t$. As is clear from the second to last column of Table 1, despite the lack of a variational principle, comparisons of ground state energies between the slave-fermion and slave-boson representation do seem meaningful for this problem. Nevertheless, we refrain from calling the concentration where energies become equal a point of first-order transition. For bipartite lattices we find analytically that at low doping the ferromagnetic slave-fermion saddle point has the lowest ground state energy, and that starting at a critical doping $\delta_c = 1/3$ it is the slave-boson paramagnetic state which wins. This critical doping is exactly the same as that of the first-order phase transition found in the Kotliar–Ruckenstein slave-boson approach.\(^9\) It is independent of dimension and is very close to the estimates obtained from numerous other approaches, except in the case of infinite dimension. The change from a slave-fermion to a slave-boson representation with doping is consistent with recent numerical simulations\(^{26,48}\) which show that exact correlation functions of the $U = \infty$ Hubbard model on a square lattice do evolve from slave-fermion like to slave-boson like with doping, the crossover occurring around the above critical value. We always found the exchange of stability of the phases to occur before the ferromagnet becomes unstable to local Gaussian fluctuations,
whether they are spin waves, amplitude or constraint gauge-field fluctuations. A softening of these fluctuations would lead to a continuous transition. Here, these fluctuations are consistent with the fact that the ferromagnetic metastability region terminates at a longitudinal $q = 0$, or slave-fermion compressibility instability.

The most obvious inadequacy of slave-fermion slave-boson mean-field theories, as revealed by Table 1, is for the case of non-bipartite lattices with $t > 0$ where both Nagaoka’s theorem and variational studies suggest a vanishing stability region contrary to the present approach which finds a small but non-vanishing critical hole density.

If comparisons of free energies are indeed truly meaningful, the estimate of the critical doping for the transition would be improved by including one-loop corrections in the calculation of the free energy itself. The critical hole concentration should then become more dependent on lattice and dimension, as in other approaches.

Note Added in Proof

The stability of the Nagaoka state to the formation of a slave-fermion Schwinger-boson bound state (S. K. Sarker, Phys. Rev. B46, 8617 (1992)) should also be considered in the present context.

Acknowledgments

We are particularly grateful to A. Ruckenstein for suggesting this problem and for many useful discussion. We also thank T. Li and R. Shankar for useful discussions. We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC), the Fonds pour la formation de chercheurs et l’aide à la recherche from the Government of Québec (FCAR) and (A.-M.S.T.) the Canadian Institute of Advanced Research (CIAR) and the Killam foundation.

Appendix A

Constraint and gauge degrees of freedom

In both slave-fermion and slave-boson representations on a lattice of $N_s$ sites, there are $N_s$ gauge degrees of freedom. We discuss only the slave-fermion representation. The slave-boson case follows trivially. In the slave-fermion representation, the $N_s$ gauge degrees of freedom correspond to the invariance of the Hamiltonian under the time-independent transformation

$$b_{j\sigma} \rightarrow e^{i\theta_j} b_{j\sigma},$$

$$f_j \rightarrow e^{i\theta_j} f_j.$$  \hspace{1cm} (A1)

The Lagrangian has the same invariance with respect to the corresponding variables. The conservation law which corresponds, by Noether’s theorem, to this gauge
symmetry is the conservation of the total number of slave-fermions plus Schwinger bosons, Eq. (4), on each site.

In the one-loop calculation of fluctuations using the functional-integral approach, we have checked that there appears a branch of excitations which satisfies $\omega(q) \equiv 0$ for all values of $q$. Since there are $N_s$ possible values of $q$, we count $N_s$ degrees of freedom with zero frequency, corresponding to the $N_s$ possible phases $\theta_i$ in Eq. (A1). Following Fadeev and Popov, the gauge degrees of freedom $\theta_i$ must not be integrated over. In other words, this spurious branch of excitation must be removed by fixing the gauge.

It is easiest to fix the gauge by first extending the gauge freedom to time-dependent transformations, as done by Read and Newns. This is done as follows. We have already noted that there are $N_s$ variables $\lambda_i$, that is one at each site. Letting this field depend on imaginary time introduces $N_s(N_r - 1)$ new redundant degrees of freedom, $N_r$ being the number of time slices (which ultimately goes to infinity). In total, there are thus now $N_sN_r$ variables that should not be integrated over: $N_s$ variables $\theta_i$ and $N_s(N_r - 1)$ extra variables $\lambda_i(\tau)$. These variables all behave as gauge degrees of freedom, as can be seen from the fact that the slave-fermion action is now invariant under the following transformation,

\[ \Phi_{i\tau}(\tau) \rightarrow e^{i\theta_i(\tau)} \Phi_{i\tau}(\tau), \]

\[ \Psi_i(\tau) \rightarrow e^{i\theta_i(\tau)} \Psi_i(\tau), \]

\[ \lambda_i(\tau) \rightarrow \lambda_i(\tau) + \frac{i}{\partial \tau} \theta_i(\tau). \]  
(A2)

