Correlated fermions on a lattice in high dimensions

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The limit of infinite dimension of the Hubbard model was recently introduced by Metzner and Vollhardt as a new type of model with interesting implications. In the present paper the same limit is applied to a family of lattice fermion models with generalized kinetic and potential energies. A simple method is introduced for investigating the important issue of handling momentum conservation at the interaction vertices. It is shown that the irrelevance of momentum conservation found by Metzner and Vollhardt applies more generally than their Gaussian density of states. Interactions between particles on different sites are shown to simplify to their Hartree substitute. This leaves on-site interactions as the only dynamical interactions in the limit of infinite dimension.

I. Introduction

Spins or other localized degrees of freedom on lattices of high dimensions $D$ are well understood: Due to its many neighbors each spin sees only small fluctuations in its effective field. This not only suppresses critical fluctuations for dimensions above a finite upper critical dimension but also makes the mean field approximation exact in the limit of $D \to \infty$.

One might ask if systems with mobile degrees of freedom, e.g. with interacting fermions, have the same tendency to get trivial in the limit of infinite dimension. What is the nature of the simplification that results in such systems from the limit $D \to \infty$? This question was recently asked by Metzner and Vollhardt [1] who showed that the free particle density of states becomes Gaussian and that momentum conservation at all skeleton vertices can be disregarded for a Hubbard model on a simple cubic lattice of infinite dimensions. Metzner and Vollhardt used these results to calculate the second order correlation energy and to evaluate the properties of variational wavefunctions. The overall conclusion to be drawn from their work is that fermion systems get much simpler in high dimensions but that they keep away from getting trivial.

In the present paper we present a simple method for demonstrating the basic findings of Metzner and Vollhardt (MV). We will rederive their results using our method in Sect. 2. This method is also able to yield corrections to the infinite-dimensional limit which we also discuss. The simplicity of our method permits us to investigate the validity of the MV results in a much more general class of models. In Sect. 3 we will discuss generalized kinetic energies containing not only nearest neighbor hopping. This is an important generalization because it allows to get away from the half-filled band perfect nesting situation. Generalized potential energies which are not site-diagonal will be considered in Sect. 4. A summary of our results and an outlook of their implications will be given in Sect. 5.

II. Hubbard model in high dimensions

In order to present our methods of investigation we rederive in this section some basic results of MV for the Hubbard model

$$H = -t/(2D)^{1/2} \sum_{\langle ij \rangle, \sigma} c_{i \sigma}^{\dagger} c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow}$$  \hspace{1cm} (1)$$

on a simple cubic lattice of dimension $D$. The parameters of the model are scaled such that the model has a finite and non-trivial limit at $D = \infty$ [1]. The nearest
neighbor hopping kinetic energy of (1) is diagonal in the momentum representation

$$H_t = \sum_{k, \sigma} \varepsilon(k) c^+_k c_k$$  \hspace{1cm} (2)

$$\varepsilon(k) = -2t/(2D)^{1/2} \sum_{n=1}^{D} \cos k_n$$  \hspace{1cm} (3)

with a cubic Brillouin zone given by $-\pi < k_a \leq \pi$. (We put the lattice constant equal to 1.) With the shorthand notation

$$\langle x(k) \rangle_k = \int \frac{x(k) \, d^D k}{(2\pi)^D}$$  \hspace{1cm} (4)

for averages over the Brillouin zone it is obvious that

$$\langle \varepsilon(k)^2 \rangle_k = t^2$$  \hspace{1cm} (5)

and the central limit theorem tells us that the density of states of the non-interacting system tends to a Gaussian in the limit of infinite dimension [1]:

$$\rho_D(\varepsilon) = \langle \delta(\varepsilon - \varepsilon(k)) \rangle_k$$

$$\rightarrow \exp(-\varepsilon^2/2t^2)/(2\pi t^2)^{1/2} \quad (D \rightarrow \infty).$$  \hspace{1cm} (6)

