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Correlated Lattice Fermions in High Dimensions

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Abstract

We discuss the properties of correlated lattice fermions in the limit of high dimensions $d \to \infty$. In this limit theoretical investigations are enormously simplified, while at the same time correlations remain non-trivial. Contact to finite dimensions can be made via systematic 1/d-expansions. We review the state-of-art of this new approach.

Introduction

Correlated Fermi systems play a particularly important role in physics. However, they are also known to be notoriously difficult to tackle. In condensed-matter physics the discovery of high-temperature superconductivity [1] has further intensified the theoretical efforts [2] to understand the effect of strong interactions among fermions. The difficulties involved are wellknown from the theory of narrow-band metals [3], liquid ^{3}He [4] and heavy-fermion systems.[5] They are all examples of Fermi systems with a strong, short-range repulsive interaction between the respective spin-1/2 fermions. These systems are often described by a lattice model, where the interaction is approximated by a Hubbard-type, i.e., on-site, interaction [6]:

$$\hat{H}_I = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{1}$$

Here $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma}$ is the number operator for fermions with spin σ on a lattice at site i. The term $\hat{H}_I$ is part of many model Hamiltonians constructed to describe the correlations between fermions. In the simplest case the interaction part $\hat{H}_I$ may be supplemented by a kinetic part

$$\hat{H}_{kin} = \sum_{ij,\sigma} t_{ij} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} = \sum_{k,\sigma} \varepsilon_k \hat{n}_{k\sigma} \tag{2}$$

where t_{ij} is an inter-site hopping matrix element, ε_k is its Fourier transform and $\hat{n}_{k\sigma}$ is the momentum distribution operator for fermions with spin σ. The single-band Hubbard Hamiltonian [6,7]

$$\hat{H} = \hat{H}_{kin} + \hat{H}_I \tag{3}$$

defines the simplest model of itinerant lattice fermions subject to a mutual short-range interaction.

In spite of its apparent simplicity, exact solutions have so far only been possible in d = 1 space dimension.[8] In view

of the special properties of one-dimensional systems it is not clear, how relevant these results are for higher-dimensional systems, e.g. for $d = 3$. In the case of models with *localized* interacting spins (e.g. Ising model or Heisenberg model) the properties are completely different in $d = 1$ and $d = 3$, respectively. In particular, the phase transitions appearing in the three-dimensional models are absent in $d = 1$. However, the existence and the order of phase transitions in $d = 3$ are correctly described by the mean-field theory (MFT), which, for localized spin models, provides the exact results for thermodynamic properties in $d \to \infty$.[9]

The investigation of correlated lattice fermions with *itinerant* degrees of freedom in $d \to \infty$ has been initiated only most recently by the present authors.[10] They showed that, provided the model parameters are properly scaled, correlations remain non-trivial even in the limit $d \to \infty$. In particular, standard mean-field solutions (e.g. unrestricted Hartree-Fock) do not provide exact results for models of correlated lattice fermions in $d \to \infty$. It was found that diagrammatic calculations become much simpler than in finite dimensions. This property makes perturbational and variational calculations tractable in $d = \infty$, which are usually prohibitively difficult in lower dimensions. Indeed, within a very short while the limit of infinite dimensions for lattice fermions has attracted a lot of researchers who showed its usefulness in a number of different problems.[11] In the following we will briefly review the main features of this approach and will at least outline the results accumulated over the year.

Limit of infinite dimensions

We first discuss the problem of how to *define* a model of correlated lattice fermions in $d \to \infty$. To obtain a non-trivial model, the parameters must be scaled such that all terms of the Hamiltonian remain finite and non-zero as $d \to \infty$. We consider the Hubbard model with next-neighbor hopping ($t_{ij} = -t$ for i,j next neighbors, 0 else) as a generic example. For $d \to \infty$, the on-site interaction $\hat{H}_I$ remains finite for fixed U,

but the hopping rate in the kinetic energy has to be scaled because the number of next neighbors diverges as $d \to \infty$. For nearest-neighbor hopping on a d-dimensional simple cubic lattice with unit lattice spacing we have

$$\varepsilon_{\mathbf{k}} = -2t \sum_{j=1}^{d} \cos k_j \qquad (4)$$

where $\mathbf{k} = (k_1 \ldots k_d)$. The corresponding density of states (DOS) in $d \to \infty$ is determined by the central-limit theorem

$$D(\varepsilon) \overset{d \to \infty}{=} \frac{1}{2t(\pi d)^{1/2}} \exp[-(\varepsilon/2td^{1/2})^2] \qquad (5)$$

Clearly, only the scaling $t = t^*/(2d)^{1/2}$ with fixed t^* (henceforth $t^* \equiv 1$) yields a finite DOS and thereby leads to a finite average kinetic energy E_0 of the noninteracting particles for arbitrary densities $n_\uparrow$, $n_\downarrow$.[10] In this way, the Hubbard model in $d \to \infty$ still describes fermions with competing potential and kinetic energies, i.e., its interpolating character between free itinerant fermions (for small U) and localized fermions (for small t^*) is retained.