This can be checked by substituting in Eq. (6) and using the periodic boundary conditions in imaginary time for the phase $\theta_i(\tau)$. This means that we can now fix the gauge by fixing either $\theta_i(\tau)$ or $\lambda_i(\tau)$. Choosing $\theta_i(\tau)$ in such a way that the field $\Phi_i(\tau)$ is real fixes the $N_sN_r$ gauge degrees of freedom. This choice is known as the radial gauge. The Jacobian associated with this choice of coordinates does not influence the saddle point nor the one-loop corrections, as discussed by Read and Newns. The gauge choice must be done before looking for the saddle point solution. Working in the radial gauge allow us to investigate real saddle points in the main body of the text.

Appendix B

**Stability of the ferromagnetic phase to one-loop order**

To investigate the local stability of the ferromagnetic state, we consider bosonic fluctuations of the type

\[ \Phi^\sigma_q = \Phi^\sigma_q(\delta_q, \theta) + \delta \Phi^\sigma_q, \quad \lambda_q = \lambda_0 \delta_q + \delta \lambda_q, \]  
(B1)

the rotational symmetry being broken as follows, $\Phi^I_q = 0$ and $\Phi^I_0 = \sqrt{(1 - \delta)}$. Our goal is to determine the excitation spectrum which is expected to include
massive longitudinal and gauge modes as well as a massless mode corresponding to the broken rotational symmetry. (In the radial gauge described in the previous appendix, the gauge mode corresponds to the fluctuations of the phase of the spin-up boson while the spin wave corresponds to fluctuations of the spin-down bosons whose phase represents the relative phase of spin-up and spin-down bosons.) We want to then check for softening of these modes.

To find the action to one loop order, one formally performs the trace over fermion variables exactly. One is left with a purely bosonic action. Introducing the fluctuating fields $(B1)$ in this effective action and expanding to quadratic order we get for the partition function

$$Z_{SF} = e^{-S_0} \int D\lambda^* D\lambda \prod_q D\Phi^* D\Phi e^{-\delta S_{SF}},$$  \hspace{1cm} (B2)

where $S_0$ is the mean field action. The Gaussian action splits into two separate parts $\delta S = S_1 + S_{\lambda \lambda}$, the first of these being given by an action for the down bosons

$$S_1 = \sum_q \delta \Phi^*_q (-i\omega_\nu (1 - \delta) + \omega_{sw}(q)) \delta \Phi_q,$$  \hspace{1cm} (B3)

where $q$ stands for both wave vector and Matsubara frequency $\omega_\nu$, and

$$\omega_{sw}(q) = \frac{1}{N_x} \sum_k \{E(k + q) - E(k)\} f(k).$$  \hspace{1cm} (B4)

As expected from the fact that fluctuations of the down bosons are responsible for restoring rotational symmetry, this last result simply is the spin-wave dispersion relation. It is trivial to see that at small wave number $q$ the frequency scales as $q^2$ as expected for ferromagnet. In one dimension, we obtain

$$\omega_{sw}(q) = \Delta^* \sin(\pi \delta)(1 - \cos q) \quad (d = 1)$$  \hspace{1cm} (B5)

with $\Delta^* = (1 - \delta)z$. We found for all lattices in Table 1 that along all the main symmetry directions illustrated in Fig. 1, the corresponding dispersion relation is positive for all hole concentrations, a fact that eliminates one possible destabilization mechanism, namely spin-wave softening. Such a conclusion contrasts with the results obtained through variational-wave-function calculations$^{39}$ which invoke a spin-wave softening destabilization at $k_f$. It must be noted that, in the present approximation, fluctuations of the down-boson field are unconstrained. A coupling of this field with the other two would occur only at two-loop order.

