

Spinless Fermions with Repulsive Interactions

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In this paper, we discuss the mean-field treatment of fermionic systems and the critical properties near the phase transitions at zero and finite temperature, respectively. Specifically, we consider the spinless fermion hopping on a square lattice, with nearest-neighbor repulsive interactions. We found that at intermediate repulsion strength there is a second-order phase transition from the Fermi liquid phase to the (π, π) charge density wave state. With stronger repulsion there seems to be coexisting density waves at different wave vectors depending on the doping.

I. INTRODUCTION

Throughout this course, we learned how to understand critical phenomena by various methods, including the Landau-Ginzberg formalism, the perturbative renormalization group, and the position-space renormalization group on lattice models. We, however, have mostly concentrated on spin systems, and fermionic systems remain undiscussed. We found it to be a good opportunity in this final project to understand how one treats criticality involving fermions.

On the other hand, the most daunting theoretical condensed matter problem nowadays is about how to understand high-temperature superconductors, the cuprates. In the last twenty years various experiments have been performed and theoretical advancement have been made; now we believe the physics of high-temperature superconductivity is captured by doping a mott insulator, which in the case of cuprates can be modeled by electrons hopping on a square lattice with large on-site repulsion. The superconductivity arises from the spin exchange which provides an effective attractive coupling between opposite spins. However, starting from here it becomes very difficult to tackle this particular model. For example, while the slave-boson mean-field theory captures the overall picture of the phase diagram, there are many degrees of freedom at choosing the mean-field ansatz and the predictability suffers. Beyond mean-field approximation it becomes a strong coupled gauge theory with finite matter density and we do not have many effective method to deal with it. The Fermi arcs seen in angular-resolved photoemission (ARPES) measurements and the quantum oscillations seen under extremely high magnetic field also lacks a coherent theoretical framework. Moreover, we have yet to have a theory (excluding holographic dual from gravity) which predicts linear resistivity from above T_c to room temperature as experiments observed.

Nevertheless, our goal is very modest here. We get rid of all the spin dynamics by considering spinless fermions. This greatly reduces the complexity of the problem at the expense of losing interesting and important physics; maybe the most important of all, in this model there is no superconductivity. The problem does not become completely trivial, however, as we can see later various density-wave states exist, which are believed to be impor-

tant for high T_c physics by some authors. In addition, in the strong repulsion limit it is not at all clear the model would behave like a Fermi liquid at high temperature when the density order is suppressed. As a technical side note, due to Pauli exclusion principle the on-site repulsive potential has no effect on a single species of fermion. We therefore consider the nearest neighbor repulsion. We then have our model Hamiltonian

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + v \sum_{\langle ij \rangle} c_i^\dagger c_i c_j^\dagger c_j. \quad (1)$$

We proceed in the following: first we introduce the way to do mean-field theory with fermions. We then numerically apply the procedure to our model in one and two dimensions and observe the result. Then we theoretically investigate the critical properties near the transition at zero or finite temperature.¹

II. MEAN-FIELD THEORY WITH FERMIONS

In the original Landau-Ginzberg formalism, we start from some phenomenological order parameter and write down an effective theory of the order parameter. Later on we realize that the theory can be formally derived from the path integral of the microscopic degrees of freedom. More specifically, the order parameter is often the coarse-grained version of the microscopic variable. Similarly, in a system with fermionic microscopic degrees of freedom, we can start from microscopically observable order parameters. Since the order parameter is necessarily of bosonic character, the natural candidate of the related microscopic degrees of freedom is a fermion bilinear. For example, $\rho(x) = \langle c_x^\dagger c_x \rangle$ and $\Delta(k) = \langle c_{k\uparrow} c_{-k\downarrow} \rangle$ are the density and the superconducting gap respectively, which are composed of fermion bilinears and could be

¹ K.-T. Chen is responsible for the introduction, part of the programming, the bosonization theory, and the theory in two dimensions. Y.-J. Chiu did the mean-field decomposition for the fermions, programmed the code in two dimensions and analyzed the data. She is also responsible for the transformation from fermions to spins in one dimension and carried out the coherence state path integral although it is not used in the end.

the order parameter of interest in certain systems. Here we introduce the Hubbard-Stratonovich transformation, in which the mean-field equations can be obtained by a saddle-point approximation, similar to the pure bosonic case.

