Correlated Lattice Fermions in $d=\infty$ Dimensions

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We show that even in $d=\infty$ dimensions the Hubbard model, when scaled properly, describes nontrivial correlations among fermions. Diagrammatic treatments are found to be substantially simpler than in finite dimensions. The weak-coupling correlation energy is seen to be a good approximation for that in $d=3$. Recent approximations based on slave-boson techniques are recovered by the exact evaluation of explicit variational wave functions in $d=\infty$.

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The spin-$\frac{1}{2}$, single-band Hubbard model[1] for interacting fermions on a lattice plays a particularly important role in condensed-matter physics. In spite of its apparent simplicity, exact solutions have so far only been possible in $d=1$ space dimension.[2] However, 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 $d=3$. There is another limiting dimension, $d=\infty$, where exact solutions have been obtained for various, mostly classical, spin systems.[3] In this case there exist close relations to mean-field-type solutions. In the case of the Hubbard model, an exact solution in $d=\infty$ is not available so far.

In this Letter properties of the Hubbard model in $d=\infty$ will be discussed. The Hubbard Hamiltonian[1] has the form

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

$$\hat{H}_{\rm kin}=\sum_{\sigma}\sum_{i,j} t_{ij}\hat{c}^{+}_{i\sigma}c^{+}_{j\sigma}=\sum_{k,\sigma}\epsilon_{\mathbf{k}}\hat{n}_{\mathbf{k}\sigma}\,, \tag{1b}$$

where $\hat{H}_{\rm kin}$ is the kinetic-energy operator expressed in position space and momentum space, respectively. For next-neighbor hopping on a d-dimensional simple cubic lattice with unit lattice spacing, we have

$$\epsilon_{\mathbf{k}}=-2t\sum_{j=1}^{d}\cos k_j\,, \tag{2}$$

where t is the hopping amplitude and $\mathbf{k}=(k_1,\ldots,k_d)$.

For $d\to\infty$, the on-site interaction is still well defined but the hopping rate in the kinetic energy has to be scaled properly to yield a nontrivial model. This is most easily seen from the corresponding density of states (DOS) for $U=0$, which in $d=\infty$ is determined by the central-limit theorem as

$$D(E)\underset{d\to\infty}{=}\frac{1}{2t(\pi d)^{1/2}}\exp[-(E/2t\sqrt{d})^2]\,. \tag{3}$$

Clearly, only the scaling $t=t^*/(2d)^{1/2}$ with fixed t^* (henceforth $t^*\equiv 1$) yields a finite DOS[4] and thereby leads to a finite average kinetic energy $\bar{\epsilon}_0(n_\uparrow,n_\downarrow)$ of the noninteracting particles for arbitrary densities $n_\uparrow,n_\downarrow$. Any other scaling makes $\bar{\epsilon}_0(n_\uparrow,n_\downarrow)$ either zero or infinite so that the model becomes immediately trivial.

We have recently shown that for weak coupling the correlation energy of the Hubbard model in $d=1,2,3$ can be calculated within ordinary Goldstone perturbation theory.[5] In particular, in the limit $d\to\infty$, the evaluation of the corresponding diagrams is greatly simplified. This may be demonstrated in the case of the second-order contribution given by

$$E_2=\frac{LU^2}{(2\pi)^{3d}}\int d\mathbf{k}\,d\mathbf{k}'\,d\mathbf{q}\,\frac{n^0_{\mathbf{k}\uparrow}n^0_{\mathbf{k}'\downarrow}(1-n^0_{\mathbf{k}+\mathbf{q}\uparrow})(1-n_{\mathbf{k}'-\mathbf{q}\downarrow})}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}'-\mathbf{q}}}\,, \tag{4}$$

where the integrations extend over a Brillouin zone; here $n^0_{\mathbf{k}\sigma}\equiv 1$ for $|\mathbf{k}|<k_{F\sigma}$ and zero elsewhere, and L is the number of lattice sites. If we write the energy denominator in (4) as an integral over an exponential factor, and express momentum conservation in (4) explicitly by an integral over a δ function, which is then converted into a lattice sum via $\delta(\mathbf{k})=(2\pi)^{-d}\sum_{\mathbf{f}}\exp(i\mathbf{k}\cdot\mathbf{f})$, (4) is written as

$$E_2/LU^2=-\int_0^\infty d\lambda\sum_{\mathbf{f}}F^{+}_{\uparrow}(\lambda;\mathbf{f})F^{+}_{\downarrow}(\lambda;\mathbf{f})F^{-}_{\uparrow}(\lambda;\mathbf{f})F^{-}_{\downarrow}(\lambda;\mathbf{f})\,. \tag{5}$$