U-Perturbation theory in high dimensions

Diagrammatic perturbation expansions about $U = 0$ are greatly simplified in $d \to \infty$. [10-13] As an example, we discuss the Feynman-Dyson expansion for Green's functions. A typical diagram contributing to the proper self-energy is depicted in fig. 1. A line running from j to j' represents a free Green's function $G^0_{\sigma jj'}$ as a factor. As $d \to \infty$, the off-diagonal elements of $G^0_{\sigma jj'}$ can be shown to decrease. For example, for nearest-neighbor hopping we have $G^0_{\sigma jj'} \propto 1/d^{\nu/2}$, where ν is the number of lattice steps neccessary to go from j to j'. As a consequence, the diagram in fig. 1 does not contribute, unless f = h, i.e. f and h "collaps" as indicated in fig. 1. Note, however, that the contributions $j \neq f,h$ in fig. 1 remain even in $d \to \infty$. For example, a term with j nearest neighbor of f = h vanishes as 1/d, but the sum of all nearest-neighbor terms

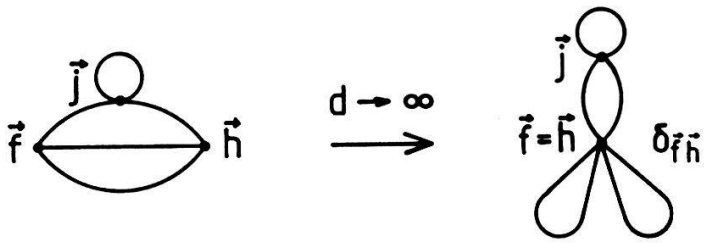

Fig.1: Collaps of a typical self-energy diagram as d → ∞.

remains finite as d → ∞, since there are 2d nearest neighbors on a d-dimensional hypercubic lattice. In general, two vertices collapse in real space as d → ∞ if they cannot be separated by cutting one or two lines in the diagram. Alternatively one may say that momentum conservation can be disregarded at the respective vertices.

In particular, the external vertices in a self-energy diagram can never be separated by cutting two lines. Hence, the self-energy becomes site-diagonal in d → ∞. As a consequence, both the shape of the Fermi surface and the spectral density at the Fermi surface are not altered by the interaction, as long as perturbation theory is applicable.[12] On the other hand, the *time*-dependence of the self-energy, which is absent in any Hartree-Fock mean-field theory, is retained in d → ∞ and implies mass renormalization and lifetime effects.[12]

A *renormalized* perturbation expansion of the self-energy involves *skeleton* diagrams; these are always two-particle irreducible. Hence, in d → ∞ all vertices of a skeleton diagram collapse onto a common site. Consequently, the self-energy is a functional only of the *local* propagator. This feature makes possible a mapping of the Hubbard model in d → ∞ onto an atomic problem with time dependent fields.[14] For the Falikov-Kimball model (a simplified version of the Hubbard model where only one spin species can hop) the corresponding atomic problem has been solved [14] while for the Hubbard model an exact solution has not been obtained so far.

Due to the diagrammatic collapse described above weak coupling expansions become much simpler in high dimensions.

As an example, we consider the second order correlation energy E_2, which is given by the Goldstone diagram in fig. 2.

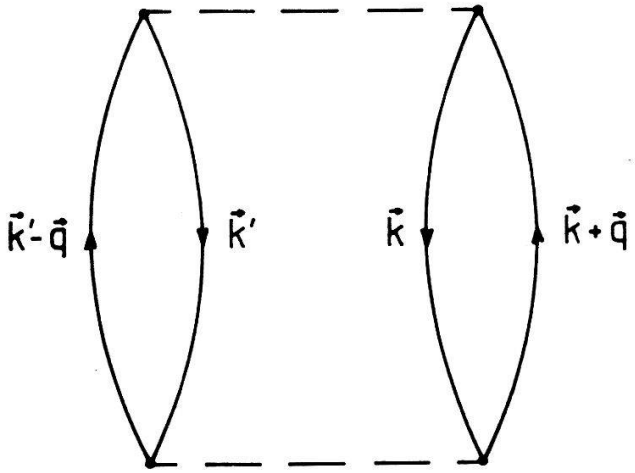

Fig.2: Second order Goldstone diagram.