Let us write our Hamiltonian as

$$H = H_0 + V, \quad (2)$$

with $V = v \sum_{\langle ij \rangle} c_i^\dagger c_i c_j^\dagger c_j$ and H_0 is the remaining part. The partition function in terms of the Euclidean path integral becomes

$$\begin{aligned} Z &= \text{Tr} e^{-\beta H} \\ &= \int Dc Dc^\dagger \exp \left(- \int_0^\beta d\tau \left(\sum_i c_i^\dagger \partial_\tau c_i + H_0 + V \right) \right) \end{aligned} \quad (3)$$

with $\tau = it$, which is the imaginary time.

Now we introduce an auxiliary field ρ , which if being integrated, would give back the exact same integral (up to some unimportant normalization factor):

$$Z = \int Dc Dc^\dagger D\rho \exp(-S'), \quad (4)$$

with

$$S' = \int d\tau \left(S_0 + \sum_{\langle ij \rangle} V(c_i^\dagger c_i \rho_j + c_j^\dagger c_j \rho_i) - V \sum_{\langle ij \rangle} \rho_i \rho_j \right), \quad (5)$$

and S_0 is the original action without the V part. Now we do the saddle point approximation, set all the derivatives respect to field to zero and obtain the following equations:

$$\begin{aligned} \rho_i &= \langle c_i^\dagger c_i \rangle; \\ -\partial_\tau c_i &= H_0 + v \sum_{j \in NN} \rho_j c_i. \end{aligned} \quad (6)$$

The first equation is the so-called self-consistency equation, determines ρ in terms of the fermion occupation number, and the second equation determines the (mean-field) fermion spectrum with a given ρ . Together the two equations determine the mean-field density ρ self-consistently. This is the Hartree approximation.

However, as one might notice, there are more than a way to take advantage of extra auxiliary fields to reproduce the same partition function. The saddle-point approximation would differ and produce very different results. In this sense, the mean field theory is quite arbitrary and one must use with caution and with a clear physical intuition of what the mean-field actually is in mind.²

Another way to understand the Hartree approximation at zero temperature is that the equation can also be derived from minimizing the ground state energy with respect to a direct-product wave function. Implementing

Pauli's exclusion principle by taking Slater determinants as the trial wave function, we can obtain a better set of mean-field equations of our model:

$$\begin{aligned} \rho_i &= \langle c_i^\dagger c_i \rangle; \quad h_{ij} = \langle c_i^\dagger c_j \rangle; \\ -\partial_\tau c_i &= H_0 + v \sum_{j \in NN} \rho_j c_i - v \sum_{j \in NN} h_{ji} c_j. \end{aligned} \quad (7)$$

This is the Hartree-Fock approximation and it can also be derived using different auxiliary fields. The extra mean-field h_{ij} acts like an effective hopping in our model. In the following section, we would solve the self-consistency equations in one and two dimensions, take ρ as our order parameter and observe if there is any phase transition.

III. NUMERICAL RESULTS

We solve the self-consistency equation by an iterative method. We start from some initial values of ρ_0 and h_0 , plug in the Hamiltonian, find the fermion spectrum and wave function, and calculate the expectation value of ρ and h , denoted as ρ_1 and h_1 . Then, in the next step, we use $\frac{\rho_0 + \rho_1}{2}$ and $\frac{h_0 + h_1}{2}$ as the new trial values for ρ and h . This procedure enhances the convergence of the iteration as compared with taking the computed expectation values directly as the new trial values, as we observed in the latter case the iteration often ends up alternating between two different set of values which therefore are not the solution to the self-consistency equations.