The second part of the Gaussian action involves the coupling between the real field $\Phi_1(\tau)$ for up-spins and the purely imaginary gauge field $\lambda_1(\tau)$. The explicit form of the action involving these field is

$$S_{\lambda \lambda} = \sum_q \langle \delta \Phi^*_q \delta \lambda^*_q \rangle \left( \begin{array}{cc} D_{\Phi \Phi}(q) & D_{\Phi \lambda}(q) \\ -D_{\Phi \lambda}(q) & D_{\lambda \lambda}(q) \end{array} \right) \left( \begin{array}{c} \delta \Phi_q \\ \delta \lambda_q \end{array} \right).$$  \hspace{1cm} (B6)
Fig. 1. Points in the reciprocal space of the lattices of Table 1 where the stability of the Nagaoka ferromagnet was tested to one-loop order. Figures are from Ref. 50. The stability was always found to occur at $q = 0$ first and for larger doping concentrations than the first-order transition.
We must be very careful to only integrate over the $N_s N_r$ independent Fourier components that $\delta \Phi_q^\dagger$ and $\delta \lambda_q$ each have. In other words, there are only half as many independent Fourier components as usual because there fields are respectively real and imaginary, leading to $\delta \Phi_q^\dagger = \delta \Phi_q^* \dagger$ and $\delta \lambda_q^* = - \delta \lambda_{-q}$. In practice, we take into account the correct number of independent Fourier components by integrating over only half of the possible wave-vector components in say the $x$ direction.

The matrix elements appearing in the above action (B6) are found to be

$$D_{\Phi \Phi}(q) = -i \omega_\nu (1 - \delta) + \omega_{\text{sw}}(q) - \frac{1}{2} \chi_2(q),$$

$$D_{\Phi \lambda}(q) = (1 - \delta) - \frac{1}{2} \chi_1(q),$$

$$D_{\lambda \lambda}(q) = \frac{1}{2} \chi_0(q),$$

(B7)

where we defined the functions

$$\chi_n(q) = -\frac{1}{N_s} \sum_k \frac{f(k+q) - f(k)}{E(k+q) - E(k) - i \omega_\nu} \left\{ E(k+q) + E(k) \right\}^n.$$

(B8)

One cannot rely on the positivity of the real parts of the matrix eigenvalues to infer the stability of the saddle point because the matrix in the action (B6) is non-Hermitian. In such a case, the result depends on the order of integration. In fact, it is easy to show that

$$D_{\Phi \Phi}(0, 0) = -2 \mu^* N \langle \mu^* \rangle \leq 0,$$

(B9)

leading to a divergence if we were to integrate over the $\delta \Phi_q^\dagger$ field in the first place. As first discussed by Ramakrishnan, we must first integrate on the gauge field $\delta \lambda_q$, an operation that should enforce the constraint to one-loop order. The stability criterion then becomes

$$D_{\lambda \lambda}(q, 0) \geq 0,$$

(B10)

$$\Delta(q, 0) = [D_{\Phi \Phi}(q, 0)D_{\lambda \lambda}(q, 0) + D_{\Phi \lambda}^2(q, 0)] \geq 0.$$

The first of these condition is automatically satisfied since the Lindhard function is always positive. A numerical calculation of the inverse correlation function

$$\langle \delta \Phi_q^\dagger \delta \Phi_q^* \rangle^{-1} = \frac{\Delta(q, 0)}{D_{\lambda \lambda}(q, 0)},$$

(B11)

along high symmetry directions in the Brillouin zone reveals that the $q = 0$ mode is the one which, for the lattices of Fig. 1, first becomes negative as the hole doping is increased from zero. Figure 2 illustrates this for two high symmetry directions on the square lattice. The critical concentration $\delta_c$ at which this happens is identical
Fig. 2. The inverse correlation function \((\delta \Phi^\dagger_q \delta \Phi^\dagger_q)^{-1} = \frac{\Delta(q_\delta)}{D_{\Delta,1}(q_\delta)}\) is plotted as a function of hole doping for selected \(q\) values along two high symmetry directions of the square lattice: a) along the diagonal, \(q_y = q_x\); (b) along the zone edge \(q_y = \pi\). Starting from small dopings, it is the \(q = 0\) correlation function which first becomes negative.

To the one found at the saddle point level by looking at the positivity of the hole compressibility. In fact, one can demonstrate explicitly that the slave-fermion compressibility Eqs. (20) and (21) and the \(q = 0\) limit of the zero-frequency longitudinal
susceptibility are proportional since
\[
\frac{\Delta(0)}{D_{\lambda\lambda}(0)} = \frac{(1 - \delta)(1 - \delta - 2\mu^* D(\mu^*))}{D(\mu^*)} = \left(\frac{1 - \delta}{\delta}\right)^2 \kappa^{-1}.
\]

(B12)

In summary, the one-loop calculation reveals that the system is locally stable to spin-wave, longitudinal, and gauge-field fluctuations of all possible wave-vectors, until an instability in the longitudinal susceptibility occurs at \(q = 0\). This corresponds to the compressibility of the holes becoming negative. For the square lattice it occurs at a critical hole concentration about twice that at which the first-order phase transition occurs. The values of this critical doping for the various lattices appear in the last column of Table 1. This defines the metastability region of the ferromagnetic phase.