In d dimensions this yields the momentum integral

$$E_2 = \frac{U^2}{(2\pi)^{3d}} \int dk\, dk'\, dq\, \frac{n_k^0\, n_{k'}^0 (1-n_{k+q}^0)(1-n_{k'-q}^0)}{\varepsilon_k + \varepsilon_{k'} - \varepsilon_{k+q} - \varepsilon_{k'-q}} \qquad (6)$$

where n_k^0 is the k-space occupation at $U = 0$. In $d \to \infty$, (6) can be simplified to a one-dimensional integration [10]:

$$E_2 = -\int_0^\infty d\lambda\, e^{2\lambda^2} P^2(\varepsilon_F - \lambda) P^2(-\varepsilon_F - \lambda) \qquad (7)$$

where $P(x)$ is the Gaussian probability function and ε_F is the Fermi energy. In fig. 3 E_2 is shown as a function of density $n = n_\uparrow + n_\downarrow$ in dimensions $d = 1,2,3, \infty$. The result for $d = 3$, which can only be calculated by considerable numerical effort, is very well approximated by that for $d = \infty$, which is given by the single integral in (7). The neglect of off-site contributions in a diagram had already been introduced previously by Kajzar and Friedel [15] as a pragmatic approximation in a perturbation treatment of transition metals. This approximation is here found to become exact in the limit of high dimensions.

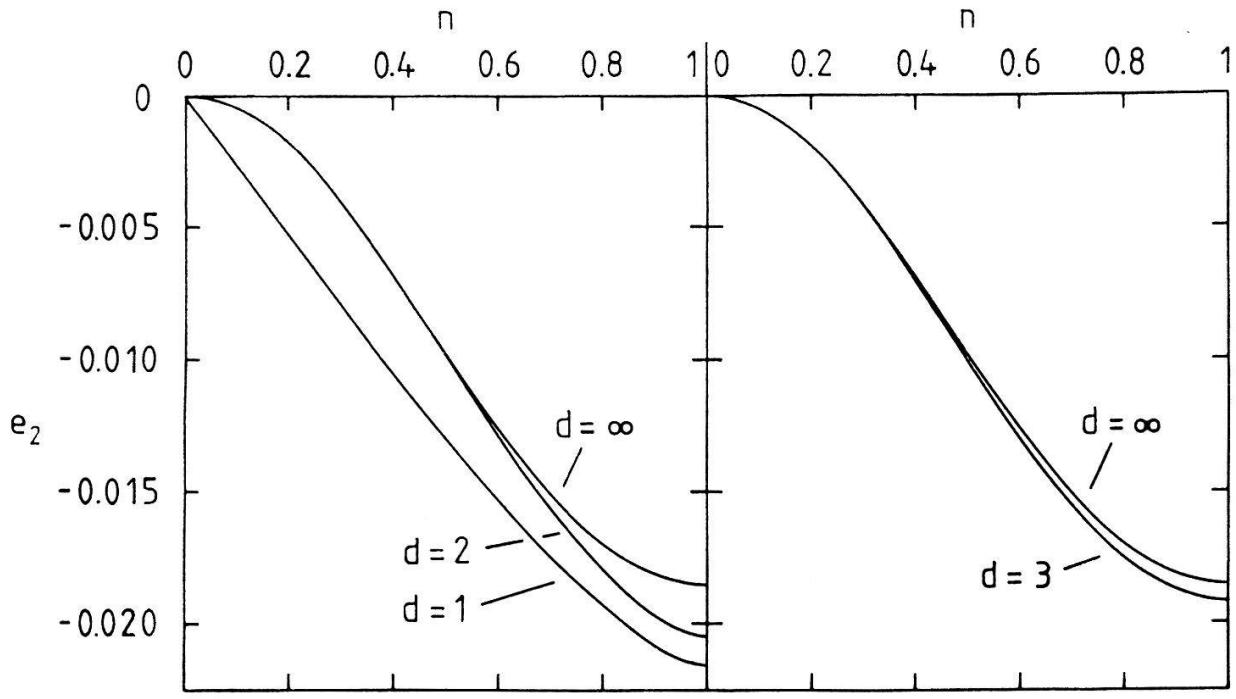

Fig.3: Second order correlation energy of the Hubbard model $e_2 = (E_2/|\bar{\varepsilon}_0|)/(U/|\bar{\varepsilon}_0|)^2$ as a function of the density n for several dimensions d; $|\bar{\varepsilon}_0|$ is the average bandwidth.

