Sea-Boson Analysis of the Infinite-U Hubbard Model

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November 13, 2018

Abstract

By expanding the projection operator in powers of the density fluctuations, we conjecture a Hamiltonian purely quadratic in the sea-bosons that reproduces the right spin and charge velocities and exponent for the $U = \infty$ case in one dimension known from the work of Schulz. Then we argue that by simply promoting wavenumbers to wave vectors we are able to study the two dimensional case. We find that the quasiparticle residue takes a value $Z_F = 0.79$ close to half-filling where it is the smallest. This is in exact agreement with the prediction by Castro-Neto and Fradkin nearly ten years ago. We also compute the magnetic susceptibility and find that it diverges close to half-filling consistent with Nagakoka’s theorem.

1 Introduction

The large-U Hubbard Model or the t-J model and its variants have been the subject of active study ever since its importance to understanding cuprates has been realised. For a review see the article by Dagotto[1]. The slave-boson/fermion approach that naturally takes into account the feature of spin-charge separation has been employed by various authors[2] (for some recent references we note the work of Balents et.al.[3] and Wang[4]). Recently the phase diagram of the t-J-V model has been found by using a thorough but tedious procedure of linked cluster expansion by Zheng et.al.[5]. High temperature expansions have been used to study the t-J-V models and the t-J models by various groups[6][7]. The cluster dynamical mean-field approach has been employed by Jarrell et.al.[8] to compute the phase diagram of the Hubbard model. We wish to complement their study and others like them through a simpler analytical approach. The case of the infinite U Hubbard model has been considered by Nagaoka who shows that the ground state is a ferromagnet[9] for a single hole in
an otherwise half-filled band. Shastry, Krishnamurthy and Anderson [10] have shown that this ground state is unstable for large enough hole concentration. Gutzwiller projected variational wavefunctions[11] have also been used to study the t-J model. Chen and Tremblay[12] have used Monte Carlo simulations to compute the magnetic susceptibility for the large but finite $U$ version. Mishra and Kishore and Mishra[13] have studied the thermodynamics of the infinite U Hubbard model and the issue of spin-charge separation using the method of orthofermions. We shall address the issue of spin-charge separation when the author’s hydrodynamic approach[14] to the Hubbard model is accepted by the community.

In this article, we wish to write down an effective low energy theory of the t-J=0 model that is local in the operators in the sea-boson language(RPA-type) that involves introducing ‘renormalised’ doping dependent hopping and onsite terms. Thus the claim is that one may treat the infinite U Hubbard model the same way as we treated the small U Hubbard model[19](RPA-like) provided we ‘renormalise’ the parameters in the hamiltonian. We find that this leads to non-trivial predictions for the quasiparticle residue and velocity of the quasiparticles in more than one dimension. We also compute the magnetic susceptibility and show that it diverges near half-filling indicating that the system exhibits ferromagnetic instability arbitrarily close to half-filling, consistent with Nagaoka’s theorem. This also indicates that the formula for the residue is also reliable as is the conjectured low energy hamiltonian for the t-J model that is local in the operators. This then sets the stage to study the large but finite U Hubbard model and also the t-J-V models in future publications.

2 The Theory

Here we describe the theory which we are going to use. Consider the t-J model in one dimension with $U = \infty$.

\[ H = \mathcal{P} \left( -t \sum_{i,\sigma} c_{i+1\sigma}^\dagger c_{i\sigma} \right) \mathcal{P} \]  \hspace{1cm} (1)

\[ \mathcal{P} = \prod_{i} (1 - n_{i\uparrow} n_{i\downarrow}) \]  \hspace{1cm} (2)

We would now like to recast this in the sea-boson language so that we may recover the results of Schulz[15]. For this we mentally expand the projection operator in powers of the density fluctuations and retain the leading terms. Thus we could write for example,

\[ \mathcal{P} = e^{\sum_{i} \log(1 - n_{i\uparrow} n_{i\downarrow} + \lambda \left[ n_{i\uparrow} n_{i\downarrow} - \langle n_{i\uparrow} n_{i\downarrow} \rangle \right])} \]  \hspace{1cm} (3)

and expand in powers of $\lambda = -1$ and retain the leading terms. We shall not do this explicitly however we may redefine effective parameters that simulate...
such an expansion. The idea is to arrive at useful answers quickly and effor-
tlessly. The above procedure for example, entails the solution of self-consistent
equations for the density correlation functions, this is clearly not desirable as
it is likely to be complicated. We adopt the point of view that making contact
with the 1d system allows us to generalise to the case of more than one dimen-
sion by simply promoting wavenumbers to wavevectors. This we justify mainly
by pointing out that the magnetic susceptibility derived using this approach is
consistent with the rigorous Nagaoka theorem\cite{9}.

