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Existence of an incommensurate ground state of interacting spinless fermions in infinite dimensions

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Abstract

We focus on the ground state phase diagram of a system of spinless fermions with repulsion on a hypercubic lattice in the limit of infinite dimensions. Spontaneous symmetry breaking into a charge density wave (CDW) occurs. Using an ansatz for the order parameter which includes the homogeneous, the AB and a large class of incommensurate phases we are able to calculate the phase diagram.

It is important to disclose the structure of the phase diagram of models with strong electron correlation. The problem is twofold. First, one has to have a clear picture of which phases are likely to be realised and second, for these phases it must be possible to calculate the free energy. In the case of the Hubbard model for example both problems can hardly be surmounted. Even if one restricts oneself to a small number of phases and to the dynamic mean field theory resulting from the limit of high dimensions [1], the problem still requires massive computational effort (e.g. Ref. [2]). The situation is different for the model of interacting spinless fermions [3] on an infinite dimensional hypercubic lattice. Although the diagrammatic theory is simple, the physics is far from trivial.

The Hamiltonian of the spinless fermion model in second quantisation is

$$\hat{H} = -\frac{t}{\sqrt{2d}} \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \frac{U}{4d} \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i. \quad (1)$$

Scaling with the inverse dimension $1/d$ is performed to ensure the continuity of the limit of infinite dimensions [1,4,5].

In a previous work, the stability of the homogeneous phase was investigated in the limit $d \rightarrow \infty$ [6]. In this limit Hartree and random phase approximation become exact [5,6]. Besides the occurrence of an AB-charge density wave (CDW) characterised by the wave vector $\mathbf{Q} = (\pi, \pi, \dots, \pi)^\dagger$, it was found that the density-density susceptibility $\chi(\mathbf{q}) = (\chi_0^{-1}(\mathbf{q}) + U\eta(\mathbf{q}))^{-1}$ diverges at incommensurate values of the wave vector $\mathbf{q}$. The parameter η is defined as $\eta(\mathbf{q}) = d^{-1} \sum_{i=1}^d \cos(q_i)$ and $\chi_0^{-1}(\mathbf{q})$ is the inverse bare susceptibility. Commensurate values of $\mathbf{q}$ which belong to a value of $\eta \neq -1, 1$ are of measure zero. The complete stability analysis is possible in $d = \infty$ because χ_0 depends on $\mathbf{q}$ only via η [5]. Thus it is sufficient to examine $\chi(\eta)$ [7].

The divergence of $\chi(\eta)$ indicates a second order transition from the homogeneous phase at high doping and/or low interaction into an incommensurate CDW. The structure of the new incommensurate phase has not yet been investigated. In finite dimensions and for related models such as the Hubbard model and the t - J model there exist many works which have different variational or approximative approaches to incom-

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mensurate phases [8]. Since the perturbation theory of the model (1) becomes exactly tractable in $d \rightarrow \infty$ it is the natural candidate to examine the energetic effects of different spatial structures of the order parameter. The resulting equations are self-consistent and include infinitely many parameters in the thermodynamic limit so that no systematic approach to their solution exists [6]. Here we give results for the following ansatz for the spatial structure of the order parameter $b(\mathbf{r}) = \langle \hat{n}_r \rangle - n$ where n is the average particle density, $b(\mathbf{r}) = b_0 \prod_{i=1}^d u_i(r_i)$. The index i counts the directions; r_i is the i th component of $\mathbf{r}$, b_0 is the overall amplitude and the new defined functions u_i take the values ± 1 . The product form of this ansatz allows us to profit best from the simplifications of $d \rightarrow \infty$. Yet it is still very general since it allows any sequence of $+1$ and -1 independently for the d directions without assuming translational invariance.

A close inspection of the free energy shows that it depends on $b(\mathbf{r})$ only via the amplitude b_0 and the relative frequency h that $b(\mathbf{r})$ has the same sign on adjacent sites [9]. These are the only parameters which are relevant for the influence of the spatial structure on the energy. In order to find an explicit functional for the energy we exploit the freedom in choosing the u_i . For $i \leq hd$, we set $u_i(r_i) \equiv 1$ and for $i > hd$, we set $u_i(r_i) \equiv (-1)^{r_i}$. This choice is special since the order parameter can be characterised by the wave vector

$$\mathbf{Q}_h = (\underbrace{0, 0, \dots, 0}_{hd}, \underbrace{\pi, \pi, \dots, \pi}_{(1-h)d})^T \quad (2)$$

but does not restrict the freedom contained in the ansatz for $b(\mathbf{r})$. This gives a general relationship $\eta = 2h - 1$, although only for special realisations can η be defined. The easy structure of the CDW with wave vector $\mathbf{Q}_h$ helps to resume the perturbation series for the grand canonical potential since the Green function is a 2×2 matrix in $\mathbf{k}$ -space.

