THE HUBBARD MODEL IN INFINITE DIMENSIONS

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INTRODUCTION

Investigations of classical spin systems in the limit of infinite dimensions ($d=\infty$) are well appreciated as a useful concept in statistical physics.[1] An exact solution in $d=\infty$ often provides the correct qualitative behavior of solutions in lower dimensions. In particular, it may serve as a starting point for systematic investigations of finite dimensional systems via 1/d-expansions. Exact solutions for systems with localized spins in $d=\infty$ are generally related to mean field solutions, since fluctuations become unimportant in infinite dimensions. In the case of fermionic systems with mobile degrees of freedom, such as the Hubbard model,[2] mean field solutions are known too, but explicit results for infinite dimensions have so far not been obtained. In fact, exact results for the Hubbard model are only available in $d=1$.[3] Therefore many fundamental questions are still open, for example, whether such quantum mechanical systems become "trivial" in $d=\infty$ and whether their exact solution corresponds to some type of mean field solution. - To answer at least parts of these questions we will first discuss a scaling of the Hubbard model such that in the limit $d=\infty$ a non-trivial model results. We will then investigate this model by calculating the correlation energy in weak coupling and by applying variational techniques.[4]

SCALING OF THE HUBBARD MODEL

The Hubbard model is given by[2]

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

$$\hat{H}_{kin} = \sum_{\sigma} \sum_{i,j} t_{ij}\, \hat{c}^{\dagger}_{i\sigma}\, \hat{c}_{j\sigma} = \sum_{k,\sigma} \varepsilon_k \hat{n}_{k\sigma} \tag{1b}$$

where $\hat{H}_{kin}$ is the kinetic energy operator written in position space and momentum space, respectively. For nearest neighbor

hopping on a hypercubic lattice in d dimensions the energy dispersion has the form

$$\varepsilon_k = -2t \sum_{n=1}^{d} \cos k_n \qquad (2)$$

where $\mathbf{k} = (k_1, \ldots k_d)$. In $d=\infty$ the central limit theorem yields the corresponding density of states (DOS) as

$$N(E) = \frac{\exp[-(E/2t\sqrt{d})^2]}{2t\sqrt{\pi d}} \qquad (3)$$

In $d=\infty$ $N(E)$ is seen to be a Gaussian without van-Hove singularities. To obtain a finite DOS[5] a scaling $t \to t^* = t/\sqrt{2d}$ is required, such that $N(E) \to N^*(E) = \exp(-E^2/2)/\sqrt{2\pi}$, where $t \equiv 1$. The average kinetic energy is then also finite, i.e. $\bar{\varepsilon}_0(n) = -2N^*(E_F)$. In this way one obtains a non-trivial model with competing potential and kinetic energy which are both of the same order of magnitude even in $d=\infty$. The naive scaling $t \to t/d$ would imply $\bar{\varepsilon}_0 = 0$, making (1) a localized model ab initio.

CORRELATION ENERGY

For small U the correlation energy E_c of the Hubbard model can be determined by Goldstone perturbation theory.[6] The second order contribution to the ground state energy in d dimensions for an equal number of up- and down spins ($n_\uparrow = n_\downarrow = n/2$) is effectively given by a 3d-dimensional integral over the Brillouin zone

$$E_2 = \frac{LU^2}{(2\pi)^{3d}} \int \prod_{i=1}^{4} d^d k_i \, \frac{n^0_{k_1} \, n^0_{k_2} \, (1-n^0_{k_3})(1-n^0_{k_4})}{\varepsilon_{k_1} + \varepsilon_{k_2} - \varepsilon_{k_3} - \varepsilon_{k_4}} \, \delta(k_1+k_2+k_3+k_4) \qquad (4)$$

where momentum conservation has been written explicitly and $n^0_k = 1$ for $k<k_F$ and zero elsewhere. L is the number of lattice sites. Writing the denominator z as $\exp(-\lambda z)$ and integrating over λ and expressing the δ-function as $\delta(\mathbf{k}) = (2\pi)^{-d} \Sigma_f \exp(i\mathbf{k}\cdot\mathbf{f})$, one obtains

$$E_2/LU^2 = -\int_0^\infty d\lambda \sum_f [F^+(\lambda,f)]^2 \, [F^-(\lambda,f)]^2 \qquad (5)$$

where $F^\pm(\lambda,f)$ are the Fouriertransforms of $n^0_k \exp(\lambda\varepsilon_k)$ and $(1-n^0_k)\exp(-\lambda\varepsilon_k)$, respectively. Since $\Sigma_f[F^\pm(\lambda,f)]^2$ is finite for all d and since the number of nearest neighbors of site f=0 increases proportional to d, $F^\pm(\lambda;f')$ vanishes at least as $1/\sqrt{d}$ for $d\to\infty$ for f' nearest neighbor to f=0. Analogous arguments hold for next-nearest neighbors etc. Consequently, only the term with f=0 contributes to (5) (i.e. $\delta(k_1+k_2+k_3+k_4) \to 1$ in (4)), such that the momentum-integrals in $F^\pm(\lambda,0)$ now depend on the momenta only via the corresponding <u>energies</u>. By use of the DOS $N^*(E)$ one finally finds

