

Process-chain approach to high-order perturbation calculus for quantum lattice models

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A method based on Rayleigh-Schrödinger perturbation theory is developed that allows to obtain high-order series expansions for ground-state properties of quantum lattice models. The approach is capable of treating both lattice geometries of large spatial dimensionalities d and on-site degrees of freedom with large state space dimensionalities. It has recently been used to accurately compute the zero-temperature phase diagram of the Bose-Hubbard model on a hypercubic lattice, up to arbitrary large filling and for $d=2, 3$, and greater [Teichmann *et al.*, Phys. Rev. B 79, 100503(R) (2009)].

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I. INTRODUCTION

Although rather simple, quantum lattice gas or spin models are known to give rise to complex strongly correlated many-body physics. Currently the interest in these paradigmatic models of condensed-matter physics is strongly amplified by the fact that it just becomes experimentally feasible to “engineer” many of them with ultracold atoms in optical lattice potentials.^{1,2} Quantum lattice models are composed of small elementary subsystems (sites), a spin or the occupation of a single-particle state, arranged in a lattice. The geometry of the lattice is reflected in the fact that only neighboring subsystems are coupled to each other directly. In general the Hamiltonian is of the form

$$\hat{H} = \sum_i \hat{h}_i + \sum_{\langle ij \rangle} \hat{v}_{ij}, \quad (1)$$

where the on-site term \hat{h}_i acts on the local state space of lattice site i only, while the coupling term \hat{v}_{ij} operates on both sites i and j with the sum $\sum_{\langle ij \rangle}$ running over all pairs of neighboring sites $\langle ij \rangle$ (bonds).

As the state-space dimensionality of the full system increases exponentially with the number of sites M , generally the treatment of models such as Eq. (1) is a hard problem. However, sometimes there exist suitable approximation schemes giving accurate results in certain regimes. One of them is given by high-order series expansions, obtained by automation of the usual Rayleigh-Schrödinger perturbation calculus. Such expansions have proven to be a useful tool for the investigation of zero-temperature properties.^{3,4} In the simplest case, the coupling terms \hat{v}_{ij} are considered as perturbation. Starting from a product $|g\rangle = \prod_i |n_i\rangle \equiv |\{n_i\}\rangle$ of local eigenstates $|n_i\rangle$ with $\hat{h}_i |n_i\rangle = \epsilon_i |n_i\rangle$, physical quantities like expectation values or static susceptibilities (characterizing the state evolving from $|g\rangle$ adiabatically when the perturbation is switched on) can be expanded in high-order power series with respect to a dimensionless coupling parameter. Also quantum phase transitions,⁵ i.e., abrupt changes in the ground-state structure, occurring when a certain parameter α passes a critical value α_c , can be inferred from such expansions.

A widely and successfully used algorithm for the application of perturbation calculus to such lattice models is given by the connected cluster expansion.^{6,7} As a first step one has

to determine all subsets C (connected clusters) of mutually connected bonds $\langle ij \rangle$ possessing not more than ν_{\max} elements, with ν_{\max} being the largest order of the expansion to be considered. Moreover, all connected subclusters (and sub-sub-clusters,...) of each of these connected clusters have to be identified. The second step consists of applying the perturbation calculus iteratively to each of the small subsystems $\hat{H}_C = \sum_{i \in C} \hat{h}_i + \sum_{\langle ij \rangle \in C} \hat{v}_{ij}$ corresponding to the connected clusters C , with C' containing all sites connected to the bonds of C . Finally, these results can be combined to give the desired expansion.

However, when trying to apply the connected cluster formalism to the Bose-Hubbard model,⁸ describing bosonic particles with short-range interaction moving in a lattice of single-particle orbitals (sites), one encounters two difficulties: (i) Finding all connected clusters as well as their sub-clusters is a demanding task for three-dimensional lattice geometries (and even more for spatial dimensionalities $d > 3$ that might be interesting in order to probe the convergence to the mean-field limit). (ii) The dimensionalities \mathcal{D}_C of the connected cluster state spaces (that have to be considered after the particle number conservation of the cluster Hamiltonians \hat{H}_C has already been taken into account) grow extremely fast with respect to the averaged lattice site occupation (filling) n . As a consequence, an iterative evaluation of the perturbation series up to eighth (tenth) order is hindered already for the moderate filling $n=5$ ($n=3$) by the fact that it requires a representation of the cluster state spaces on the machine.⁹ While difficulty (i) appears for every quantum lattice model of large spatial dimensionality $d \geq 3$, difficulty (ii) is noticed for systems with the relevant local on-site state-space dimensionalities being too large. In the following, a method based on Kato’s formulation of Rayleigh-Schrödinger perturbation calculus¹⁰ will be described that circumvents both difficulties (i) and (ii). Here, perturbative corrections are obtained as sums over chains of processes acting in the “classical” space containing the unperturbed states but not their superpositions. These process chains, in turn, are generated from paths through the d -dimensional lattice. As an example, using this approach one is able to accurately compute the Bose-Hubbard phase diagram at any integer filling n and for spatial dimensionalities $d=2, 3$, and larger.¹¹ An implementation of the method presented here is straightforward and can be accomplished from scratch with

reasonable effort. The present approach is found to be related to the ones described previously in Refs. 12–14 where contributions to the perturbation series are equally expressed in terms of sequences of processes. Differences to these approaches lie both in the way contributions are organized¹⁵ and in the generation of diagrams from paths through the lattice.

For clarity, the process-chain method will be introduced in terms of the simple Bose-Hubbard model.⁸ The generalization of the method to more involved or just different lattice Hamiltonians (such as those of Heisenberg-type spin models) is, however, straightforward; later on the properties of a general model amenable to the approach will be sketched. The Bose-Hubbard Hamiltonian reads

$$\hat{H}_{\text{BH}} = \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + (\varepsilon_i - \mu) \hat{n}_i \right] - J \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i), \quad (2)$$

with \hat{b}_i^\dagger , \hat{b}_i , and $\hat{n}_i \equiv \hat{b}_i^\dagger \hat{b}_i$ denoting the bosonic creation, annihilation, and number operator for a single-particle orbital located at site i . The first line of Eq. (2) includes an on-site interaction characterized by the energy cost U for each pair of particles occupying the same site. Moreover, it assigns the local potential energy $\varepsilon_i - \mu \equiv -\mu_i$ to particles sitting at site i , including an overall chemical potential μ introduced to control the total particle number N . The terms of the second line implement the kinetics, being exhausted by tunneling of particles between neighboring sites. Although rather simple, this model provides a quantitative description of ultracold bosonic alkali atoms in optical lattice potentials.^{1,16,2} It shows quantum phase transitions between a gapless, compressible superfluid phase with (quasi) long-range order present at large values of the ratio J/U and various gapped incompressible Mott-insulator phases (at sufficiently small J/U) with exponentially decaying correlations, each characterized by an integer filling factor $n = \sum_i \langle \hat{n}_i \rangle / M$ (depending on the chemical potential μ/U).^{5,8}

This paper is organized as follows: Section II is devoted to the general perturbation expansion. It is briefly reviewed how expectation values and static susceptibilities can be obtained via the computation of energy corrections. Starting from Kato's formulation of the ν th energy correction,¹⁰ then a way to reduce the number of terms that have to be taken into account to a minimum is described. This is the first step that has to be accomplished on the machine. Finally, the perturbative corrections are written as sums over process chains. This formulation will serve as a fruitful starting point for customizing perturbation calculus to quantum lattice models in the way developed in Sec. III. The main conceptual step of Sec. III consists in considering groups of operations (to be visualized by diagrams) such that each sequence of the operations contained in a group/diagram gives a process chain contributing to the desired perturbative correction. It is explained that the generation of the relevant diagrams can be put down to the rather simple task of generating paths through the lattice (this allows one to address also large d), and it is described how the evaluation of diagrams can be performed. These are the two final steps to be implemented

on the computer. In order to give a comprehensive presentation of the approach, the computation of perturbative corrections is first discussed in the context of the Bose-Hubbard model (2). Following along the lines given by this instructive example the application of the method to the large class of quantum lattice models described at the end of Sec. III should be straightforward. Section IV summarizes the basic steps of the approach, before Sec. V closes with concluding remarks.