We assume our order parameter takes a periodic form on the lattice with period of n sites, and from Bloch theorem, the wavefunction is periodic in n up to a phase. We therefore use the Bloch basis to diagonalize our Hamiltonian, which effectively becomes a $n^d \times n^d$ matrix at different Bloch momentum k . We assume the total size of the lattice is $n \times l$, and thus k can take value from 0 to 2π with steps $2\pi/l$. To solve the eigenvalue equation, a $n \times n$ matrix takes time proportional to n^3 , so the time required is greatly reduced from $(n \times l)^3$ to $n^3 \times l$ by using the Bloch wave functions. However, the price we pay is that we can only observe certain wave numbers of the order parameter. Since, our main focus is on the $\pi - \pi$ order, we ignore this fact for the time being.

At $T = 0$, we use the canonical ensemble to fix the number of fermions N , find the N lowest energy states, and calculate the order parameter. This method is used instead of the grand canonical ensemble. In the latter case, we fill eigenstates with energy lower than the chemical potential μ . However, the interaction V would strongly affect the energy eigenvalues and make the process unstable at given μ . For example, with a large v , the density would oscillate between a completely empty and a completely full band. At finite T , theoretically, one can first use fixed N to find μ , and then using the calculated μ to acquire the order parameter. However, the iteration process still has to be polished to have better convergence. Here we assume that at low temperature,

the situation would not be too different from zero temperature and we can just extrapolate.

We present here the results of self-consistent mean-field approximation in 1D and 2D lattices. We compare the results with the presence of the Hartree term only with both the Hartree and the Fock term. We also look at the charge density wave (CDW) throughout different v and different doping. In our simulation, we choose the range of v to go from 0.5 to 5, and doping from 1/8 to 1/2.

For the 1D simulation, we choose a lattice of 80 sites with $n = 4$ and $l = 20$. With only the Hartree term, the result is shown in Fig. 1. With the Hartree term, we

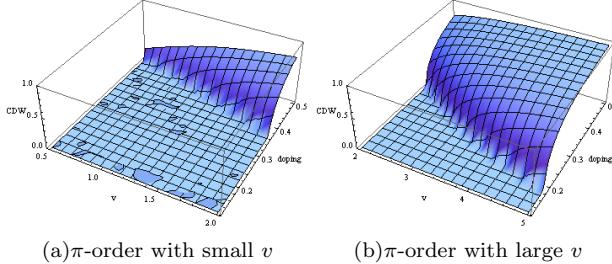


FIG. 1: 1D results with the Hartree term

observe only π -order throughout the entire range of v . We should mention here that despite in our simulation only π -order and $\pi/2$ -order is observable, generically we would expect different commensurate ordering would be likely for different doping. Here around doping = $\frac{1}{2}$ we do not see the $\pi/2$ order and we would therefore postulate that orders at other ordering wave vectors are also absent. Here we observe at mean-field level the transition to the CDW state is a second-order phase transition.

The results at the presence of both the Hartree and the Fock terms are shown in Fig 2. With Hartree-Fock, the

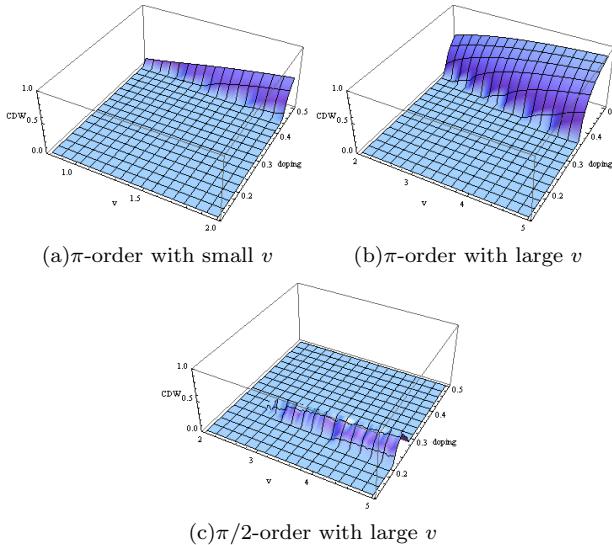


FIG. 2: 1D results of Hartree-Fock

π -order is suppressed compared with the previous case.

The ordering does not appear at small v until very close to half-filling. At half-filling both approximations would predict a CDW order with a very small v though. With larger repulsion we can see a $\pi/2$ -order CDW showing up at doping $\sim 1/4$ with the Hartree-Fock approximation.