In infinite dimensions the diagram for the free energy is simple. Compared to the free fermion system the grand potential gains a term $\Delta\Omega = T \text{Tr} \int_0^1 d\lambda \lambda^{-1} G \Sigma|_{U \rightarrow U\lambda}$, where G is the Green function and Σ the self-energy. At $T=0$ this yields the ground state energy

$$E(\Delta, \eta) = \frac{Un^2}{2} - \frac{\Delta^2}{2\eta U} + \int_{-\infty}^{\infty} dv \frac{\exp\left(-\frac{v^2}{1-\eta}\right)}{2\sqrt{\pi(1-\eta)}} \times \left\{ \frac{\sqrt{v^2 + \Delta^2}}{\text{sgn}(v)} \text{erf}(P) - \frac{\sqrt{1+\eta}}{\sqrt{\pi}} \exp(-P^2) \right\}, \quad (3)$$

$$P := \frac{\tilde{\mu} - \text{sgn}(v)\sqrt{v^2 + \Delta^2}}{\sqrt{1+\eta}}$$

where $\tilde{\mu} = \mu - nU$ and $\Delta = -\eta U b_0$. The doping $\delta = 0.5 - n$ is given by

$$\delta = \int_{-\infty}^{\infty} dv \frac{\exp\left(-\frac{v^2}{1-\eta}\right)}{2\sqrt{\pi(1-\eta)}} \text{erf}(P) \quad (4)$$

and the equations which define the energetic minimum are $\partial E / \partial \Delta|_n = 0$ and $\partial E / \partial \eta|_n = 0$. For a particular value of the interaction U it is possible to determine for each doping the parameters Δ and η which describe the physical state. Additionally, one has to be on the watch for first order phase transitions.

As example we look at the case $U = 1.2$. We plotted ground state energy as a function of doping in Fig. 1. For large doping and at half-filling, the situation is clear. For the former the system is in the homogeneous phase whereas for the latter the system is in the commensurate CDW characterised by $\eta = -1$ (AB-phase). In between four special points at $\delta_{\text{div-AB}}$, $\delta_{\text{PS-IP}}$, $\delta_{\text{PS-AB}}$, and $\delta_{\text{div-IP}}$ can be identified.

Let us focus on the situation with fixed $\eta = -1$. The system is forced to choose between the homogeneous phase and the AB-phase. The response of the system

Fig. 1. Ground state energy for $U = 1.2$. Dotted curve, homogeneous phase; dotted-dashed curve, AB phase; solid curve, incommensurate phase (η optimised). Divergence of $\chi(-1)$ at $\delta_{\text{div-AB}}$. Divergence of $\chi(\eta)$ for optimised η at $\delta_{\text{div-IP}}$. Maxwell constructions between $\delta = 0$ and $\delta_{\text{PS-AB}}$ or $\delta_{\text{PS-IP}}$. Incommensurate phase between $\delta_{\text{PS-IP}}$ and $\delta_{\text{div-IP}}$. To facilitate visibility a linear function of δ has been added: $a \approx 0.5561$, $b \approx 0.1946$.

towards fluctuations with wave vector Q_0 becomes infinite at $\delta_{\text{div-AB}}$. The ground state energy is indicated by a dotted and a dotted-dashed curve, respectively in Fig. 1. For smaller doping the ground state energy is concave so that a first order phase transition will occur. The Maxwell construction gives rise to the value $\delta_{\text{PS-AB}}$. Thus, there is phase separation between the homogeneous phase and the AB phase for $0 < \delta < \delta_{\text{PS-AB}}$. This situation turns out to be generic for $U < U_{\text{IPL}} \approx 0.5716$ and $U > U_{\text{IPH}} \approx 1.9145$. In between, and thus for the case $U = 1.2$, a different scenario is realised.

The divergence of $\chi(\eta)$ is at $\delta_{\text{div-IP}}$ for general values of η . For $U_{\text{IPL}} < U < U_{\text{IPH}}$ holds $\delta_{\text{div-IP}} > \delta_{\text{PS-AB}}$. By minimizing $E(\Delta, \eta)$ we obtain the solid curve in Fig. 1. Again, the curve is concave for low dopings so that a Maxwell construction must be made. The doping where the phase separation sets in is $\delta_{\text{PS-IP}}$. It is important to realise that $\delta_{\text{PS-IP}} < \delta_{\text{PS-AB}}$. For dopings $\delta_{\text{PS-IP}} < \delta < \delta_{\text{div-IP}}$ the pure incommensurate phase is the absolute energy minimum.

The overall result is depicted in Fig. 2. At half-filling the system is in the AB-phase for all $U > 0$. For large doping the system is in the homogeneous phase. For $U < U_{\text{IPL}}$ and $U > U_{\text{IPH}}$ there is phase separation between the AB-phase and a hole-enriched homogeneous phase. For $U_{\text{IPL}} < U < U_{\text{IPH}}$ there exists a region where an incommensurate phase is present, and a region of phase separation between the AB-phase and the hole-enriched incommensurate phase.

Fig. 2. Phase diagram. HOM, homogenous phase; AB, AB phase; IP, incommensurate phase; PS-AB, phase separated region between homogeneous and AB phase; PS-IP, phase separated region between incommensurate and AB phase. U_{IPL} , U_{IPH} , lower and upper interaction bound of the IP.

Fig. 3. The value of η along the phase borders of the incommensurate phase. Solid curve, right border; dashed curve, left border.

The parameter η is close to -1 in the incommensurate phase. To give an impression we plotted those values of η in Fig. 3 which arise at the borders of the incommensurate phase in Fig. 2. The function $\eta(\delta)$ at constant U is monotonic so that the figure gives a good impression of the deviation of η from -1 . Note that the values for η belonging to the left border (Fig. 2), given by the solid curve in Fig. 3, are important for the whole region of phase separation.

In summary, we have demonstrated the complexity of the ground state phase diagram of the model of interacting spinless fermions in infinite dimensions. Most important is the existence of an incommensurate phase and of the phase separation between the AB-phase and the incommensurate or homogeneous phase.

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