II. GENERAL PERTURBATION EXPANSION

A. Problem

Consider a system described by the time-independent Hamiltonian

$$\hat{H} = \hat{H}_0 + \lambda \hat{V} \quad (3)$$

consisting of an unperturbed part \hat{H}_0 that is already diagonalized,

$$\hat{H}_0 = \sum_e E_e |e\rangle \langle e|, \quad (4)$$

and a perturbation

$$\hat{V} = \sum_{e,e'} V_{e',e} |e'\rangle \langle e| \quad (5)$$

multiplied by a dimensionless factor λ finally to be set equal to 1. The standard nondegenerate Rayleigh-Schrödinger perturbation calculus¹⁷ gives a power-law expansion

$$E_G = E_g + \lambda E_g^{(1)} + \lambda^2 E_g^{(2)} + \dots \quad (6)$$

for the energy of the state $|G\rangle$ evolving adiabatically from an eigenstate $|g\rangle$ of the unperturbed Hamiltonian (e.g., its ground state) when the perturbation is switched on. In the following the question of convergence will not be discussed, but an algorithm for the computation of such series expansions for many-body quantum lattice models is devised.

Usually, one is not interested in high-order perturbative corrections to the *state* of a many-body system containing a vast amount of mostly unwanted information. One rather wishes to compute selected quantities such as expectation values $\langle G | \hat{A} | G \rangle$. It is known, however, that the computation of ground-state expectation values and static susceptibilities can be reduced to the evaluation of energy corrections. Introducing the extended Hamiltonian

$$\hat{H}_{AB} = \hat{H}_0 + \lambda \hat{V} + x \hat{A} + y \hat{B}, \quad (7)$$

with operators \hat{A} and \hat{B} , a perturbative treatment of $\hat{V}' \equiv \lambda \hat{V} + x \hat{A} + y \hat{B}$ yields the expansion

$$E_{G_{AB}} = \sum_{v,m,k} E_g^{(v,m,k)} \lambda^v x^m y^k \quad (8)$$

for the energy of the perturbed eigenstate $|G_{AB}\rangle$ evolving from $|g\rangle$. [In the case of non-Hermitian operators \hat{A} one can consider instead the Hermitian ones $\hat{A}^{(+)} \equiv \frac{1}{2}(\hat{A} + \hat{A}^\dagger)$ and

$\hat{A}^{(-)} \equiv \frac{1}{2i}(\hat{A} - \hat{A}^\dagger)$ such that $\hat{A} = \hat{A}^{(+)} + i\hat{A}^{(-)}$.] The low-order coefficients with respect to x and y then give series in powers of λ for the expectation value

$$\langle G|\hat{A}|G\rangle = \sum_{\nu} \lambda^{\nu} E_g^{(\nu,1,0)}, \quad (9)$$

and the static susceptibilities

$$\chi_{AB} = \sum_{\nu} \lambda^{\nu} E_g^{(\nu,1,1)} \quad (10)$$

and

$$\chi_{AA} = \frac{1}{2} \sum_{\nu} \lambda^{\nu} E_g^{(\nu,2,0)} \quad (11)$$

describing the linear response of $\langle \hat{A} \rangle$, when the full Hamiltonian \hat{H} is perturbed by \hat{B} or \hat{A} , respectively. One can obtain these relations, e.g., by using the Hellmann-Feynman theorem $\frac{d}{dz} \langle \psi(z) | \hat{H}(z) | \psi(z) \rangle = \langle \psi(z) | [\frac{d}{dz} \hat{H}(z)] | \psi(z) \rangle$ [valid if $|\psi(z)\rangle$ is a normalized eigenstate of $\hat{H}(z)$] or by interpreting them as first-order energy corrections to the unperturbed problem given by the full Hamiltonian \hat{H} . Hence, solely by using a formalism for the evaluation of energy corrections, one can obtain series expansions for many important quantities characterizing the system.

B. Minimal expression for the ν th order energy correction

The ν th energy correction appearing in Eq. (6) is given by Kato’s closed expression¹⁰ (see also Ref. 17)

$$E_g^{(\nu)} = \sum_{(\nu-1)} \text{tr}\{\hat{S}^{\alpha_{\nu+1}} \hat{V} \hat{S}^{\alpha_{\nu}} \dots \hat{V} \hat{S}^{\alpha_3} \hat{V} \hat{S}^{\alpha_2} \hat{V} \hat{S}^{\alpha_1}\} \quad (12)$$

with the sum $\sum_{(\nu-1)}$ running over all combinations of the $\nu+1$ non-negative integers α_k such that $\sum_{k=1}^{\nu+1} \alpha_k = \nu-1$, $\text{tr}\{\cdot\} \equiv \sum_e \langle e | \cdot | e \rangle$, and

$$\hat{S}^{\alpha} \equiv \begin{cases} -|g\rangle\langle g| & \text{for } \alpha = 0 \\ \sum_{e \neq g} \frac{|e\rangle\langle e|}{(E_g - E_e)^{\alpha}} & \text{for } \alpha \geq 1. \end{cases} \quad (13)$$

Since on the right-hand side of Eq. (12) there are always at least two α_i equal to zero, by cyclic permutation under the trace and using

$$\hat{S}^{\alpha} \hat{S}^{\alpha'} = \begin{cases} -\hat{S}^0 & \text{for } \alpha = 0 \text{ and } \alpha' = 0 \\ 0 & \text{for } \alpha = 0 \text{ and } \alpha' \neq 0 \\ & \text{or } \alpha \neq 0 \text{ and } \alpha' = 0 \\ \hat{S}^{\alpha+\alpha'} & \text{for } \alpha \neq 0 \text{ and } \alpha' \neq 0 \end{cases} \quad (14)$$

the energy correction can always be expressed as a sum over expectation values with respect to the unperturbed state $|g\rangle$. This gives

$$E_g^{(\nu)} = \sum_{(\nu-1)} G_{\{\alpha_k\}} \langle g | \hat{V} \hat{S}^{\alpha_{\nu-1}} \hat{V} \dots \hat{S}^{\alpha_2} \hat{V} \hat{S}^{\alpha_1} \hat{V} | g \rangle \quad (15)$$

with $\sum_{k=1}^{\nu-1} \alpha_k = \nu-1$ according to the constraint of sum (12) and with (not uniquely determined) weight factors $G_{\{\alpha_k\}}$ tak-

ing into account how often each matrix element is generated with positive and negative prefactor during the elimination of the trace. Below the short hand

$$(\alpha_{\ell}, \dots, \alpha_2, \alpha_1) \equiv \langle g | \hat{V} \hat{S}^{\alpha_{\ell}} \hat{V} \dots \hat{S}^{\alpha_2} \hat{V} \hat{S}^{\alpha_1} \hat{V} | g \rangle, \quad (16)$$

for the matrix elements appearing in sum (15) will be used, with $(\) \equiv \langle g | \hat{V} | g \rangle$ denoting the first-order energy correction.