$$E_2/LU^2 = -\int_0^\infty d\lambda \, e^{2\lambda^2} P^2(E_F - \lambda) P^2(-E_F - \lambda) \qquad (6)$$

with P(x) as the probability function. The result for E_2 in $d=\infty$ is therefore seen to be particularly simple. The reason

for this is that for an arbitrary choice of momenta meeting at a vertex the corresponding energies are randomized by Umklapp-processes which makes them mutually independent. This allows one to go from a momentum integration to an energy integration. - The result for E_2 as a function of density n is shown in Fig. 1 together with the results in d = 1,2,3. The result for d=3, which can only be obtained by Monte-Carlo integration, is obviously very well approximated by that in d=∞, which is so simple to calculate. For n not too close to n=1 even the result for d=2 is well approximated by that in d=∞, while the case d=1 is quite distinct from all finite dimensions. - The existence of a finite U^2-contribution to E_c for small U shows that the mean field solution obtained within unrestricted Hartree-Fock cannot be exact in d=∞ since in that solution an asymptotic expansion yields $E_2 = 0$.

VARIATIONAL WAVE FUNCTIONS

Simplifications similar to those described above also occur in the evaluation of expectation values $\langle\hat{O}\rangle = \langle\Psi|\hat{O}|\Psi\rangle/\langle\Psi|\Psi\rangle$ in terms of generalized Gutzwiller wave functions

$$|\Psi\rangle = g^{\hat{D}} |\Phi_0\rangle \qquad (7)$$

in d = ∞. Here $|\Phi_0\rangle$ is an arbitrary, not necessarily translational invariant one-particle wave function, $g \in [0,1]$ is a variational parameter and $\Sigma_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \hat{D}$, the interaction part of (1a), counts the doubly occupied sites. The actual Gutzwiller wave function (GWF)[8] is obtained with $|\Phi_0\rangle$ as the simple Fermi sea.

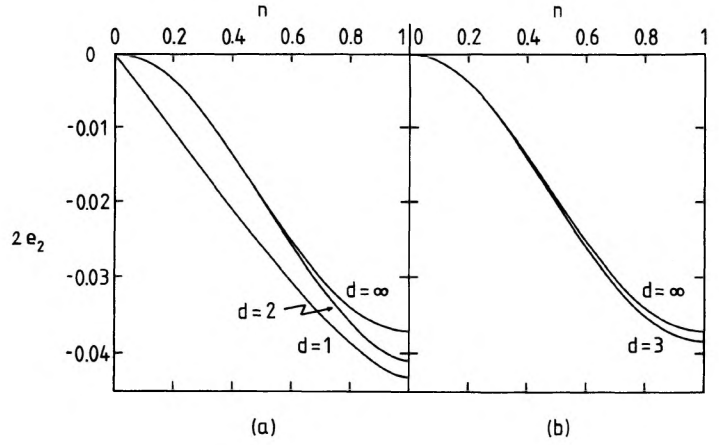

Fig. 1. The second order contribution to the correlation energy $E_2=e_2(LU^2/|\bar{\varepsilon}_0(1)|)$ as a function of density n for various dimensions d; (a) d=1,2,∞, (b) d=3,∞.

Expectation values $\langle\hat{O}\rangle$ can be expanded in powers of (g^2-1) by using standard field-theoretical methods and their diagrammatic representation in analogy with the Green's function approach to a Φ^4-theory.[10] In particular, the ensueing diagrams may be conveniently expressed by the "self energy" S.[4] Thereby the one-particle density matrix $P_{\sigma fh} \equiv \langle\hat{c}^+_{f\sigma}\hat{c}_{h\sigma}\rangle$, which determines the momentum distribution and thus the kinetic energy in (1a) and the interaction term in (1a) are determined on the same footing:

$$P_{\sigma fh} = P^0_{\sigma fh} + 1_{fh}\,[(1-g^2)(P^0_\sigma S_\sigma)_{ff} - (S_\sigma)_{ff}]\,/(1+g)^2$$

$$+ \,[(P^0_\sigma-(1+g)^{-1})S_\sigma(P^0_\sigma-(1+g)^{-1})]_{fh} \qquad (8a)$$

$$\langle\hat{D}\rangle = \frac{g^2}{1-g^2}\,\frac{1}{L}\,\mathrm{Tr}(P^0_\sigma S_\sigma) \qquad (8b)$$

Here $P^0_{\sigma fh} = \langle\phi_0|\hat{c}^+_{f\sigma}\hat{c}_{h\sigma}|\phi_0\rangle$ and P^0_σ, P_σ, S_σ are taken as matrices with elements $S_{\sigma fh}$ etc. and $\mathrm{Tr}(\,) = \Sigma_f(\,)_{ff}$.