Müller-Hartmann [12] calculated the self-energy of the infinite-dimensional Hubbard model in a self-consistent weak coupling expansion. In second order the expressions for the corresponding diagram can again be reduced to a one-dimensional integral. The results show all Fermi liquid features of a correlated Fermi system. Similarly, Schweitzer and Czycholl [13] investigated the periodic Anderson model within a self-consistent perturbation theory in the on-site Coulomb interaction between the f-electrons in $d = \infty$. Such an investigation had not been feasible in finite dimensions, since this requires an enormous numerical effort. The simplification arising in $d = \infty$ reduces these difficulties by several orders of magnitude. At the same time the physical behavior (Fermi liquid properties, spectral density etc.) was found to be essentially the same as that expected for finite dimensions.

It will surely be very interesting to carry out more sophisticated conserving perturbational calculations in $d \to \infty$. In particular, the parquet equations should be tractable in this limit.

Correlated variational wave functions

Variational wave functions play an important role in the investigations of interacting many body systems, and of strongly correlated Fermi systems in particular.[16] They provide an approximate, but explicit and physically intuitive tool for the treatment of correlations and quite generally go beyond the range of perturbation theory. In the case of fermionic lattice models with a strong on-site repulsion $\hat{H}_I$, (1), the suppression of doubly occupied sites is of prime importance. This is achieved by a wave function of the form

$$|\Psi\rangle = g^{\hat{D}} |\Phi_0\rangle \qquad (8)$$

where $\hat{D} \equiv \Sigma_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the number operator for doubly occupied sites, $g \in [0,1]$ is a variational parameter and $|\Phi_0\rangle$ is a one-particle wave function. With $|\Phi_0\rangle$ as the Fermi sea, $|\Psi\rangle$ reduces to the well-known Gutzwiller wave function (GWF).[7] More generally, $|\Phi_0\rangle$ may be chosen as a spin density wave with antiferromagnetic long range order. Insertion of a BCS wave function for $|\Phi_0\rangle$ leads to a resonating valence bond (RVB) state in the limit $g \to 0$, where all doubly occupied sites are projected out.[17]

Evaluations of expectation values

$$\langle\hat{O}\rangle \equiv \frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \qquad (9)$$

of observables $\hat{O}$ in terms of correlated wave functions $|\Psi\rangle$, (8), are extremely difficult. Exact analytic evaluations have so far only been possible for the GWF in d = 1 dimension.[18,19] Numerical investigations of expectation values for finite systems have been initiated by Kaplan, Horsch and Fulde [20] and have recently been performed by several researchers.[21] These calculations gave important insight into the properties of $|\Psi\rangle$, (8), in low dimensions d = 1,2. In d = 3 there are no reliable numerical evaluations, since the largest lattice studied so far contained only 6·6·6 sites.

In this situation an exact evaluation of expectation values in $d = \infty$ combined with a systematic calculation of finite-d corrections is probably the best approach to $d = 3$ and may also supplement the numerical data in $d = 1,2$. Exact evaluations in the limit of high dimensions are indeed possible by using a diagrammatic expansion of expectation values and by exploiting the simplifications of diagrams in $d \to \infty$.[10,22] We will now mention some particularly interesting examples.

(i) $|\Phi_0\rangle$ is chosen as the Fermi see, i.e. $|\Psi\rangle$ corresponds to the Gutzwiller wave function (GWF).[7] The result obtained for the energy expectation value $E(g) = \langle\hat{H}\rangle$ with $\hat{H}$, (3), is the same as that provided by the well-known Gutzwiller approximation (GA) [23], which corresponds to a semi-classical counting method of spin configurations. Hence, the GA becomes the exact result for $\langle\hat{H}\rangle$ within the GWF as $d \to \infty$.