An example for an expression such as Eq. (15) is given by the formula¹⁸ (see also Ref. 17)

$$E_g^{(\nu)} = \sum'_{(\nu-1)} (\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1), \quad (17)$$

where all $G_{\{\alpha_k\}}$ are either zero or one, as it is encoded in the set of constraints $\sum_{k=1}^s \alpha_k \geq s$ with $s=1, 2, \dots, (\nu-2)$, additional to the requirement $\sum_{k=1}^{\nu-1} \alpha_k \geq \nu-1$. A further way to obtain an expression of type (15) similar to formula (17) is to start with the matrix element $(1, 1, \dots, 1, 1)$, with all $\alpha_k=1$, and to generate successively further matrix elements to be considered by applying the recursive scheme described in Ref. 19.

Many matrix elements $(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1)$ that appear in the sum (15) or sum (17) give identical contributions: writing explicitly $\hat{S}^0 = -|g\rangle\langle g|$, each matrix element $(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1)$ breaks up into elementary matrix elements (EME) $(\beta_{\ell}, \dots, \beta_2, \beta_1)$, containing strictly positive (i.e., nonzero) integers β_i only. Thus, e.g., one has

$$\begin{aligned} (1, 1, 0, 0, 3, 0, 2, 1) &= - (1, 1) () (3) (2, 1) \\ &= - (1, 1) () (3) (1, 2) = (1, 1, 0, 0, 3, 0, 1, 2) \\ &= - (1, 1) () (2, 1) (3) = (1, 1, 0, 0, 2, 1, 0, 3) \\ &= - (1, 1) () (1, 2) (3) = (1, 1, 0, 0, 1, 2, 0, 3) \\ &= \dots \end{aligned} \quad (18)$$

Here two basic operations were applied leaving the expression unchanged, the permutation of EMEs and the “reflection” of an EME, $(\beta_{\ell}, \dots, \beta_2, \beta_1) \rightarrow (\beta_1, \beta_2, \dots, \beta_{\ell})$. The latter is allowed since both \hat{V} and the \hat{S}^{α} are Hermitian. Hence, one has families of matrix elements $(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1)$ with all members giving the same contribution. In contrast, different EMEs $(\beta_{\ell}, \dots, \beta_2, \beta_1)$ generally give different contributions, if, by convention, one considers EMEs differing just by a “reflection” to be identical. Accordingly, each family of equally contributing matrix elements $(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1)$ is uniquely determined by a set of EMEs. In order to take into account only one representative of each family the energy correction can be rewritten as

$$E_g^{(\nu)} = \sum_{(\nu-1)} G_{\{\alpha_k\}}^{\min} (\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1) \quad (19)$$

with a minimum number of nonvanishing weight factors $G_{\{\alpha_k\}}^{\min}$. Obtaining such a minimal expression for the orders to be considered is the first problem that has to be solved on a computer for an implementation of the method described here. Since so far one is dealing with the general perturbation expansion, this step has to be performed once only.

TABLE I. Minimum number K_ν of matrix elements that have to be considered for the ν th order energy correction. The number of contributing terms is significantly reduced to K'_ν if the first-order energy correction vanishes, $\langle g|\hat{V}|g\rangle=0$. The data for $\nu\geq 12$ are taken from Ref. 20.

Order ν	K_ν (No. of terms)	K'_ν (No. of restrict. terms)
1	1	0
2	1	1
3	2	1
4	4	2
5	10	3
6	22	7
7	53	12
8	119	26
9	278	47
10	627	97
11	1433	180
12	3216	357
13	7253	668
14	16169	1297
15	36062	2427
16	79876	4628
17	176668	8637
18	388910	16260
19	854493	30188
20		56252
21		103848
22		191873
23		352204
24		646061

A routine (R1) for the generation of a minimal set of matrix elements contributing to sum (19) and their weights can be based on one of two alternative approaches. The first one is to generate all matrix elements appearing in an expression such as Eq. (15) by starting either from formula (12) or Eq. (17), and then to identify members of the same matrix element family by decomposition into EMEs. The second approach is to generate all EMEs and all combinations of them describing families of matrix elements $(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1)$ appearing in sum (15). The weight factor $G_{\{\alpha_k\}}^{\min}$ of a given family can then be obtained from a simple expression.²⁰ The minimum number K_ν of matrix elements to be considered in ν th order is listed in Table I. It is drastically reduced, if it is known that the first-order energy correction $\langle g|\hat{V}|g\rangle=0$ vanishes. Generally, given knowledge about the vanishing of corrections in certain orders ν that are, say, even, odd or smaller than a value ν_0 can be used to reduce the number of matrix elements that has to be taken into account. For example, if all corrections appearing in orders smaller than ν_0 are known to vanish, then there is at most one relevant matrix element appearing in order ν_0 .

C. Energy corrections as sums over process chains

One can interpret each matrix element $(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1)$ appearing in Eq. (19) as a weighted sum $\sum_{\{e_k\}}$ over paths $|g\rangle \rightarrow |e_1\rangle \rightarrow |e_2\rangle \rightarrow \dots \rightarrow |e_{\nu-1}\rangle \rightarrow |g\rangle$ in a “classical” space containing the unperturbed states $|e\rangle$ but not their superpositions. All paths lead from $|g\rangle$ back to $|g\rangle$ via $\nu-1$ intermediate states $|e_k\rangle$: by plugging definitions (5) and (13) into Eq. (16), one obtains

$$(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1) = \sum_{\{e_k\}} V_{g,e_{\nu-1}} W_{e_{\nu-1}}^{(\alpha_{\nu-1})} \dots \times \dots W_{e_2}^{(\alpha_2)} V_{e_2,e_1} W_{e_1}^{(\alpha_1)} V_{e_1,g} \quad (20)$$

with

$$W_e^{(\alpha)} \equiv -\delta_{\alpha,0} \delta_{e,g} + (1 - \delta_{\alpha,0})(1 - \delta_{e,g})[E_g - E_e]^{-\alpha}. \quad (21)$$

In that way a formulation involving huge quantum mechanical state spaces is avoided.