For the 2D simulation, we use a lattice of 256 sites with $n = 4$ and $l = 4$. The results of the Hartree approximation are presented in Fig. 3. The results in 2D with

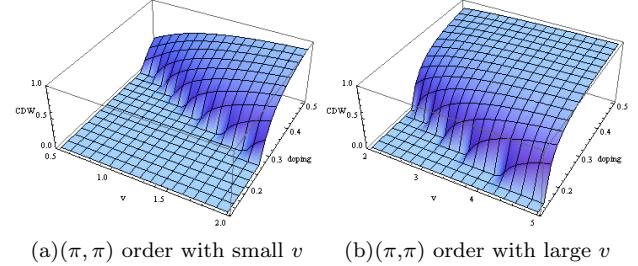


FIG. 3: 2D results of Hartree

only the Hartree term is similar to what we observe in 1D except that the order becomes more profound. Again We observe no other order throughout the range of v .

The results with Hartree-Fock are shown in Fig. 4. For small v , again we only see (π, π) order similar to

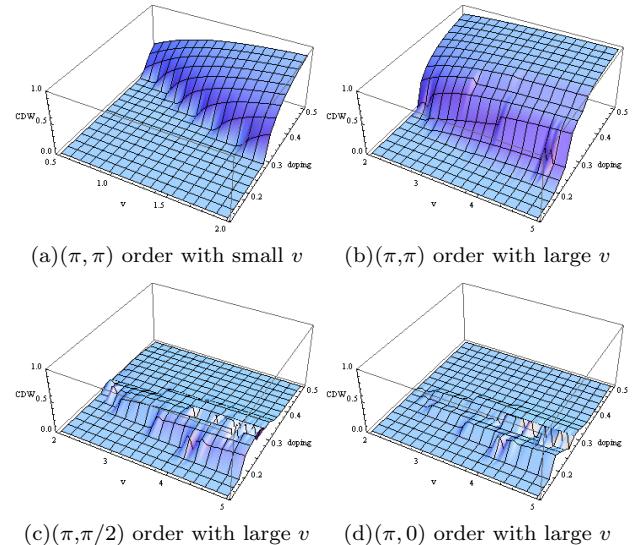


FIG. 4: 2D results of Hartree-Fock

the case in 1D. However, with a large v , other orderings such as $(\pi, \pi/2)$ ad $(\pi, 0)$ start to appear and we see a coexistence of two order parameters which compete against each other. If we look only at the (π, π) order, the difference between the Hartree and the Hartree-Fock approximation becomes minute at smaller v .

IV. THEORY IN ONE DIMENSION

First we demonstrate that the Hamiltonian of 1D fermions can be effectively be expressed in terms of 1D Heisenberg spin- $\frac{1}{2}$ s.⁴

Define the lowering and raising operators on site i :

$$S_i^\pm = S_i^x + iS_i^y \quad (8)$$

where $S^k = \frac{1}{2}\sigma^k$. From the Jordan-Wigner transformation, one can show that the creation and annihilation operators on site i , c_i^\dagger and c_i , are related to S by

$$\begin{aligned} S_i^+ &= c_i^\dagger (-1)^{\sum_{j=1}^{i-1} c_j^\dagger c_j}, \\ S_i^- &= (-1)^{\sum_{j=1}^{i-1} c_j^\dagger c_j} c_i. \end{aligned} \quad (9)$$

Since terms like $c_i^\dagger c_{i+1}$, $c_{i+1}^\dagger c_i$, and $c_i^\dagger c_i$ are present in the Hamiltonian in Eq. (1), let us compute $S_i^+ S_{i+1}^-$, $S_i^- S_{i+1}^+$, and $S_i^+ S_i^-$ and in terms of c^\dagger and c .