This result and corrections at finite $D$ are easily obtained by looking at the Fourier transform

$$\Phi_D(s) = \int_{-\infty}^{\infty} \rho_D(\varepsilon) e^{i\varepsilon s} \, d\varepsilon = \langle e^{i\varepsilon s(k)} \rangle_k.$$  \hspace{1cm} (7)

Due to the additivity of the kinetic energy (3) the Brillouin zone average in (7) factorizes into $D$ one-dimensional integrals

$$\Phi_D(s) = \left[ \int_{-\pi}^{\pi} \exp(-2is \cdot \cdot \cos k/(2D)^{1/2}) \, dk/2\pi \right]^D.$$  \hspace{1cm} (8)

The straightforward expansion of the integral in terms of powers of $s$ now yields

$$\Phi_D(s) = \exp[-(s \cdot t)^2/2 - (s \cdot t)^4/16D + O(D^{-2})]$$  \hspace{1cm} (9)

which after transforming back corresponds to

$$\rho_D(\varepsilon) = \exp[-(\varepsilon/t)^2/2$$

$$- (\varepsilon/t)^4 - 6(\varepsilon/t)^2 + 3]/16D$$

$$+ O(D^{-2}))/2\pi t^2)^{1/2}. \hspace{1cm} (10)$$

From the derivation we see that the Gaussian and its asymptotic corrections result from the “short time regime” ($s \geq 1$) of $\Phi$. The density of states for small dimensions deviates from the Gaussian mostly due to its van Hove singularities which are discontinuities of order $D/2 - 1$ and which result from the “long time regime” ($s \geq 1$) of $\Phi$. This regime is also easy to investigate because the integral in (8) is equal to the Bessel function $J_0(2s \cdot t/(2D)^{1/2})$. The asymptotic expansion (10) is controlled to all orders in $1/D$ by the maximum of $J_0$ at $s = 0$. Van Hove singularities result from the other maxima of $J_0$ which add exponentially small contributions (of order $e^{-2D}$) to the expansion (10). Quantitative comparison shows that even the density of states for $D = 3$, despite of its square root van Hove singularities, is surprisingly close to the Gaussian. (The average deviation is only 10%).

We wish to emphasize that the short wavelength cut-off associated with the lattice is absolutely essential for obtaining a meaningful limit for fermion models of infinite dimension. For a continuum model the density of states is proportional to $e^{2/1} - 1$ which is impossible to scale to a well-behaved limit like (10).

Let us now have a look at perturbation expansions with respect to the interaction $U$. Alternatively we might look at expansions with respect local correlations in a variational wavefunction as it was done in ref. [1]. The basic problem is the same in both cases: we have to perform $D$-dimensional momentum integrations paying attention to momentum conservation at each vertex. Since the interaction matrix elements $U$ do not depend on momenta for the on-site Hubbard interaction in (1) and since the free propagators depend on momenta only through $\varepsilon(k)$, the whole issue of momentum integration and momentum conservation at an internal vertex is comprehended in the vertex function

$$v_D(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4) = \prod_{i=1}^{4} \delta(\varepsilon_i - \varepsilon(k))$$

$$\cdot \Delta(k_1 - k_2 + k_3 - k_4)_{all_k}. \hspace{1cm} (11)$$

Here $k_1, k_3$ and $k_2, k_4$ are the ingoing and outgoing momenta, respectively, and the Laue function

$$\Delta(k) = \sum_R \exp(iR \cdot k)$$  \hspace{1cm} (12)

takes proper care of momentum conservation modulo reciprocal lattice vectors. (The sum extends over all lattice vectors $R$.)

In high dimensions the vertex function (11) can be analysed with the same method we applied above to the density of states. In analogy to (7) we consider the fourfold Fourier transform of $v_D$:

$$\Psi_D(s_1, s_2, s_3, s_4)$$

$$= \exp[i(s_1 \cdot \varepsilon(k) - i(\cdot(-1)^{R \cdot k})]_s.$$  \hspace{1cm} (13)