However, usually we have to deal with several perturbing terms at once, $\hat{V} = \hat{V}^{(1)} + \hat{V}^{(2)} + \dots$ with $\hat{V}^{(m)} = \sum_{e',e} V_{e',e}^{(m)} |e'\rangle \langle e|$, and we wish to keep track of them independently. Therefore, it is convenient to reformulate Eq. (20) once more, namely, as a sum over *process chains* P each of them being given by an ordered sequence $V_{e_1,g}^{(m_1)} |e_1\rangle \langle g|, V_{e_2,e_1}^{(m_2)} |e_2\rangle \langle e_1|, \dots, V_{g,e_{\nu-1}}^{(m_\nu)} |g\rangle \langle e_{\nu-1}|$ of basic processes $V_{e',e}^{(m)} |e'\rangle \langle e|$ leading from $|g\rangle$ back to $|g\rangle$ in the classical space of unperturbed states introduced above. One has

$$(\alpha_{\nu-1}, \dots, \alpha_2, \alpha_1) = \sum_P V_{g,e_{\nu-1}}^{(m_\nu)} W_{e_{\nu-1}}^{(\alpha_{\nu-1})} \dots \times \dots W_{e_2}^{(\alpha_2)} V_{e_2,e_1}^{(m_2)} W_{e_1}^{(\alpha_1)} V_{e_1,g}^{(m_1)}, \quad (22)$$

or, in combination with Eq. (19),

$$E_g^{(\nu)} = \sum_P \sum_{\{\alpha_k\}} G_{\{\alpha_k\}}^{\min} V_{g,e_{\nu-1}}^{(m_\nu)} \dots W_{e_2}^{(\alpha_2)} V_{e_2,e_1}^{(m_2)} W_{e_1}^{(\alpha_1)} V_{e_1,g}^{(m_1)} \quad (23)$$

for the ν th order energy correction.

The strategy for the computation of energy corrections proposed here is to generate all process chains P appearing in a given order n in a first step, and then to compute the contributions arising from each chain according to the different sets $\{\alpha_k\}$ possessing nonvanishing weight factors $G_{\{\alpha_k\}}^{\min}$ in the general perturbation expansion in the form given by Eq. (19). In the next section it is shown how both steps can be accomplished efficiently for a lattice system with short-range coupling.

III. LATTICE SYSTEM

A. Bose-Hubbard problem

In this section, the above formalism is applied to the Bose-Hubbard Hamiltonian (2) on a hypercubic lattice geometry. All terms that are diagonal with respect to the lattice-site occupation numbers n_i will be considered as unperturbed problem

$$\hat{H}_0 = \sum_i \left[\frac{1}{2}(\hat{n}_i - 1) - \frac{\mu_i}{U} \right] \hat{n}_i, \quad (24)$$

and the remaining tunneling terms as perturbation

$$\hat{V} = - \frac{J}{U} \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i). \quad (25)$$

Energies have been expressed in units of the positive interaction parameter U , such that J/U is identified to be the dimensionless coupling parameter. A basis of unperturbed states $|e\rangle$ is given by the lattice-site occupation-number states

$$| \{n_i\} \rangle \equiv \prod_i \frac{(\hat{b}_i^\dagger)^{n_i}}{\sqrt{n_i!}} | \text{vacuum} \rangle. \quad (26)$$

Let us assume that the state we want to investigate is the one evolving adiabatically from the unperturbed state

$$|g\rangle \equiv | \{n_i = g_i\} \rangle \quad (27)$$

when the perturbation is switched on. If $|g\rangle$ denotes the unperturbed ground state its occupation numbers g_i minimize $[(g_i - 1)/2 - \mu_i/U]g_i$ and read

$$g_i = \begin{cases} 0 & \text{if } \mu_i/U < 0 \\ h & \text{if } (h - 1) < \mu_i/U < h \\ (h - 1) \text{ or } h & \text{if } \mu_i/U = h - 1 \geq 0, \end{cases} \quad (28)$$

with non-negative integers h . As long as the marginal case of integer μ_i/U is avoided, this state is protected by an energy gap.

In the following first a thorough discussion of the computation of (actual) energy corrections is given as an instructive example. Then it will be shown that this example already contains everything one needs also for the computation of other quantities of interest, such as single particle correlations $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$, number correlations $\langle \hat{n}_i \hat{n}_j \rangle$, or the static susceptibility $\chi_{\hat{a}_0, \hat{a}_0^\dagger}$ for the annihilation and creation operators of the condensate mode, \hat{a}_0 and \hat{a}_0^\dagger . The divergence of the latter indicates the quantum phase transition from a Mott-insulator to a superfluid.^{11,21,22} The approach can easily be generalized to more complicated or just different lattice models. A general model that is amenable to the procedure described below is sketched at the end of this section.

B. Corrections to the energy

The perturbation \hat{V} to be considered consists of tunneling processes, i.e., the annihilation of one particle at a given site in combination with the creation of one particle at a neighboring site. Denoting a tunneling operation by an arrow, one can visualize sets of tunneling operations graphically by drawing diagrams. Obviously all process chains P starting and ending at the same (arbitrary) unperturbed state $|g\rangle$ must contain the same number of creation and annihilation processes at each site. Hence, those *diagrams contributing to the energy corrections contain closed paths only*. In Fig. 1 typical diagrams describing sets of tunneling operations in the two-dimensional square lattice are sketched. The number of

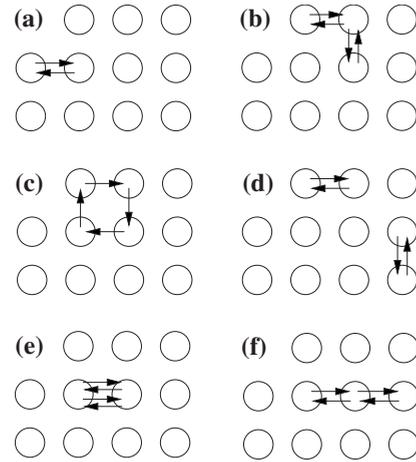


FIG. 1. Typical diagrams characterizing sets of tunneling operations between neighboring sites in the two-dimensional square lattice that appear in the energy correction of second and fourth order. Tunneling operations are denoted by arrows, lattice sites by circles. Diagrams contributing to the perturbation expansion are those that can be interpreted as a single closed path, i.e., all except (d).

arrows corresponds to the power of J/U to which the diagram contributes. In principle one can obtain all process chains P appearing in the general formula (23) by generating all diagrams (sets of tunneling operations) contributing to a given order in a first step, and by ordering the operations of each diagram in all possible ways in a second step. Hence, before energy corrections can be evaluated all contributing diagrams have to be generated.

It has been noted that only diagrams containing closed paths of tunneling operations contribute, since only these have the same number of creation and annihilation operations at each site. In correspondence with the connected cluster theorem,⁷ one can also show that *only connected diagrams give a nonvanishing contribution to the energy correction*, i.e., those diagrams that cannot be divided into two or more subdiagrams with no lattice site in common or, in other words, that can be interpreted to consist of a single closed path only. For example, the energy corrections stemming from the different process chains that can be obtained from diagram (d) of Fig. 1 must add up to zero. The basic idea for a proof of this statement goes as follows:⁷ A connected diagram would equally appear in the perturbation expansion for a system differing from the one considered here by the fact that it consists of two completely independent subsystems that are not coupled to each other by tunneling and with one part of the diagram lying in each of them. In that case, however, the perturbed state evolving from an unperturbed product state will obviously be a product state with respect to both decoupled subsystems, and its energy will be the sum of both subsystem energies. Thus, contributions to the energy depending in a nonadditive way on the properties of both subsystems cannot occur.