$$\begin{aligned} S_i^+ S_{i+1}^- &= c_i^\dagger (-1)^{2\sum_{j=1}^{i-1} (-1)^{c_j^\dagger c_j}} (-1)^{c_i^\dagger c_i} c_{i+1} \\ &= c_i^\dagger (1 - 2c_i^\dagger c_i) c_{i+1} \\ &= c_i^\dagger c_{i+1}, \end{aligned} \quad (10)$$

where we have used

$$\begin{aligned} (-1)^{c_i^\dagger c_i} &= e^{-i\pi c_i^\dagger c_i} \\ &= 1 + \sum_{n=1}^{\infty} \frac{(-i\pi c_i^\dagger c_i)^n}{n!} \\ &= 1 + \sum_{n=1}^{\infty} \frac{(-i\pi)^n}{n!} c_i^\dagger c_i \\ &= 1 + (e^{-i\pi} - 1)c_i^\dagger c_i \\ &= 1 - 2c_i^\dagger c_i. \end{aligned} \quad (11)$$

Similarly, we get

$$\begin{aligned} S_i^- S_{i+1}^+ &= c_i (-1)^{c_i^\dagger c_i} c_{i+1}^\dagger \\ &= c_i (1 - 2c_i^\dagger c_i) c_{i+1}^\dagger \\ &= c_i c_{i+1}^\dagger - 2c_i c_{i+1}^\dagger \\ &= c_{i+1}^\dagger c_i. \end{aligned} \quad (12)$$

And last,

$$S_i^+ S_i^- = c_i^\dagger c_i. \quad (13)$$

Using the above equations, we can rewrite the Hamiltonian in Eq. (1) as

$$H = -t \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + v \sum_i S_i^+ S_i^- S_{i+1}^+ S_{i+1}^-. \quad (14)$$

Recollecting terms, we found the Hamiltonian of repulsive fermions is equivalent to an anisotropic Heisenberg model:

$$H = \sum_{\langle ij \rangle} (-2t(S_i^x S_j^x + S_i^y S_j^y) + v S_i^z S_j^z) + \sum_i v(1 + S_i^z). \quad (15)$$

If we rotate our fermions by a staggered π -phase so that the hopping between the nearest neighbor becomes $+t$, the spin Hamiltonian becomes antiferromagnetic. For a given doping which translates to fixed total S_z , we have to apply a magnetic field to maintain the average value of S_z . Combine with above, our model at some fixed doping can be written as the following spin- $\frac{1}{2}$ model:

$$H = \sum_{\langle ij \rangle} (-2t(S_i^x S_j^x + S_i^y S_j^y) + v S_i^z S_j^z) + \sum_i h S_i^z, \quad (16)$$

where h is determined by the doping, and specifically, $h = 0$ at half-filling.

In the spin model, the π or (π, π) CDW order corresponds to Neel order in the z direction. A similarly staggered hopping corresponds to the spin Peierls order. CDWs at other ordering vectors, corresponding to other ordering of spins, however, are not commonly seen but that may be due to the finite magnetic field present at those dopings.

We can already gain some insight by looking at the equivalent spin model. Firstly, at finite temperature since the quantum nature of the spin can be ignored near the phase transition, we immediately find that there cannot be any kind of ordering present. The mean-field result, therefore, is incorrect in finite temperature (as it usually is not in 1D.) At zero temperature, the situation is more complicated. Nevertheless, we know that antiferromagnetic Heisenberg model is solved by the Bethe ansatz, and the Neel order does not exist in 1D, therefore at $v = 2t$ the system should still be in the Fermi liquid state. The Hartree approximation therefore greatly exaggerates the order, adding the Fock term cures it a bit but it is still favors the order state too much. On the other hand, we can see that with a large v which favors the Neel order in the z direction, at $h = 0$ the Neel order would ultimately prevail. Therefore there is an ordered state at zero temperature. The detail of the transition, however, requires more work.

One can use the coherent basis to write down a path integral presentation of the partition function of the spin model, and take the continuum limit. However, in the antiferromagnetic spin- $\frac{1}{2}$ chain, the result contains a topological term in addition to the nonlinear sigma model. The nonlinear sigma model itself in 1D just goes into the disorder state with finite correlation under renormalization group (RG) but the topological term does not renormalize and messes up the property. Thus, it becomes unclear how the 1D system would behave in this approach.