Here $F^{+}_{\sigma}(\lambda;\mathbf{f})$, $F^{-}_{\sigma}(\lambda;\mathbf{f})$ are the Fourier transforms of $n^0_{\mathbf{k}\sigma}\exp(\lambda\epsilon_{\mathbf{k}})$ and $(1-n^0_{\mathbf{k}\sigma})\exp(-\lambda\epsilon_{\mathbf{k}})$, respectively. If we make use of the fact that $\sum_{\mathbf{f}}[F^{\pm}_{\sigma}(\lambda;\mathbf{f})]^2$ is finite and count the number of nearest neighbors, next-nearest neighbors, etc., of the site $\mathbf{f}=0$, it follows that $F^{\pm}_{\sigma}(\lambda;\,\mathbf{f}\neq 0)$ vanishes at least as $1/\sqrt{d}$ for $d\to\infty$. Consequently, the off-site ($f\neq 0$) contributions in (5) vanish as $1/d$, such that only the $\mathbf{f}=0$ term remains. Using the DOS (3) we thus find

$$E_2/LU^2=-\int_0^\infty d\lambda\, e^{2\lambda^2}\prod_{\sigma}P(E_{F\sigma}-\lambda)P(-E_{F\sigma}-\lambda)\,. \tag{6}$$

Here $P(x)$ is the Gaussian probability function. Hence the evaluation of E_2 for $d \to \infty$ is seen to reduce to a *single* integral over probability functions and is therefore the simplest of all dimensions. The simplification is due to the fact that in $d=\infty$, and for an arbitrary choice of the momenta $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{q}$ in (4), the energies $\epsilon_{\mathbf{k}}$, $\epsilon_{\mathbf{k}'}$, $\epsilon_{\mathbf{k}+\mathbf{q}}$, and $\epsilon_{\mathbf{k}'-\mathbf{q}}$ are randomized by umklapp processes generated when the lattice momenta are added.[6] Hence the energies become mutually *independent*, which allows one to replace the momentum integrations in (4) by energy integrations over the DOS (3). The energy E_2, plotted as a function of density n ($n_\uparrow = n_\downarrow = n/2$), is shown in Fig. 1 in comparison with the respective numerical evaluation for $d=1$ and 3.[5] The result for $d=\infty$ is seen to be very close to that for $d=3$ and can therefore be considered as an easily tractable, reliable approximation. The existence of a nonzero second-order contribution to the exact ground-state energy also shows that the antiferromagnetic Hartree-Fock approximation[7] is *not* the exact result even in $d=\infty$, since the asymptotic expansion of the latter terminates after the linear term in U.

We note that $F_\sigma^+(0;\mathbf{f}-\mathbf{h})$ is just the one-particle density matrix of the noninteracting system

$$F_\sigma^+(0;\mathbf{f}-\mathbf{h}) = P^0_{\sigma,\mathbf{fh}} \equiv \langle \Phi_0 | \hat{c}^+_{\mathbf{f}\sigma} \hat{c}_{\mathbf{h}\sigma} | \Phi_0 \rangle ,$$

where $|\Phi_0\rangle$ is the noninteracting ground state. Hence $P^0_{\sigma,\mathbf{fh}}$ vanishes at least as $1/\sqrt{d}$ for $d \to \infty$, if $\mathbf{f} \neq \mathbf{h}$. The result remains true even if $|\Phi_0\rangle$ is chosen to be a more general one-particle wave function, e.g., a Hartree-Fock spin-density wave. This property allows for an exact evaluation of expectation values $\langle \hat{0} \rangle = \langle \Psi | \hat{0} | \Psi \rangle / \langle \Psi | \Psi \rangle$ in terms of variational wave functions of the form