Unless one is not dealing with a rather small system, computing perturbative corrections to an extensive quantity like the energy will generally involve too many diagrams to be accomplished in reasonable time. Nevertheless, it is possible to compute these corrections for a homogeneous system with

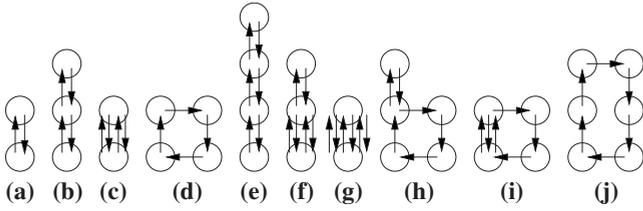


FIG. 2. All topological diagrams contributing to the energy correction of a hypercubic lattice in the leading orders 2, 4, and 6.

$\mu_i = \mu$ (or a system that shows a different kind of translational symmetry). In that case topologically identical diagrams—such as (b) and (f) of Fig. 1—will give identical contributions. In Fig. 2 all types of topologically different diagrams appearing in the leading orders²³ 2, 4, and 6 are plotted. The multiplicity M_T of a topological diagram T is a weight factor being defined as the number of ways it can be embedded into the given lattice geometry. Note that disconnected diagrams would give rise to unphysical multiplicities increasing with a power larger than one with the system size. In the following diagrams like those of Fig. 1 containing operations that are located in the lattice will be called *geographical diagrams*, while diagrams like those of Fig. 2 that are characterized by topology only will be called *topological diagrams*.

C. Computing high-order energy corrections

In order to obtain all topological diagrams contributing to the energy correction and their multiplicities on a computer, one needs two basic routines, R2a and R2b, that will also serve to evaluate corrections to other expectation values than that of the energy. The first routine (R2a) computes all paths through the lattice via neighboring sites starting from a given site i to another site j containing ν steps. By choosing $i=j$ and associating each step with a tunneling operation, in that way one obtains all sets of tunneling operations, i.e., all geographical diagrams, contributing in order ν . However, two corrections have to be taken into account. First, for closed loops a path visiting s different lattice sites could equally be associated to each of the $s-1$ sites different from i . Hence, such a diagram must be weighted by a factor of s^{-1} . Second, it might happen that different paths contain exactly the same tunneling operations (just in a different order). An example for that is given by the diagram shown in Fig. 1(b) that—starting from the site all arrows are connected to—might be obtained by first moving vertically and then horizontally or vice versa. If two paths include the same tunneling operations, only one of them should be taken into account. For that purpose a further routine (R2b) is needed that identifies paths containing the same tunneling operations.

For a homogeneous Bravais lattice all sites are equal and it suffices to consider just a single site i ; moreover only topologically distinct diagrams give distinct contributions. The relevant topological diagrams and their multiplicities can be obtained by collecting geographical ones of the same topology. Note that this step serves only to reduce the number of diagrams that have to be evaluated. Hence, the algorithm used to probe the topological equivalence of two geo-

graphical diagrams does not need to be perfect. A very simple way of identifying identical topologies is to enumerate the sites appearing in a geographical diagram by a single index in the order they appear the first time in an associated path. Then routine R2b can be used to compare the diagrams. For the closed loop diagrams contributing to the ground state energy, with site i not being distinguished from the other ones appearing in the diagram, this approach has to be improved by probing enumerations starting at different sites.

One advantage of the diagram generation via paths consist in that fact that it is easily implemented, even for high spatial dimensionalities d . Assuming, for example, a hypercubic lattice, it is not difficult to design a routine R2a that in principle works for arbitrary d and also practically allows to consider values of d well above 3 that might be interesting to study the convergence toward mean-field behavior.

Once all diagrams of a given order have been obtained, their contribution to energy (23) can be evaluated by a last routine (R3). Each sequence of the operations contained in a diagram corresponds to a different process chain P , with the permutation of two identical operations—as they appear, e.g., in Fig. 2(c)—not giving a new process chain. Thus, the diagrams (a), (b), and (c) of Fig. 2 give rise to $2! = 2$, $4! = 24$, and $4! / (2!)^2 = 6$ different process chains, respectively. By applying the processes of a given chain one after the other to a small array of occupation numbers $\{n_i\}$ initialized with $n_i^{(0)} = g_i$, giving a sequence $\{n_i^{(0)}\}, \{n_i^{(1)}\}, \{n_i^{(2)}\}, \dots$, one can compute (i) the matrix elements $V_{e_{k+1}, e_k}^{(m_k)}$ [being $-(J/U)[n_i^{(k)}(n_j^{(k)} + 1)]^{1/2}$ for tunneling from site i to site j], (ii) the unperturbed energy differences $E_{e_k} - E_g$ of the intermediate states [given by $\sum_i [n_i^{(k)}(n_i^{(k)} - 1) - g_i(g_i - 1) - (\mu/U)(n_i^{(k)} - g_i)]$], and (iii) whether an intermediate state $|e_k\rangle$ equals $|g\rangle$ (i.e., whether $n_i^{(k)} = g_i$ for all i) or not. Afterward one can choose only those matrix elements $(\alpha_{n-1}, \dots, \alpha_2, \alpha_1)$ appearing in the minimal expression (19) that have $\alpha_k = 0$ if $|e_k\rangle = |g\rangle$ and $\alpha_k \neq 0$ if $|e_k\rangle \neq |g\rangle$ for all intermediate states $k = 1, 2, \dots, n-1$. Only these give a nonvanishing contribution to energy correction (23) that now can be evaluated with the help of Eq. (21) employing the energy differences $E_{e_k} - E_g$.

The scheme described in the preceding paragraph is not affected by the filling (the averaged particle number per site), since no representation of a quantum-mechanical state space is needed. Moreover, while applying the process chain to a set of occupation numbers those unperturbed basis states $\{|n_i\rangle\}$ that are relevant for a given order of perturbation calculus (and only those) are generated automatically.

D. Corrections to expectation values and static susceptibilities

Perturbative corrections to an expectation value $\langle \hat{A} \rangle$ (or a static susceptibility $\chi_{\hat{A}, \hat{B}}$) in ν th order of the perturbation \hat{V} can be obtained by computing energy corrections for the combined perturbation $\hat{V}' = \lambda \hat{V} + x \hat{A} + y \hat{B}$ in first order in x (and y) and in ν th order in λ , as expressed in Eq. (9) [and Eq. (10)] of Sec. II. Hence, in order to compute such quantities, one can proceed exactly as before. Now just one process $A_{e', e} |e'\rangle \langle e|$ associated to the operator $\hat{A} \equiv \sum_{e', e} A_{e', e} |e'\rangle \langle e|$ (and another one associated to \hat{B}) has to be included in each

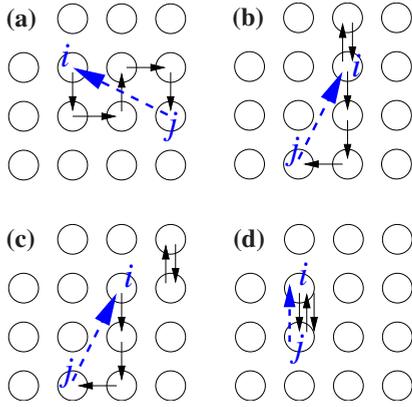


FIG. 3. (Color online) Typical diagrams appearing in the perturbation expansion of correlation functions $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$ in a 2D square lattice. The dashed arrow is associated to an operator $\hat{b}_i^\dagger \hat{b}_j$. Again, all diagrams contain closed loops only, with the solid arrows describing a path from site i to site j , and disconnected diagrams like (c) give zero contribution.

process chain, in addition to ν tunneling processes stemming from \hat{V} . The weight factors $G_{\{\alpha_k\}}^{\min}$ entering the general perturbation expansion (23) are those referring to energy corrections of order $\nu+1$ for the computation of expectation values (or $\nu+2$ for susceptibilities).