Appendix C

Finite-temperature saddle-point solutions

In this appendix we outline a fermion–boson decoupling scheme which allows us to treat both fermions and bosons on the same footing. This method applies equally well to slave-fermions and slave-bosons formulations of the infinite \(U\) Hubbard model. For definiteness, let us consider the case of slave-fermions. The Lagrangian (6) involves a fermion–boson interaction. In some sense, the saddle point approximation applied to the Schwinger-boson fields represents a way of decoupling fermions and bosons in a mean-field way. Here, instead of keeping only the uniform component of the bosonic field and loosing the Schwinger boson’s dynamics, we perform this decoupling systematically at finite temperature through a Hubbard-Stratonovich transformation. More specifically, we use the identity
\[
e^{-2 \sum_{\alpha} (A_{\alpha}^* B_{\alpha} + h.c.)} = \int \int D\xi^* D\zeta e^{-\sum_{\alpha} \left( \xi_{\alpha}^* \xi_{\alpha} + \zeta_{\alpha}^* (B_{\alpha} - A_{\alpha}) + \zeta_{\alpha} (B_{\alpha}^* - A_{\alpha}^*) \right)} 
\times \int \int D\xi^* D\zeta e^{-\sum_{\alpha} \left( \xi_{\alpha}^* \zeta_{\alpha} - \zeta_{\alpha}^* (B_{\alpha} + A_{\alpha}) - \xi_{\alpha} (B_{\alpha}^* + A_{\alpha}^*) \right)},
\]

where \(A\) and \(B\) are commuting operators while \(\xi\) and \(\zeta\) are complex bosonic fields.

Again, one starts with the partition function written as a coherent state functional integral. Using the above identity, the Hamiltonian part of the argument of the functional integral can be expressed as
\[
e^{i \sum_{\langle i, j \rangle} \cdot \oint d\tau (A_{ij}^* B_{ij} + h.c.)}
\]
\[
= \int \int D\xi^* D\zeta e^{\sum_{\langle i, j \rangle} \cdot \oint d\tau \left( -\xi_{ij}^* \xi_{ij} + \sqrt{3} \xi_{ij}^* (A_{ij} - B_{ij}) + \sqrt{3} \xi_{ij} (A_{ij}^* - B_{ij}^*) \right)}
\times \int \int D\xi^* D\zeta e^{\sum_{\langle i, j \rangle} \cdot \oint d\tau \left( -\xi_{ij}^* \xi_{ij} + \sqrt{3} \xi_{ij}^* (A_{ij} + B_{ij}) + \sqrt{3} \xi_{ij} (A_{ij}^* + B_{ij}^*) \right)}
\]
where the bosonic link variables $A_{ij}(\tau) = \phi^{*}_i(\tau)\psi_i(\tau)$ and $B^{\sigma}_{ij}(\tau) = \phi^{*}_{i\sigma}(\tau)\phi^{\sigma}_j(\tau)$ have been defined. Note that in the above integral, the time dependencies have been omitted to simplify the notation. Also, the integration measures take the form $D\xi^* D\xi = \prod_{(i,j)} \frac{d\xi^*_{ij} d\xi_{ij}}{2\pi i}$ (and similarly for $\zeta$), where $(i, j)$ denotes sums or products over nearest-neighbor links. The integration over spinless fermions and Schwinger bosons then becomes trivial since both fields appear quadratically. After these two Gaussian integrals are done, we are left with an effective action that only involves the bosonic Hubbard-Stratonovitch fields $\xi$ and $\zeta$. In the saddle-point approximation, these fields are assumed to be uniform in space and imaginary time.

The effective free-energy functional then takes the form

$$F_0(T, h, \mu, N_s) = zt \sum_{\sigma} \alpha^{\sigma}_0 \beta^{\sigma}_0 - \frac{1}{N_s\beta} \sum_k \log \left( 1 + e^{-\beta((-\sum_{\sigma} \alpha^{\sigma}_0)(-\lambda_0 - \mu))} \right)$$

$$+ \frac{1}{N_s\beta} \sum_{k\sigma} \log \left( 1 - e^{-\beta((\beta^{\sigma}_0 t(k) - \lambda_0 - \sigma h))} \right) + \lambda_0$$

