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Angaben zur Veröffentlichung / Publication details:

Metzner, Walter, and Dieter Vollhardt. 1989. "The Hubbard model in infinite dimensions." In *Interacting electrons in reduced dimensions*, edited by Dionys Baeriswyl and David K. Campbell, 129–34. Boston, MA: Springer US.
https://doi.org/10.1007/978-1-4613-0565-1_15.

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.

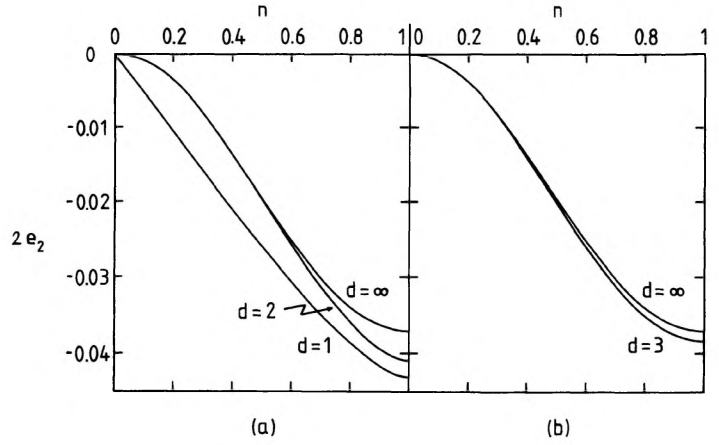

Fig. 1. The second order contribution to the correlation energy $E_2=e_2(LU^2/|\bar{\varepsilon}_0(1)|)$ as a function of density n for various dimensions d; (a) d=1,2,∞, (b) d=3,∞.

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]

References

1. See, for example, H. E. Stanley in Phase Transitions and Critical Phenomena, vol. 3 , eds. C. Domb and M.S. Green (Academic Press, London, 1974), p. 485.
2. M. C. Gutzwiller, Phys. Rev. Lett. 10 159 (1963); J. Hubbard, Proc. R. Soc. London, A276 238 (1963); J. Kanamori, Prog. Theor. Phys. 30 275 (1963).
3. E. H. Lieb and F.Y. Wu, Phys. Rev. Lett. 20 1445 (1968).
4. W. Metzner and D. Vollhardt, Phys. Rev. Lett., in press (January 16, 1989).
5. U. Wolff, Nucl. Phys B225 391 (1983).
6. W. Metzner and D. Vollhardt, Phys. Rev. B (in press).
7. D. R. Penn, Phys. Rev. 142 350 (1966); M. Cyrot; J. Physique 33 125 (1972).
8. M. C. Gutzwiller, Phys. Rev. A137 1726 (1965).
9. For a review, see the accompanying article by D. Vollhardt appearing in this volume of the proceedings.
10. W. Metzner and D. Vollhardt, Phys. Rev. Lett. 59 121 (1987); Phys. Rev. B37 7382 (1988).
11. H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 56, 3582 (1987).
12. G. Kotliar and A.E. Ruckenstein, Phys. Rev. Lett. 57 1362 (1986) .
13. For a detailed discussion, see D. Vollhardt, Rev. Mod. Phys. 56, 99 (1984) ; D. Vollhardt, P. Wölfle and P. W. Anderson, Phys. Rev. B35 6703 (1987).
14. T. Ogawa, K. Kanda and T. Matsubara, Prog. Theor. Phys. 53 614 (1975); F. Takano and M. Uchinami, Prog. Theor. Phys. 53 1267 (1975); J. Florencio and K.A. Chao,Phys. Rev. B14 3121 (1976).
15. See the accompanying article by F. Gebhard and D. Vollhardt appearing in this volume of the proceedings.
16. E. Müller-Hartmann, preprint; G. Czycholl, preprint.