For the computation of a correlation function $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$, the additional operation to be taken into account is the transfer of a particle from site j to site i described by the operator $\hat{b}_i^\dagger \hat{b}_j$. Denoting such an operation by a dashed arrow, one can again use diagrams to describe sets of operations. Typical diagrams are shown in Fig. 3. As before, the requirement that any sequence of the operations contained in a diagram must lead from a given unperturbed state $|g\rangle$ back to it (i.e., that the number of particle annihilations equals that of particle creations at every site) ensures that only closed loops (containing the dashed as well as solid arrows) contribute. Since, moreover, again disconnected diagrams such as (c) do not need to be considered, the tunneling operations stemming from \hat{V} can be interpreted as a single path leading from i to j . (One immediately sees that the perturbative treatment in the tunneling term discussed here is not sensitive to single-particle correlations between sites that are more than ν steps between neighboring sites apart.) Also the generation of diagrams via the generation of paths through the lattice can be accomplished in a similar way as before by using routine R2a. Paths lead now from i to j and must not be corrected by the weight s^{-1} , since no other starting point than the distinguished site i will be taken into account. Note that if i and j are neighboring sites, as it is the case in diagram (d) of Fig. 3, the operation related to the dashed arrow still gives a factor of x rather than λ , such that it is well distinguished from a parallel tunneling operation stemming from \hat{V} described by a solid arrow. Therefore, e.g., in diagram (d) the permutation of both upward tunneling operations (the “solid” and the “dashed” one) in a sequence does lead to a new process chain, such that here $4!/2!=12$ different process chains have to be taken into account.

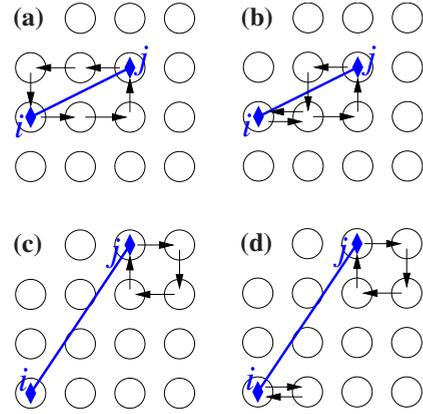


FIG. 4. (Color online) Typical diagrams appearing in the perturbation expansion of the number correlations $\langle \hat{n}_i \hat{n}_j \rangle$ in a 2D square lattice. The operation associated with the linked diamonds is described by the operator $\hat{b}_i^\dagger \hat{b}_i \hat{b}_j^\dagger \hat{b}_j$ that leaves occupation numbers unaltered.

Another example is the computation of number correlations $\langle \hat{n}_i \hat{n}_j \rangle$. The corresponding operator $\hat{n}_i \hat{n}_j = \hat{b}_i^\dagger \hat{b}_i \hat{b}_j^\dagger \hat{b}_j$, with matrix elements depending on the occupation of both sites i and j , leaves any unperturbed occupation number state unaltered. Nonetheless one can associate this “operation” with a diagrammatic symbol that is chosen to be given by two diamonds at sites i and j , connected by a line. Figure 4 shows some diagrams appearing in the perturbative expansion of expectation values $\langle \hat{n}_i \hat{n}_j \rangle$. Obviously, the tunneling operations must form closed paths, such that the number of creation and annihilation operations at each site are equal. Since, moreover, again only connected diagrams contribute, the closed tunneling paths must visit either i or j . For given i and j , one can generate all contributing diagrams by generating all combinations of two paths, such that one leads from i back to i and the other from j back to j (including paths of zero length).

In the spirit of the examples treated so far, single-site expectation values $\langle \hat{n}_i^p \rangle$ with arbitrary power p are obtained from diagrams that are generated by paths leading from site i back to site i .

It is worth mentioning that the expectation value of an operator like $\hat{n}_i \hat{n}_j$, acting on a few sites only, can be computed even in the case of a large inhomogeneous system (provided, of course, perturbation theory is meaningful). Since the contributing geographic diagrams are just those exploring the neighborhood of i and j , their number is limited and does not depend on the system size. Correlations between i and j that are induced by the perturbing coupling term (such as $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$ in the present case) will, however, only be taken into account in orders of perturbation theory that are comparable to the distance between i and j (measured in steps between neighboring sites). This directly reflects the limitation of the perturbative approach to systems with such correlations decaying on a distance being at most equal to the order of perturbation theory (at least as long as additional extrapolation techniques are not applicable or considered).

Finally, it shall be outlined how the static susceptibility $\chi_{\hat{a}_0, \hat{a}_0^\dagger} \equiv \chi$ for the annihilation and creation operators of the

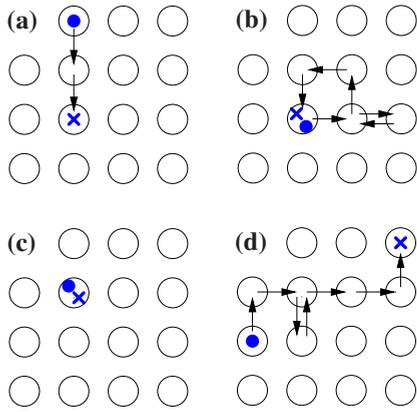


FIG. 5. (Color online) Typical diagrams contributing to the static susceptibility $\chi_{\hat{a}_0, \hat{a}_0^\dagger}$ that indicates the quantum phase transition from a Mott-insulator to a superfluid.

condensate mode, \hat{a}_0 and \hat{a}_0^\dagger , with $\hat{a}_0 \propto \sum_i \hat{b}_i$ for the homogeneous system can be computed. This quantity is proportional to the contribution $\propto |\xi|^2$ to the energy obtained from the effective Hamiltonian $\hat{H}_{\text{eff}} = \hat{H} + \sum_i (\xi \hat{b}_i + \xi^* \hat{b}_i^\dagger)$. The process chains contributing to it contain (apart from tunneling processes) one creation process and one annihilation process that will be represented diagrammatically by a bullet \bullet and a cross \times , respectively. Examples for relevant diagrams are given in Fig. 5. They can be obtained from connected paths starting and ending anywhere in the lattice [including the zeroth order contribution shown in diagram (c)]. All topological diagrams appearing in the leading orders 0, 1, 2, and 3 are shown in Fig. 6. In the limit of large spatial dimensionalities d , tunneling several times along the same bond becomes very unlikely such that diagrams like (a), (b), (d), and (h) of Fig. 6 that can be interpreted as a path visiting each site only once give the major contribution to the susceptibility.