It turns out in 1D, one can deal with the antiferromagnetic spin- $\frac{1}{2}$ problem with bosonization.³ The strategy is first to turn the spins into fermions by the inverse transformation mentioned above (so we return to our original model) and then use the density fluctuations to express the fermionic operators. In general dimensions this is not possible but in 1D indeed there always is a one-to-one correspondence between density operators and fermionic

creation/annihilation operators. The physical reasoning behind is that the Fermi surface becomes Fermi points in 1D and the low energy particle-hole excitations have the same measure as the single particle excitations. It is easy to express the density or the particle-hole creation operator using the fermionic operators, but what may not be so trivial is that the free low energy Hamiltonian of the fermion system

$$H_F = -iv_F \int dx \left(\Psi_R^\dagger \frac{\partial \Psi_R}{\partial x} - (R \leftrightarrow L) \right), \quad (17)$$

where $\Psi_R(\Psi_L)$ is the right(left)-moving fermionic field, can be written as

$$H' = \frac{\pi v_F Q_R^2}{L} + \frac{2\pi v_F}{L} \sum_{n=1}^{\infty} (\rho_{R-n} \rho_{Rn} + R \leftrightarrow L) \quad (18)$$

which is still quadratic in the bosonic field ρ . ρ_n is the n th Fourier component of the density $\rho(x) \equiv \Psi^\dagger \Psi$ and Q_R is the total charge of the right movers. In the derivation we have used

$$[\rho_{Rn}, \rho_{R-n'}] = \delta_{nn'} \cdot n. \quad (19)$$

Let us change variables to ϕ and θ :

$$\begin{aligned} \phi(x) &= -\phi_0 + \frac{\pi Qx}{L} - \frac{i}{2} \sum_{n \neq 0} \frac{e^{i2n\pi x/L}}{n} \rho_n \\ \theta(x) &= -\theta_0 + \frac{\pi Jx}{L} - \frac{i}{2} \sum_{n \neq 0} \frac{e^{i2n\pi x/L}}{n} (\rho_{Rn} - \rho_{Ln}), \end{aligned} \quad (20)$$

with $Q = Q_R + Q_L$ and $J = Q_R - Q_L$. We can see $\nabla\phi = \pi\rho$. Plugging in, H' now takes the form

$$H' = \frac{v_F}{2\pi} \int_0^L dx [(\nabla\phi)^2 + (\nabla\theta)^2]. \quad (21)$$

Note that we have

$$[\nabla\phi(x), \theta(y)] = [\nabla\theta(x), \phi(y)] = i\pi\delta(x-y), \quad (22)$$

therefore $\nabla\theta$ is the conjugate momentum of ϕ . Switching to Lagrangian formalism and using the Euclidean path integral, we have

$$S = \frac{1}{2\pi v_F} \int dx d\tau [(\partial_\tau \phi)^2 + v_F^2 (\nabla\phi)^2]. \quad (23)$$

We recognize that this is a free Gaussian model, with finite correlation length since the coupling in front is below the Kosterlitz-Thouless threshold. This does not contradict the fact that we are describing free fermions, as we have yet to express the fermionic operators in terms of our bosonic field. This is actually a highly nontrivial task, and somehow the expression even depends on the actual form of the Hamiltonian. In the end we have

$$\Psi_F(x) = \sum_{m \text{ odd}} A_m \exp(imk_F x + im\phi(x) - i\theta(x)) \quad (24)$$

where the long-range behavior is dominated by $m = \pm 1$ terms. If H_F describes free fermion, we would only have the smallest m and we can recover the fermionic correlation.

With the expression of the fermion operator at hand, we can easily add interactions. Our V term corresponds to

$$V = \sum_{<ij>} v \rho_i \rho_j \sim 2av \int dx \rho^2 = \frac{2av}{\pi^2} \int dx (\nabla\phi)^2. \quad (25)$$

This renormalizes v_F , and give us a different coupling constant in front of the action. Now we can smell how the CDW transition comes about. The situation is a little bit more complicated, though; let us start right at half filling. Here, the repulsion contributes to umklapp processes as well which in terms of the bosonic fields looks like $\cos 4\phi$. Now while this looks like a potential in ϕ if we write in terms of θ this term allows us to tunnel between different states with 4π vortices in θ . Therefore, the increase in v helps the proliferation of 4π vortices in the θ field. In terms of the θ field, at low v vortices are scarce and the renormalization group flows to the Gaussian theory which in terms of the fermions there is infinite correlation length and the fermions are gapless. As v increases, the coupling becomes smaller (in the θ theory) and the vortices start to appear. Once it crosses the Kosterlitz-Thouless threshold, the vortices destroy the quasi long-range order of θ completely but establishing true long-range order of ϕ at the same time. The critical properties of the phase transition at zero temperature is of the same type as the classical 2D XY model.