$$|\Psi\rangle = g^{\hat{D}} |\Phi_0\rangle , \tag{7}$$

which are generalizations of the Gutzwiller wave function.[8] Here $|\Phi_0\rangle$ is an arbitrary, not necessarily translationally invariant, one-particle wave function, g is a variational parameter, $0 \le g \le 1$, and $\hat{D} = \sum_i \hat{D}_i = \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ is the number operator for doubly occupied sites. Generalizations of $|\Phi_0\rangle$ to BCS-type wave functions, leading to a resonating-valence-bond-type state in the limit $g=0$,[9] are only slightly more complicated. The case where $|\Phi_0\rangle$ is a simple Fermi sea has already been discussed earlier,[6] where it was shown that an analytic evaluation of ground-state properties of the Hubbard model is possible in $d=1$. This earlier analysis may be simplified and further generalized by employment of well known many-body techniques. To this end we recall that the diagrams which determine the one-particle density matrix $P_{\sigma,\mathbf{fh}} = \langle \hat{c}^+_{\mathbf{f}\sigma} \hat{c}_{\mathbf{h}\sigma} \rangle$ are identical in form to the ones for the two-point functions of a Φ^4 theory with lines corresponding to $P^0_{\sigma,\mathbf{fh}}$. In analogy to the diagrammatic representation of Green's functions, one may therefore define a "self-energy" $S_{\sigma,\mathbf{fh}}$, which is built up by the same diagrams as the self-energy for Green's functions, and a "proper" self-energy $S^*_{\sigma,\mathbf{fh}}$ being the sum over all one-particle irreducible diagrams. S_σ and S^*_0 are related by the usual Dyson equation. The one-particle density matrix then takes the form

$$P_{\sigma,\mathbf{fh}} = P^0_{\sigma,\mathbf{fh}} + \mathbf{1}_{\mathbf{fh}} \left(\frac{1-g}{1+g} P^0_\sigma S_\sigma - \frac{S_\sigma}{(1+g)^2} \right)_{\mathbf{ff}} + \left[\left(P^0_\sigma - \frac{1}{1+g} \right) S_\sigma \left(P^0_\sigma - \frac{1}{1+g} \right) \right]_{\mathbf{fh}} . \tag{8}$$

Here P_σ, P^0_σ, and S_σ are taken as matrices, with $\mathbf{1}$ as the unit matrix, with elements $P_{\sigma,\mathbf{fh}}$, etc. The expectation value for the interaction term of the Hubbard Hamiltonian can be expressed in terms of S as

$$\bar{d} \equiv L^{-1} \langle \hat{D} \rangle = L^{-1} [g^2/(1-g^2)] \mathrm{Tr}(P^0_\sigma S_\sigma) , \tag{9}$$

where $\mathrm{Tr}(\,) = \sum_{\mathbf{f}} (\,)_{\mathbf{ff}}$. To investigate the consequences of the fact that $P^0_{\sigma,\mathbf{fh}}$, $\mathbf{f} \neq \mathbf{h}$, vanishes at least as $1/\sqrt{d}$ for $d \to \infty$, we consider a diagram in which two vertices $\mathbf{f},\mathbf{h}$ are connected by three or more separate paths. The evaluation of the diagram involves the lattice sum over $\mathbf{f},\mathbf{h}$ and all other vertices. However, the contributions from $\mathbf{f} \neq \mathbf{h}$, are suppressed by factors of order $1/\sqrt{d}$. Consequently, in the limit $d \to \infty$, only the on-site terms ($\mathbf{f}=\mathbf{h}$) remain, i.e., the two vertices collapse into a single vertex. Consequently, since external vertices of proper diagrams are always connected by three separate paths, $S^*_{\sigma,\mathbf{fh}}$ is seen to be *diagonal*, i.e., $S^*_{\sigma,\mathbf{fh}} \equiv \delta_{\mathbf{fh}} S^*_{\sigma\mathbf{f}}$.

As a first application, we treat the simple Gutzwiller wave function[8] with $|\Phi_0\rangle$ in (7) given by the Fermi sea. Because of translational invariance $S^*_{\sigma\mathbf{f}}$ is independent of $\mathbf{f}$: $S^*_{\sigma\mathbf{f}} = S^*_\sigma$ for all $\mathbf{f}$. The evaluation of $\langle \hat{n}_{\mathbf{k}\sigma} \rangle$, the Fourier transform of $P_{\sigma,\mathbf{fh}}$ in (8), and of $\langle \hat{D} \rangle$ in (9) is thus reduced to the calculation of a single *number* S^*_σ.

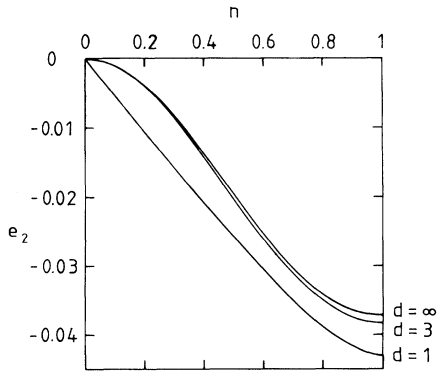

FIG. 1. Second-order correlation energy $e_2 \equiv E_2/[LU^2/|\bar{\epsilon}_0(\frac{1}{2},\frac{1}{2})|]$ vs density for lattice dimensions $d=1$, 3, and ∞.