This means we may suspect that the t-J model with

\[ H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}^\ \ + \ \ \frac{U_{\text{eff}}}{N_a} \sum_{q\neq 0} \rho_{q1} \rho_{q-\uparrow} \]  

(4)

for some suitable ‘renormalized’ dispersion \( \epsilon_k = -2t_{\text{eff}} \cos(ka) \) and \( U_{\text{eff}} \). The
spin and charge velocities may be written as follows. \( v_s = v_{F,\text{eff}} (1 - \frac{U_{\text{eff}}}{\pi v_{F,\text{eff}}})^{1/2} \)
and \( v_c = v_{F,\text{eff}} (1 + \frac{U_{\text{eff}}}{\pi v_{F,\text{eff}}})^{1/2} \), where \( v_{F,\text{eff}} = 2t_{\text{eff}} \sin(\pi n_e/2) \) (lattice spacing \( a = 1 \). From the work of Schulz we know, \( v_c = 2t \sin(\pi n_e) \). Here
\( n_e = N_e/N_a \) is the number of electrons per site and \( v_s = 0 \). Also we know
that the anomalous exponent for the momentum distribution is \( \gamma = 1/8 \). Thus
we would like to compute \( t_{\text{eff}} \) and \( U_{\text{eff}} \) in terms of \( t \) and \( n_e \) given these
facts. From our earlier work\cite{19} we may read off a formula for the exponent
\( \gamma = \frac{U_{\text{eff}}^2}{4\pi^2} v_{F,\text{eff}} \frac{\rho_{q1}}{(v_c + v_{F,\text{eff}})^2} \). Thus we may write, \( U_{\text{eff}} = \pi \sqrt{\frac{v_c}{2v_{F,\text{eff}}}} (v_c + v_{F,\text{eff}}) \) and \( v_{F,\text{eff}} + v_{F,\text{eff}} = 0 \), we may solve this to yield, \( v_{F,\text{eff}} = \frac{1}{2} \left( -\frac{U_{\text{eff}}}{\pi} + \sqrt{\frac{U_{\text{eff}}^2}{\pi^2} + 4v_c^2} \right) \). We choose the positive solution, \( U_{\text{eff}} > 0 \) since we
know that the negative U Hubbard model possesses a spin gap \cite{17} whereas the
\( U = \infty \) Hubbard model does not. These may be solved via a scaling argument,
\( U_{\text{eff}} = u_{\text{eff}} v_c \) and \( v_{F,\text{eff}} = y_{\text{eff}} v_c \). This may be solved using mathe-
matica to yield \( u_{\text{eff}} = 4.71 \) and \( y_{\text{eff}} = 0.5 \). In order for \( v_s = 0 \) we must have
\( U_{\text{eff}} > \pi v_{F,\text{eff}} \). We may see that this is being obeyed. Hence we may claim
that Eq.( 4) captures the low energy physics of the Hubbard model at \( U = \infty \)
exactly. Now we make the following non-obvious assertion that the same Eq.( 4)
also captures the same physics in more than one dimension by simply promoting
wavenumbers to wavevectors. We make this plausible by pointing out that the
one dimensional Hubbard model may be generalised to higher dimensions by
precisely such a procedure, namely by promoting wavenumbers to wavevectors.
On the other hand, the prediction (see below) that the magnetic susceptibility
diverges as half-filling is approached is consistent with the rigorous Nagaoka
theorem, thus lending credibility to our approach.
2.1 $Z_F$ in Two Dimensions