Away from half-filling, we need to modify two things: first we have to include a magnetic field which couples to $\nabla\phi$ in the bosonized theory, and then the umklapp process no longer presents. The $\nabla\phi$ term is a total derivative which integrates to be a constant as we require specific boundary conditions for the ϕ field. Without the umklapp term, it seems there would be no phase transition. Nevertheless, above the threshold the Gaussian state becomes unstable, and a tiny Neel order runs away. The critical coupling would be higher due to the absence of the umklapp term. Comparing to our mean-field result, it seems the Hartree-Fock approximation captured this sharp difference a little bit as it ordered almost immediately at half filling but becomes resilient very soon after the doping being decreased. On the other hand, whether the system stays gapless even after the onset of the Neel order (as in mean-field treatment) requires some further understanding.

V. THEORY IN TWO DIMENSIONS

None of our discussion in the previous section can be applied in 2D. In two and higher dimensions in general there is no way to transform gapless fermions into anything else. Nevertheless, with our auxiliary field we can

still formally integrate out the fermions and look at the effective action of the auxiliary field. If we then allow a power and gradient expansion in our auxiliary field, take the Hartree field ρ for example, clearly the finite temperature result belongs to the Ising universality class since the order parameter has only one component. At zero temperature, we have to be more careful about the fermion integration. For a given ordering wave vector, in 2D generically one can only find a finite set of discrete points on the Fermi surface which connects via the wave vector. In this case, the low energy fermions are around those points, doing the vacuum bubble integral would give a k^2 as well as $|\omega|$ in front of $|\rho(k, w)|^2$. This means $z = 2$ and the effective theory of the order parameter is at the upper critical dimension. Therefore a perturbation theory in the ρ^4 coupling is viable (which runs logarithmatically) and we can calculate the critical exponents perturbatively. The mean field result in this case might have been good enough, though.

If we look back at our mean-field result, maybe the closeness between the Hartree and Hartree-Fock approximations is a good indication that mean-field treatment is not bad.

VI. DISCUSSIONS

In this paper, we presented a coherent picture of phase transitions between charge density waves and Fermi Liquid in one and two dimensions. However, as mentioned in the introduction, one of the big question is that whether this CDW state has any effect on higher temperatures,

as in realistic situations the lower temperatures are covered by the superconducting dome. Theory of quantum phase transition predicts a quantum-critical regime at finite temperature above the quantum critical point. This could be a way to get non-Fermi liquid (NFL) behavior.

On the other hand, in the high temperature phase there is no phase boundary, only crossover between this regime and the Fermi liquid regime. One thus could imagine doing a high temperature expansion to investigate the properties in the NFL regime. This is originally planned as the third part of our project.

However, the high temperature expansion of fermions turned out to be extremely difficult. In addition to the difficulty of interactions (which we would take the strong interaction limit to forbid occupation on nearest neighbors), we have trouble even to formulate a high temperature expansion for free fermions. The key problem is that the single-particle eigenstates can only be summed up independently only when the energy is in a exponential, and the high temperature expansion ruins that. The best we can do is just to replace fermions with classical particles, but then the model is just a Van Der Waal gas on a lattice. We hope to come back to this problem if we have some new idea in the future.

Acknowledgments

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² Negele, J. and Orland, H., 1988, *Quantum Many-Particle Systems* (Addison Wesley)

³ Sachdev, S., 1999, *Quantum Phase Transitions* (Cambridge Press)

⁴ Fradkin, E., 1991, *Field Theories of Condensed Matter Systems* (Addison-Wesley)