With $L^{-1}\sum_{\mathbf{k}} n_{\mathbf{k}\sigma}=n_\sigma$ the latter is determined by a quadratic equation, yielding

$$S_\sigma^*=\{A_\sigma-[A_\sigma^2-4(1-g^2)(1-n_\sigma)n_{-\sigma}]^{1/2}\}/2(1-n_\sigma)\,, \tag{10}$$

with $A_\sigma=1-(1-g^2)(n_\sigma-n_{-\sigma})$. By Dyson's equation, the self-energy $S_\sigma(\mathbf{k})$ is then given by $S_\sigma=S_\sigma^*/(1-S_\sigma^*)$ for $k<k_{F\sigma}$ and by $S_\sigma=S_\sigma^*$ for $k>k_{F\sigma}$. The momentum distribution $\langle\hat{n}_{\mathbf{k}\sigma}\rangle$ is therefore a step function with a discontinuity

$$q_\sigma=1-[S_\sigma^*/(1+g)^2][1-g^2/(1-S_\sigma^*)]$$

and

$$\langle\hat{D}\rangle=L[g^2 n_\sigma/(1-g^2)]S_\sigma^*/(1-S_\sigma^*)\,.$$

These are precisely the results of the Gutzwiller *approximation*[8] (for a detailed discussion, see Ref. 10), which is therefore seen to become the exact result for the expectation value of $\hat{H}$ in terms of the Gutzwiller wave function in the limit $d=\infty$.[6]

To determine $S_{\sigma\mathrm{f}}^*$ for general starting wave functions $|\Phi_0\rangle$ we introduce skeleton diagrams by defining dressed lines $\bar{P}_\sigma=P_\sigma^0+P_\sigma^0 S_\sigma P_\sigma^0$. The first three diagrams appearing in a skeleton expansion of S^* are shown in Fig. 2. Solid (broken) loops correspond to factors $\bar{P}_{\uparrow\mathrm{ff}}$ ($\bar{P}_{\downarrow\mathrm{ff}}$). Because of their simple structure, the collapsed skeleton diagrams can be summed up exactly, yielding

$$S_{\sigma\mathrm{f}}^*=-\{1-[1+4(1-g^2)\bar{P}_{\sigma,\mathrm{ff}}\bar{P}_{-\sigma,\mathrm{ff}}]^{1/2}\}/2\bar{P}_{\sigma,\mathrm{ff}}\,, \tag{11}$$

which, together with the definition of $\bar{P}_\sigma$ and the Dyson equation, determines $S_{\sigma\mathrm{f}}^*$ and $S_{\sigma,\mathrm{fh}}$ for given $P_{\sigma,\mathrm{fh}}^0$ and g. We note that the series of diagrams in Fig. 2 contains all diagrams, i.e., does not represent a particular subclass.

The above formalism enables one to evaluate the Hubbard Hamiltonian in terms of increasingly refined wave functions. For example, $|\Phi_0\rangle$ in (7) may allow for antiferromagnetic long-range order

$$|\Psi_{\mathrm{AF}}\rangle=g^{\hat{D}}\prod_\sigma\prod_{|\mathbf{k}|<k_F}[\cos\theta_{\mathbf{k}}\hat{a}_{\mathbf{k}\sigma}^+ +\sigma\sin\theta_{\mathbf{k}}\hat{a}_{\mathbf{k}+\mathbf{Q},\sigma}^+]\,|0\rangle\,. \tag{12}$$

Here $\mathbf{Q}$ is half a reciprocal-lattice vector, for which the perfect nesting property $\epsilon_{\mathbf{k}+\mathbf{Q}}=-\epsilon_{\mathbf{k}}$ is supposed to be valid (AB lattice). For detailed numerical investigations of $|\Psi_{\mathrm{AF}}\rangle$ in $d=1,2$, see Ref. 11. In the case of $|\Psi_{\mathrm{AF}}\rangle$, $P_{\sigma,\mathrm{fh}}^0$ is no longer translationally invariant, although translations among points of the A- and the B-type sublattice, respectively, are still allowed. This particular situation may be treated conveniently by the introduction of a matrix representation distinguishing between translations from A to A, A to B, B to A, and B to B.