(ii) To take into account the antiferromagnetic tendencies of the Hubbard model for $n \to 1$, $|\Phi_0\rangle$ may be chosen as a spin density wave, i.e.

$$|\Psi\rangle = g^{\hat{D}} \prod_{\sigma} \prod_{k < k_F} (\cos\theta_k \, \hat{a}^{\dagger}_{k\sigma} + \sigma \sin\theta_k \, \hat{a}^{\dagger}_{k+Q,\sigma})|0\rangle \qquad (10)$$

where Q is half a reciprocal lattice vector and $|0\rangle$ is the vacuum. The energy expectation value $E\{g,\theta_k\} = \langle\hat{H}\rangle$, which is a functional of g and θ_k, can be calculated exactly in $d = \infty$ and can be minimized in closed form.[10,22] One finds that the optimal θ_k is in general more complicated than the Hartree-Fock form often used for simplicity in numerical evaluations.[21] The variational energy obtained by inserting the optimal θ_k in $E\{g,\theta_k\}$ is identical to the ground state energy calculated by Kotliar and Ruckenstein [24], who used a slave-boson technique.

(iii) Anderson [17] proposed the so-called resonating valence bond (RVB) state

$$|\Psi\rangle = \lim_{g\to 0} g^{\hat{D}}\,\hat{P}_N\,|\mathrm{BCS}\rangle \qquad (11)$$

as an appropriate ground state to describe high-T_c superconductivity. Here $|\mathrm{BCS}\rangle$ is a BCS wave function and $\hat{P}_N$ projects onto states with a fixed particle number N. A modified version of $|\Psi\rangle$, where $\hat{P}_N$ is omitted, has also been investigated. [21,25] An exact evaluation of expectation values within the latter state is possible in $d \to \infty$ and yields a systematic and consistent single-site approximation. The results for the kinetic energy of holes, which have been calculated for s-wave and d-wave RVB states [26], are in good agreement with numerical results in low dimensions.[21]

(iv) The periodic Anderson model (PAM) involves almost localized f-electrons ($\hat{f}_{k\sigma}$) on a periodic lattice in a sea of conduction electrons ($\hat{a}_{k\sigma}$), which hybridize with the f's. The wave function

$$|\Psi\rangle = \lim_{g\to 0} g^{\hat{D}} \prod_{\sigma} \prod_{k<k_F} [1+ A_\sigma(\mathbf{k})\ \hat{f}^{\dagger}_{k\sigma}\hat{a}_{k\sigma}]\,|\mathrm{cFS}\rangle \qquad (12)$$

has been suggested for an investigation of the correlations within the PAM.[27] Here $|\mathrm{cFS}\rangle$ is the Fermi sea of conduction electrons and $A_\sigma(\mathbf{k})$ describes the hybridization. The variational energy of the PAM within $|\Psi\rangle$, (12), can be evaluated exactly in $d = \infty$ [28] and the results agree with those obtained earlier by semi-classical counting arguments à la Gutzwiller [27], and with those of a slave-boson approach.[24]

(v) Correlation functions within correlated wavefunctions as in (8) have been evaluated exactly in $d = \infty$ by van Dongen, Gebhard and Vollhardt.[29] The result obtained for the nearest-neighbor spin-spin correlation function within the GWF was seen to be identical to that obtained earlier by semi-classical counting methods.[25] However, in general, i.e. for further separations and, in particular, for more refined wave functions, counting methods cannot provide an exact evaluation of correlation functions in $d = \infty$. [30] Using the exact results for the spin-spin correlation function within the GWF in $d = 1$ and $d = \infty$ and employing general scaling arguments,

one can show [29] that the Brinkman-Rice transition [31], i.e. the localization of particles at finite U which is obtained within the Gutzwiller approximation [23], is absent in any finite dimension.

Most recently, Gebhard [30] has worked out an improved, more economic method for the calculation of expectation values within correlated wave functions in high dimensions. He was able to show the general equivalence of variational results based on correlated wave functions $|\Psi\rangle$, (8), in $d \to \infty$ and the slave-boson approach of Kotliar and Ruckenstein.[24] The method is particularly useful for calculating 1/d-corrections. [30] Numerical results obtained for expectation values within the GWF are well described by the analytic expansion up to order 1/d.

Conclusion

Within a short time the limit of infinite lattice dimensions has turned out to be a particularly useful approach to the problem of correlated lattice fermions. While correlations in the many-body system remain non-trivial, theoretical investigations become much simpler than in finite dimensions. This fact, in conjunction with the possibility to calculate explicit 1/d-corrections, gives rise to great hopes for the success of future investigations of correlated lattice fermions in dimensions $1 < d < \infty$.

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