For $d \geq 2$ the susceptibility χ diverges when J/U reaches some critical value $(J/U)_c$, indicating the quantum phase transition from a Mott-insulator to a superfluid.^{21,22} However, the approximate value of χ in ν th order, $\chi^{(\nu)} \equiv \sum_{k=0}^{\nu} \beta_k (J/U)^k$ with the coefficients β_k depending on μ/U , will always be finite for finite J/U as long as μ/U is noninteger. Thus, in order to extract the critical parameter $(J/U)_c$ one has to resort to extrapolation to infinite order ν . The critical parameter can be associated with the radius of convergence of the series for χ with respect to J/U , namely $(J/U)_c = \lim_{k \rightarrow \infty} \beta_{k-1} / \beta_k$, assuming all β_k to have the same

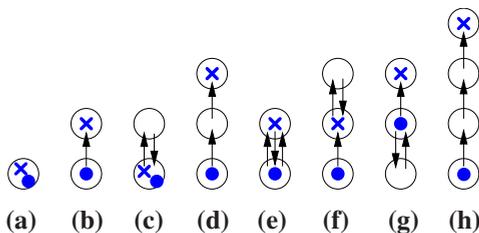


FIG. 6. (Color online) All topological diagrams contributing to the static susceptibility $\chi_{\hat{a}_0, \hat{a}_0^\dagger}$ in the leading orders 0, 1, 2, and 3.

sign. Plotting β_{k-1} / β_k versus $1/k$, one finds to good approximation all data points to lie on a straight line, suggesting the very simple phenomenological extrapolation scheme to extend the line to $1/k=0$ by a linear fit.²⁴ This procedure gives the phase boundary $(J/U)_c$ versus μ/U with an estimated error of 1%–2% for arbitrary large filling n and spatial dimensionalities $d=2, 3$, and greater.¹¹ The errors have been estimated by monitoring deviations of the approximate phase boundary while successively taking into account more and more coefficients β_k . For $n=1$ these results agree with those obtained by a strong coupling expansion^{25,26} ($d=2$) and by quantum Monte Carlo simulations^{27,28} ($d=2$ and 3). This simple example illustrates that extrapolation can be a valuable tool augmenting high-order perturbation calculus. A brief introduction to more advanced extrapolation techniques as well as further references can be found in chapter 1 of Ref. 4.

E. More general quantum lattice models

So far, in this section the method has been developed in terms of the Bose-Hubbard model (2). However, the approach is not restricted to this model, and following along the lines of the above example, it can be applied to a variety of quantum lattice models of the form given by Eq. (1). This includes fermionic Hubbard models or Heisenberg-type spin models. In the remaining part of this section the properties of quantum lattice models that are amenable to the method described in this paper will be sketched.

First of all the splitting of the full Hamiltonian (1) into an unperturbed part \hat{H}_0 and a perturbation \hat{V} does not necessarily have to be such that \hat{H}_0 contains just all on-site terms \hat{h}_i , while \hat{V} covers all coupling terms \hat{v}_{ij} . Both terms \hat{H}_0 and \hat{V} can contribute to both on-site terms \hat{h}_i and coupling terms \hat{v}_{ij} . Moreover, the site index i can be generalized to run over several degrees of freedom at every lattice point, or, similarly, the sum $\sum_{\langle ij \rangle}$ can be extended to include not only pairs of nearest neighbors, but also further pairs of near sites. It is, however, required that the relevant set of eigenstates of \hat{H}_0 is characterized by a set of on-site quantum numbers $\{n_i\}$ taking values $n_i = n_i^{\min}, n_i^{\min} + 1, n_i^{\min} + 2, \dots, n_i^{\max}$ (with the possibility of arbitrary large on-site state-space dimensionalities $\mathcal{D}_i = n_i^{\max} - n_i^{\min} + 1$). In other words, \hat{H}_0 should be expressed in terms of number operators \hat{n}_i with $\hat{n}_i |n_1 n_2 \dots n_i \dots\rangle = n_i |n_1 n_2 \dots n_i \dots\rangle$. For each site i there should also be a pair of ladder operators, $\hat{\ell}_i^+$ and $\hat{\ell}_i^-$, being defined by $\hat{\ell}_i^\pm |n_1 n_2 \dots n_i \dots\rangle = \eta_i^\pm |n_1 n_2 \dots n_i \pm 1 \dots\rangle$. The perturbation \hat{V} can be expressed in terms of both number and ladder operators. Given the structure described in this paragraph, it will be possible to define diagrams and to evaluate them in a similar fashion as described for the Bose-Hubbard model above.

Lattice systems covered by the scheme just outlined are bosonic or fermionic Hubbard models as well as spin Hamiltonians. In the former case the n_i are just occupation numbers running from $n_i^{\min}=0$ to $n_i^{\max}=\infty$ for bosons and $n_i^{\max}=1$ for fermions. The index i can also distinguish between different

internal degrees of freedom (or species) of particles. For spins, n_i would be associated with the magnetic quantum number characterizing the spin at site i along a distinguished quantization axis, taking values between $\pm S$ with half-integer total spin S . Concerning just the implementation, the systems (or the unperturbed states) amenable to the approach described here do not need to be homogeneous and they can be defined on various lattice geometries; also frustration, disorder, and certain types of long-range interaction can be present. But, of course, apart from being implementable the perturbation expansion must as well be a suitable approximation scheme for a given problem.

For particles (i.e., in the Hubbard case) the unperturbed Hamiltonian \hat{H}_0 can contain site-dependent potential terms $\propto \hat{n}_i$ and two-particle density-density interaction terms $\propto \hat{n}_i \hat{n}_j$, also three- and more particle terms are possible. In spin models, corresponding terms can be considered, describing, e.g., local magnetic fields along the quantization axis or Ising-type coupling. Nonlocal density-density interaction terms appearing in the unperturbed Hamiltonian \hat{H}_0 can, in fact, be long-ranged. In that case the unperturbed energies computed during the evaluation of a given diagram will depend on the unperturbed quantum numbers n_i at sites not contained in that diagram (these will be unaltered by the operations contained in the diagram). Considering a homogeneous unperturbed state, this will cause only little extra computational effort, for an inhomogeneous state the additional effort will just grow as the number of sites within the range of interaction. Clearly, the perturbative approach is limited to such strongly correlated phases that can be explored by starting from an unperturbed product state. However, the treatment of the bosonic Mott-transition^{11,25} is an example showing that even the boundaries of such phases in parameter space can be obtained by applying suitable extrapolation schemes. One should also note that (near) degeneracies between the unperturbed state considered and other unperturbed states can spoil the results obtained by perturbation theory. As a simple example, this can happen for varying on-site potentials (or magnetic fields) that cause at some sites two different quantum numbers to lead to similar unperturbed energies. As a remedy, in these cases one might consider to include degeneracy breaking terms in \hat{H}_0 and to subtract them again in the perturbation \hat{V} , cf. chapter 8 of Ref. 4 and references therein.

The perturbation \hat{V} can contain the ladder operators $\hat{\ell}_i^\pm$. For the Hubbard models these correspond to the bosonic or fermionic creation and annihilation operators, for a spin model they are given by the raising and lowering operators for the given quantization axis at site i . For bosonic and spin models the factors η_i^\pm just depend on the local quantum number n_i . In the case of the fermionic Hubbard model, the factors η_i^\pm accompanying the creation or annihilation of particles take the values $+1$ and -1 , depending on all occupation numbers $\{n_i\}$ (according to a given convention for the ordering of all sites i). Taking care of these signs will cause additional effort. While the unperturbed Hamiltonians \hat{H}_0 can contain long-range coupling terms, the coupling between different sites i and j appearing in the perturbation \hat{V} should be rather short-ranged, since the number of diagrams to be

evaluated grows rapidly with the number of coupling terms contained in \hat{V} . If the coupling between different sites i and j is of the familiar form $\hat{\ell}_i^+ \hat{\ell}_j^-$, diagrams can, again, be generated conveniently by finding paths through the lattice as described above for the Bose-Hubbard model. This form is, however, quite typical, as it describes both hopping of particles as well as spin-spin coupling in spin directions transverse to the quantization axis.