The ground-state energy $E\{g;\theta_{\mathbf{k}}\}=\langle\hat{H}\rangle$ is then obtained as a functional of g and $\theta_{\mathbf{k}}$. The minimization with respect to the function $\theta_{\mathbf{k}}$ can be performed exactly yielding

$$|\sin 2\theta_{\mathbf{k}}|=\frac{[\mu/(\mu^2-1)]\epsilon_{\mathbf{k}}^2+\Delta(\epsilon_{\mathbf{k}}^2+\Delta^2)^{1/2}}{[\mu^2/(\mu^2-1)]\epsilon_{\mathbf{k}}^2+\Delta^2}\,, \tag{13}$$

where μ is a parameter related to g and Δ parametrizes the sublattice magnetization

$$m\equiv|\langle n_{i\uparrow}-n_{i\downarrow}\rangle|=2\Delta L^{-1}\sum_{|\mathbf{k}|<k_F}(\epsilon_{\mathbf{k}}^2+\Delta^2)^{-1/2}\,.$$

We note that $\theta_{\mathbf{k}}$ in (13) is, in general, different from the Hartree-Fock form, which has been used in numerical calculations,[11] and which is seen to be a special case ($g=1$, i.e., $\mu=-\infty$). If we use (13) and express $E\{g;\theta_{\mathbf{k}}\}$ in terms of m and $\bar{d}$ (9), E may be cast into the form

$$E(m,\bar{d})/L=q\bar{\epsilon}_{\mathrm{HF}}(m)+U\bar{d}\,, \tag{14a}$$

where $\bar{\epsilon}_{\mathrm{HF}}(m)$ is the antiferromagnetic Hartree-Fock result for the kinetic energy and

$$q=\frac{4(n-2\bar{d})[\bar{d}(\bar{d}+1-n)]^{1/2}+2(2\bar{d}+1-n)[(n-2\bar{d})^2-m^2]^{1/2}}{\{(n^2-m^2)[(2-n)^2-m^2]\}^{1/2}} \tag{14b}$$

is a renormalization factor. The minimization of E with respect to $m,\bar{d}$ has to be performed numerically. The result (14) is seen to be identical to that by Kotliar and Ruckenstein,[12] who obtained their results by a slave-boson technique. Here we have constructed the explicit *wave function* $|\Psi_{\mathrm{AF}}\rangle$, for which this result is exact in the limit $d=\infty$.

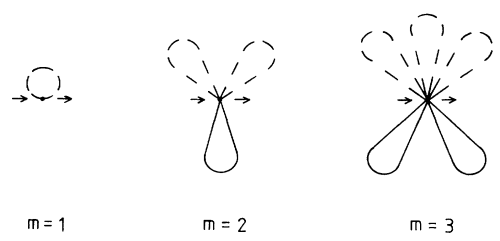

FIG. 2. Skeleton diagrams for the first three orders of the proper self-energy.

For $n=1$, the minimization shows that for all $U>0$ one has $m>0$ and $q<1$, i.e., there is a transition at $U=0$ to an antiferromagnetic insulator as is expected from the perfect nesting property. This is in contrast to earlier attempts to generalize the Gutzwiller approximation to the antiferromagnetic case.[13] The energy is always lower than that obtained by use of the Gutzwiller wave function or the Hartree-Fock results. For $U\to\infty$, $|\Psi_{\mathrm{AF}}\rangle$ approaches the Néel state which is, in fact, the *exact* ground state of the half-filled Hubbard model in $d=\infty$ for large U.[14] [However, for smaller U neither $|\Psi_{\mathrm{AF}}\rangle$ (12) nor the Gutzwiller wave function is the exact ground state in $d=\infty$, e.g., they yield only 85% of the

exact second-order correlation energy E_2 (6).] For less than half-filling there exists a critical density $n_c \approx 0.85$ below which $m=0$ for all U, while for $n_c < n < 1$ there exists a bounded regime in U with $m > 0$. One finds $q < 1$ for all n and $U > 0$.

In summary, we have investigated the Hubbard model in the limit $d=\infty$ using perturbation theory and variational wave functions. Applying well known many-body techniques to the case $d=\infty$, we have shown that (i) in $d=\infty$ the diagrammatic calculation of ground-state properties is greatly simplified; (ii) at least in the weak-coupling limit, the correlation energy in $d=3$ is very close to that in $d=\infty$; (iii) the mean-field antiferromagnetic Hartree-Fock solution does *not* yield the exact results in $d=\infty$; (iv) calculations with variational wave functions of increasing refinement are analytically tractable. In this way the results of several well known approximations[8,12] used in finite-dimensional systems are recovered. The methods developed here for $d=\infty$ may equally be used to study correlation functions and other Hamiltonians such as the periodic Anderson model.[15] In particular, our results should also be valuable for the investigation of these models within a general Green's-function approach. Indeed, preliminary results for the Hubbard model in $d=\infty$, obtained by application of the above methods and ideas to the one-particle propagator, are very promising.[16]

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