The t-J model in two dimensions is relevant to cuprates\[2\] [11] and cobalt oxide superconductors\[16\]. In the two-dimensional case, we may solve for the sea-boson occupation as follows\[19\]. The energy dispersion for a square lattice is $\epsilon_k = -2t_{eff} [\cos(k_x a) + \cos(k_y a)]$. The sea-boson method is well-known and hence we shall refer the reader to our earlier work for details\[19\]. Suffice it to say that we have to compute the boson occupation numbers in order to derive a formula for the quasiparticle residue. Therefore we write,

$$< A_{k-q}^{k\sigma} (t^+) A_{k-q}^{k\sigma} (t^+) > = \frac{U_{eff}^2 P(q, \omega_c)}{N_a} \frac{[A_{k-q}^{k\sigma}, A_{k-q}^{k\sigma}]}{\epsilon_{k-q}(q, \omega_c) (-\omega_c - \epsilon_k + \epsilon_{k-q})^2}$$

$$< A_{k-q}^{k\sigma} (t^+) A_{k-q}^{k\sigma} (t^+) > = -\frac{U_{eff}}{N_a} \frac{1}{\epsilon_{s}(q, \omega_s)} \frac{[A_{k-q}^{k\sigma}, A_{k-q}^{k\sigma}]}{(-\omega_s - \epsilon_k + \epsilon_{k-q})^2}$$

where $P(q, \omega) = \sum_k \frac{n_{s}(k) - n_{s}(k-q)}{\omega - \epsilon_k - \epsilon_{k-q}}$ and $\epsilon_{s}(q, \omega) = 1 - \frac{U_{eff}^2}{N_a} P^2(q, \omega)$, also, $\epsilon_{s}(q, \omega) = 1 + \frac{U_{eff}}{N_a} P(q, \omega)$. In order to evaluate these expressions, we turn the cosine dispersion into a parabolic one by demanding that the slope of the two be the same at the Fermi momentum. $-2t_{eff} \cos(k_x) = -2t_{eff} + \frac{k^2_{F}}{2m}$. Thus we set $2t_{eff} \sin(k_{F}/\sqrt{2}) = k_{F}/(\sqrt{2}m)$. Also, $k_{F} = \sqrt{2\pi n_{c}}$. This approximation captures the important physics while leaving the integrals analytically computable. From our earlier work we may read off the formula for the velocity of the charge carriers. Here $v_{F,2d} = k_{F}/m$. We find that there is only one velocity and $\epsilon_{s} = 0$ does not have a solution.

$$v_{cc} = v_{F,2d} \frac{1 + \frac{2\pi}{mU_{eff}}}{\sqrt{(1 + \frac{2\pi}{mU_{eff}})^2 - 1}}$$

and the formula for the quasiparticle residue has been derived in an earlier work\[19\].

Close to half-filling, $2t_{eff} \approx y_{eff} 2t \sin(\pi n_{c})$, $U_{eff} = u_{eff} 2t \sin(\pi n_{c})$. Furthermore, $y_{eff} 2t \sin(\pi n_{c}) \sin(\sqrt{\pi}) = \sqrt{\frac{\pi}{m}}$. Therefore we may write the following formula for the quasiparticle residue.

$$Z_F = Exp \left[ -\frac{(m^2v_{cc}^2 - k_F^2)^2}{\pi k_F^2 m v_{cc}} \frac{1}{\pi} \frac{4mv_{cc} ArcTan \left[ \frac{mv_{cc} - k_F}{\sqrt{m^2v_{cc}^2 - k_F^2}} \right]}{\sqrt{m^2v_{cc}^2 - k_F^2}} \right]$$

This may be evaluated to yield,

$$Z_F \approx 0.79$$
This result is in exact agreement with the prediction by Castro-Neto and Fradkin nearly ten years ago\[18\]. They considered spinless fermions interacting via short-range interactions in two dimensions. Thus it would appear that the same physics is operating. In general we may conclude that the same mechanism that makes the anomalous exponent saturate in one dimension to a rather small value (1/8) also makes the quasiparticle residue to saturate to an equally small deviation from unity. In one dimension it suggests that the residual Fermi surface persists all the way to infinite onsite repulsion. In two dimensions it says that the actual Fermi surface persists all the way to infinite onsite repulsion. Since the functional dependence on the onsite repulsion is monotonic, we may conclude that there is no chance for Fermi liquid theory to break down in two dimensions with short-range interactions. In fact if anything these results show that the system is strongly metallic all the way to infinite repulsion.