For large d the evaluation of diagrams is again greatly simplified, since - as in the case of $F^\pm$ in (5) - $P^0_{\sigma fh}$ vanishes as least as $1/\sqrt{d}$ for $f\neq h$. We now consider two vertices f,h in a diagram which are connected by three or more separate paths. The evaluation of the diagram involves the lattice sum over f,h and all the other vertices. Since the contributions from $f\neq h$ are suppressed at least as $1/\sqrt{d}$, only the on-site (f=h) terms remain in $d=\infty$, i.e. the two vertices collapse into a <u>single</u> vertex. In particular, the proper self-energy $S^*_{\sigma fh}$, defined as the sum over all one-particle irreducible diagrams, now becomes diagonal, i.e. $S^*_{\sigma fh} \equiv \delta_{fh}S^*_{\sigma f}$. S^* can be written as a sum over all skeleton diagrams with dressed lines $\bar{P}=P^0+P^0SP^0$. In $d=\infty$ all the vertices of a skeleton diagram are then seen to collapse into one vertex. The structure of the collapsed skeleton diagrams is so simple that an exact summation is possible, yielding

$$S^*_{\sigma f} = -\frac{1}{2\,\bar{P}_{\sigma ff}}\,\left[1 - \sqrt{1+4(1-g^2)\bar{P}_{\sigma ff}\bar{P}_{-\sigma ff}}\;\right] \qquad (9)$$

This, together with the Dyson equation, determines S* and S for given P^0 and g.

One is now in the position to evaluate the Hubbard-Hamiltonian in terms of arbitrary variational wave functions of the form (7) in $d=\infty$. For example, $|\Phi_0\rangle$ in (7) may be choosen as a Hartree-Fock spin density wave with antiferromagnetic long range order

$$|\Psi_{AF}\rangle = g^{\hat{D}} \prod_\sigma \prod_{k<k_F} \left[\cos\,\theta_k\hat{a}^+_{k\sigma} + \sigma\,\sin\,\theta_k\hat{a}^+_{k+Q}\right]|0\rangle \qquad (10)$$

where $Q = (\pi,\ldots,\pi)$ is half a reciprocal lattice vector. This wave function has already been investigated in detail. Using the above formalism and employing the remaining translational invariance on A- and B-sublattices, the ground state energy $E\{g;\theta_k\} = \langle H\rangle$ is obtained as a functional of g and θ_k. The minimization of E can be performed in closed form, i.e. without assuming any particular form for the function θ_k. The

optimal θ_k is in general different from the Hartree-Fock form[7] which has been used in numerical calculations.[11] E may equivalently be expressed as a function of the sublattice magnetization $m \equiv |< \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} >|$ and the density of doubly occupied sites $\bar{d} \equiv L^{-1} <\hat{D}>$ as

$$E(m,\bar{d})/L = q\bar{\varepsilon}_{HF}(m) + U\bar{d} \tag{11}$$

where $\bar{\varepsilon}_{HF}(m)$ is the result for the kinetic energy within unrestricted Hartree-Fock,[7] and

$$q = \frac{4(n-2\bar{d})\sqrt{\bar{d}\ (\bar{d}+ 1- n)} + 2(2\bar{d}+ 1- n)\sqrt{(n -2\bar{d})^2 - m^2}}{\sqrt{(n^2 - m^2)\ [\ (2- n)^2 - m^2\ ]}} \tag{12}$$

is a renormalization factor. This result is identical to the result of a slave boson approximation by Kotliar and Ruckenstein.[12] Here we have found an explicit wave function, $|\Psi_{AF}>$, for which this result is exact in $d=\infty$.[4] Assuming $m = 0, |\Psi_{AF}>$ in (10) reduces to the GWF [8] and (12) becomes identical to the formula of the much-employed, semi-classical Gutzwiller approximation.[8,13] Therefore the Gutzwiller approximation provides an exact evaluation of the GWF in $d= \infty$.[4]

For $n = 1$ the minimization of the energy $E(m,\bar{d})$ obtained with the more general wave function (10) yields $m > 0$ (antiferromagnetic insulator) and $q < 1$ for all $U > 0$, in contrast to earlier attempts to generalize the Gutzwiller approximation to antiferromagnetism.[14] For $U \to \infty$, $|\Psi_{AF}>$ approaches the Neél state. For $0.85 < n < 1$ there exists a bounded regime in U with $m > 0$, while for smaller densities m is always zero. The fact that the minimum of E is attained for $g < 1$, shows that the additional correlations, introduced by the factor $g^{\hat{D}}$ into the antiferromagnetic starting wave function in (10), are important for all n and $U > 0$.

SUMMARY

The Hubbard model has been investigated in the limit of infinite spatial dimensions. The most important finding is that the model possesses a non-trivial limit, where diagrammatic calculations are substantially simpler than in finite dimensions. The weak coupling correlation energy is found to be a very good approximation for d = 3. As to variational wave functions, the results of the wellknown Gutzwiller approximation[8,13] and of a recent slave boson approach[12] have been recovered by evaluating a class of variational wave functions exactly in $d = \infty$. - The concept derived here is equally applicable to the evaluation of correlation functions[15] and to the general Green's function approach for the Hubbard model and related models.[16]

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