IV. SUMMARY

Let us briefly recapitulate the three basic steps of the approach described above in Secs. II and III. The first task to be accomplished is to generate the leading order energy corrections (19) as they appear in standard Rayleigh-Schrödinger perturbation theory such that in every order ν only a minimum number of different matrix elements (16), each characterized by $\nu-1$ non-negative integers α_k , has to be taken into account. This can be done, e.g., by starting from Kato's expression (12), and merging matrix elements that (via a decomposition into elementary matrix elements) are identified to give identical contributions. The number of relevant terms can further be reduced if *a priori* knowledge is available about the vanishing of all matrix elements appearing in certain orders ν with, e.g., ν being even, odd, or smaller than some value ν_0 . The obtained results also serve for the computation of expectation values and static susceptibilities.

The contributing matrix elements are interpreted as sums over process chains in a classical state space containing only the unperturbed states and not their superpositions, cf. Eq. (22). For the lattice problems considered, this formulation allows one to organize the perturbation expansion in terms of simple connected diagrams, each representing a collection of different operations. The second and the final third step to be accomplished are the generation and the evaluation of these diagrams. It has been shown that the generation of diagrams can be put down to the generation of paths through the lattice, a rather simple task that can be done on a computer even for large spatial dimensionalities d . Finally, the evaluation of diagrams is straightforward; one has to go through all possible sequences of the operations contained in a given diagram and map them according to Eq. (22) to the terms of the general perturbation expansion (19) obtained before. Since this procedure does not require a representation of the quantum-mechanical state space on the sublattice associated to a given diagram, it is not affected by large dimensionalities of the on-site state spaces.

V. CONCLUSION

A method to compute high-order series expansions for ground-state properties of quantum lattice models has been described that is based on Rayleigh-Schrödinger perturbation calculus. The approach can be divided into three basic steps that have to be accomplished on a computer; each of them can be implemented with reasonable effort. Since the treatment of high spatial dimensionalities as well as of large lattice-site state-space dimensionalities is not connected to serious difficulties, the presented approach complements the

well-known connected cluster method.^{6,7} Recently, the method described here has been used to compute the phase diagram of the Bose-Hubbard model on a d -dimensional hypercubic lattice, describing ultracold bosonic atoms in optical lattices.¹¹ It allowed not only to monitor in detail the convergence toward both the quantum-rotor limit of high filling n and the mean-field limit of large d , but also provided experimentally relevant data for two- and three-dimensional systems at moderate filling $n=2-10$. However, as outlined in Sec. III E a wide class of quantum lattice models including Heisenberg-type spin and Hubbard-type tight-binding models are amenable to the approach described in this paper. These models can be frustrated and inhomogeneous and they can contain disorder as well as long-range interaction of the density-density or Ising type. Especially in view of the enormous interest in quantum lattice systems made of ultracold

atoms,¹ the ease of treating three-dimensional systems can make the method a valuable tool for current research.

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¹M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen(de), and U. Sen, *Adv. Phys.* **56**, 243 (2007).

²I. Bloch, J. Dalibard, and W. Zwerger, *Rev. Mod. Phys.* **80**, 885 (2008).

³M. P. Gelfand and R. R. P. Singh, *Adv. Phys.* **49**, 93 (2000).

⁴B. J. Oitmaa, C. Hamer, and W. Zheng, *Series Expansion Methods for Strongly Interacting Lattice Models* (Cambridge University Press, Cambridge, UK, 2006).

⁵S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, UK, 1999).

⁶L. G. Marland, *J. Phys. A* **14**, 2047 (1981).

⁷M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *J. Stat. Phys.* **59**, 1093 (1990).

⁸M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, *Phys. Rev. B* **40**, 546 (1989).

⁹In order to compute corrections to the ground-state energy in ν th order, one has to consider connected clusters containing up to $M_C = \nu$ sites, such that \mathcal{D}_C is given by the number of possibilities to place $N_C = \nu M_C$ indistinguishable particles on these sites. If about 500 bytes are needed per state space dimension, this gives 100 gigabyte of required RAM already for the filling of either $n=3$ in tenth order or $n=5$ in eighth order.

¹⁰T. Kato, *Prog. Theor. Phys.* **4**, 514 (1949).

¹¹N. Teichmann, D. Hinrichs, M. Holthaus, and A. Eckardt, *Phys. Rev. B* **79**, 100503(R) (2009).

¹²M. Parrinello, M. Scirè, and T. Arai, *Lett. Nuovo Cimento Soc. Ital. Fis.* **6**, 138 (1973).

¹³C. J. Hamer and A. C. Irving, *Nucl. Phys. B* **230**, 336 (1984).

¹⁴P. Prelovšek, I. Sega, and J. Bonča, *Phys. Rev. B* **42**, 10706 (1990).

¹⁵By taking Kato’s expression (12) as a starting point here subcluster subtractions (or cumulant corrections) do not have to be performed on the level of each single diagram, as it is the case in Refs. 12 and 13. In contrast, the approach briefly sketched in Ref. 14 is more similar to the one presented here; it does, however, not include the (huge) reduction of terms contributing to

the general perturbation expansion that will be described in Sec. II B.

¹⁶D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).

¹⁷A. Messiah, *Quantenmechanik 2, 3. Auflage* (de Gruyter, Berlin, 1990).

¹⁸C. Bloch, *Nucl. Phys.* **6**, 329 (1958).

¹⁹R. Huby, *Proc. Phys. Soc.* **78**, 529 (1961).

²⁰V. Steenhoff (unpublished).

²¹J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Westview Press, Reading, MA, 1998).

²²F. E. A. dos Santos and A. Pelster, *Phys. Rev. A* **79**, 013614 (2009).

²³For any bipartite lattice geometry, as the hypercubic one, only an even number of tunneling operations leads back to the initial state such that only energy corrections of even power in J/U (not depending on the sign of the tunneling matrix element) appear. This fact can also be exploited to reduce the number of matrix elements considered in the general perturbation expansion (23).

²⁴Since the slope of the line is relatively low, the coefficients β_k resemble approximately those of a geometric series. Thus, also an exponential fit to the β_k already gives a good estimate to the phase boundary.

²⁵N. Elstner and H. Monien, *Phys. Rev. B* **59**, 12184 (1999).

²⁶Though using series expansions in powers of J/U , the approach of Ref. 25 is different from the one described here. Instead of computing the susceptibility χ to obtain the phase boundary, the authors compare the energy of a state with integer filling to the energies of defect states having one additional particle or hole. Moreover, they use a connected cluster expansion to obtain energy corrections.

²⁷B. Capogrosso-Sansone, N. V. Prokofev, and B. V. Svistunov, *Phys. Rev. B* **75**, 134302 (2007).

²⁸B. Capogrosso-Sansone, S. G. Soyler, N. Prokofev, and B. Svistunov, *Phys. Rev. A* **77**, 015602 (2008).