where $z$ is the number of nearest neighbors, $t(k)$ is the dispersion relation and $h$ is an external magnetic field introduced to break the rotational symmetry. The order parameters $\alpha^{\sigma}_0 = \frac{1}{\sqrt{2\pi}}(\xi^{\sigma}_0 + i\zeta^{\sigma}_0)$ and $\beta^{\sigma}_0 = \frac{1}{\sqrt{2\pi}}(\xi^{\sigma}_0 - i\zeta^{\sigma}_0)$ have been defined in terms of the saddle-point values of the Hubbard-Stratonovitch fields $\xi^{\sigma}_0$ and $\zeta^{\sigma}_0$. These are both real since we are again using the radial gauge (Appendix A). In this free-energy functional, bosons and fermions are clearly treated on equal footing. Minimizing this functional leads to the five saddle-point equations:

$$\frac{\partial F_0}{\partial \lambda_0} = \frac{1}{N_s} \sum_k f(k) + \frac{1}{N_s} \sum_{k\sigma} n_\sigma(k) - 1 = 0,$$

$$\frac{\partial F_0}{\partial \alpha^{\sigma}_0} = zt \beta^{\sigma}_0 - \frac{1}{N_s} \sum_k t(k) f(k) = 0 \quad (\sigma = \uparrow, \downarrow),$$

$$\frac{\partial F_0}{\partial \beta^{\sigma}_0} = zt \alpha^{\sigma}_0 + \frac{1}{N_s} \sum_{k\sigma} t(k) n_\sigma(k) = 0 \quad (\sigma = \uparrow, \downarrow),$$

where

$$n_\sigma(k) = \frac{1}{e^{\beta((\beta^{\sigma}_0 t(k) - \lambda_0 - \sigma h))} - 1}$$

and

$$f(k) = \frac{1}{e^{\beta((-\sum_\sigma \alpha^{\sigma}_0)(-\lambda_0 - \mu))} + 1}$$

are respectively the renormalized Bose-Einstein and Fermi occupation factors. Similar saddle-point equations have been obtained in Ref. 2, using Hamiltonian methods. We notice from these occupation factors that $\lambda_0$ act as the chemical potential of the bosons while $\mu + \lambda_0$ is the effective chemical potential of the quasi-holes. The
first of these saddle-point equations is the finite-temperature version of (17) which expresses the mean-field thermal average of the constraint. This mean-field theory exhibits spin-charge separation at the one-particle level for it leads to different effective bandwidths for the spinless fermions and for up and down bosons. More specifically, for hypercubic lattices we have respectively $|2zt \sum_\sigma \alpha_\sigma^0|$ and $|2zt \beta_0^0|$.

We shall now show that as $T \to 0$, we recover the results of Sec. 4. As temperature is lowered, Bose condensation occurs only for bosons whose spin points in the direction of the symmetry-breaking field $\theta$. If, for example, the magnetic field is taken to be positive, it follows from the properties of the Bose–Einstein distribution that the up bosons's chemical potential reaches the bottom of the band from below \( \lim_{T \to 0} \lambda_0(T) = \beta_0^0 \hat{t}(0) + h = z t \beta_0^0 - 0^+ \) whereas for the down bosons, the argument of the Bose factor tends to a positive limit \( \lim_{T \to 0} (\beta_0^0 \hat{t}(0) - \lambda_0(T) + h) = 2h \). Consequently, only the up bosons condense. In the zero temperature limit, the saddle-point equations give

\[
\alpha_0^0 = \delta_{\sigma, \uparrow} \alpha_0^\uparrow = \frac{1}{zt N_s} \sum_k t(k) n_k(k) \left( \lim_{T \to 0} \lim_{h \to 0^+} \right) \left( \frac{T}{h} \right) = -\delta
\]

since the band-bottom state $k = 0$ is macroscopically occupied. We also have

\[
\beta_0^0 = \frac{1}{zt N_s} \sum_k t(k) f(k) \quad (\sigma = \uparrow, \downarrow).
\]

Substituting this equation in the above expression for $\lambda_0(T)$ at Bose condensation, we find the same result as in Sec. 4, namely \( \lim_{T \to 0} \lim_{h \to 0^+} \lambda_0(T) = \frac{1}{N_s} \sum_k t(k) f(k) \).

Therefore, Bose condensation occurs when the effective boson chemical potential equals the mean kinetic energy of the spinless fermions.

References

18. As is well-known, it suffices to consider the case of hole doping away from half-filling since the case of electron doping may be obtained from a particle-hole transformation which maps the electron problem to the hole problem with the opposite sign for t. For bipartite lattices, only one sign of t needs to be considered because of the additional particle-hole symmetry.
20. For a review of exact results, see also E. H. Lieb in Advances in Dynamical Systems and Quantum Physics, Proceedings of a conference held in Capri, May 1993 (World Scientific, Singapore, 1993).