3 Magnetic Susceptibility

The dynamic spin susceptibility may be computed using the Kubo formula.

\[ \chi(\omega) = i \int_0^\infty dt e^{i \omega t} \langle [S^+(t), S^- (0)] \rangle \] (10)

\[ S^+(t) = \sum_k c^\dagger_{k\uparrow}(t)c_{k\downarrow}(t) \] (11)

\[ S^-(0) = \sum_k c^\dagger_{k\downarrow}(0)c_{k\uparrow}(0) \] (12)

To use the sea-boson formalism, we have to take special care to account for possible infrared divergences. This is the crucial aspect that leads to the correct solution of the Luttinger model\[20\] and also leads to the solution of the problem of quenched disorder for scattering across the Fermi surface\[?\]. Define \( n_{\uparrow\downarrow}(k) \equiv c^\dagger_{k\uparrow}c_{k\downarrow} \). Now we would like to compute the correlation function,

\[ N(kt; k't') \equiv \langle n_{\uparrow\downarrow}(kt)n_{\downarrow\uparrow}(k't') \rangle \] (13)

This may be decomposed as follows.

\[ N(kt; k't') = (1 - n_F(k))(1 - n_F(k'))S_{AA}(kt; k't') + n_F(k)n_F(k')S_{BB}(kt; k't') \]

\[ -(1 - n_F(k))n_F(k')S_{AB}(kt; k't') - (1 - n_F(k'))n_F(k)S_{BA}(kt; k't') \] (14)

\[ S_{mn}(kt; k't') = e^{-2<\tilde{S}_{m,\uparrow}(k)>}e^{-2<\tilde{S}_{n,\downarrow}(k')>}S^0_{mn}(kt; k't') \] (15)

\[ \tilde{S}_A(k\sigma\sigma', t) = \sum_{q\sigma_1} A^\dagger_{k-q/2\sigma_1}(q\sigma, t)A_{k-q/2\sigma_1}(q\sigma', t) \] (16)
\[ \tilde{S}_{B}(k\sigma\sigma',t) = \sum_{q\sigma} A_{k+q/2\sigma'}(q\sigma_1,t) A_{k+q/2\sigma}(q\sigma_1,t) \] (17)

\[ S^0_{mn}(kt; k't') = <\tilde{S}_m(k\uparrow\downarrow,t)\tilde{S}_n(k'\downarrow\uparrow,t')> - <\tilde{S}_m(k\uparrow\downarrow,t)> <\tilde{S}_n(k'\downarrow\uparrow,t')> \] (18)

Since the \((\sigma,\sigma)\) part of the hamiltonian is distinct from the \((\sigma,\bar{\sigma})\) part of the hamiltonian, we may conclude that \(<S_A> = <S_B> = 0\). Thus in this case there are no difficulties associated with the infra-red regulator. After some tedious calculations we may see that the most divergent part of the magnetic susceptibility is given by,

\[ \chi(\omega = 0) \sim m \sim (1 - n_e)^{-1} \] (19)

As pointed out before, this is consistent with Nagaoka’s theorem and also with Shastry et.al.’s\[10\] work that shows that the ferromagnetic ground state is unstable with respect to the addition of holes. We find that unless the filling is arbitrarily close to half-filling, the susceptibility does not diverge.

4 Conclusions

To conclude, we have computed the quasiparticle residue of the infinite-U Hubbard model in two dimensions saturates to a value \( Z_F = 0.79 \). This is in exact agreement with the prediction of Castro-Neto and Fradkin\[18\]. The velocity of the quasiparticles is also found to shrink to zero as expected. The magnetic susceptibility is found to diverge as half-filling is approached which is consistent with a ferromagnetic ground state for a small\(^1\) concentration of holes. This is consistent with Nagaoka’s theorem\[9\] and also the with the work of Shastry et.al.,\[10\]. This shows that the effective low energy hamiltonian for the t-J model that is local in the operators is now reliable and can be expected to yield similar nontrivial results when generalised to include J terms and so on.

It is a pleasure to acknowledge email correspondence with Debanand Sa and Pinaki Majumdar and useful comments by Sourin Das.

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