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Perturbative calculation of Jastrow factors: Accurate description of short-range correlations

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We present a perturbative treatment of Jastrow-type correlation factors which focus on an accurate description of short-range correlations. Our approach is closely related to coupled cluster perturbation theory with the essential difference that we start from a variational formulation for the energy. Such kind of perturbation theory is especially suited for multiscale bases, such as wavelets, which provide sparse representations for Jastrow factors. Envisaged applications in solid-state physics are confined many-particle systems such as electrons or multiexcitons in quantum dots. The resulting Jastrow factors can be further used as trial wave functions in quantum Monte Carlo calculations for these systems. First applications to a screened homogeneous Fermi gas model demonstrate that first-order Jastrow factors already recover 95% of the correlation energy in variational Monte Carlo calculations over a fairly large range of densities and screening parameters. The corresponding second- and third-order perturbation energies turned out to be more sensitive to the specific choice of the model parameters. Furthermore, we have compared our first-order Jastrow factors with those obtained from Fermi hypernetted chain calculations, where excellent agreement at short and intermediate interparticle distances has been observed.

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I. INTRODUCTION

The determination of ground-state properties for interacting many-particle systems is a central topic in condensed matter physics and quantum chemistry. It can be either treated by density-functional theory (DFT), or through a more direct approach based on certain kinds of many-particle wave functions. Within DFT, the original many-particle problem is mapped, via the Kohn-Sham equation,[1] into an effective one-particle problem and thus considerably reduces the computational effort. Despite the great success of DFT for a large variety of systems, it has the basic drawback that there exists no systematic way to improve the exchange-correlation potential in the Kohn-Sham equation. On the contrary, various schemes for a systematic improvement of many-particle wave functions exist. We just want to mention the coupled cluster (CC) theory[2,3] and the Fermi hypernetted chain (FHNC) method.[4,5] By construction, CC theory is aiming toward a direct approximation of the exact wave function, while the FHNC method deals with a more restricted class of Jastrow-type wave functions, which is supposed to be very close to the exact one. A common feature of both methods is the ansatz

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)=\mathcal{F}\Phi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N), \tag{1}$$

where a correlation operator $\mathcal{F}$ acts on a single Slater determinant Φ. Here and in the following, $\mathbf{x}_i:=(\mathbf{r}_i,\sigma_i)$ denotes the combined spatial and spin coordinate of a particle. Their distinguished role in condensed matter physics is due to the fact that both methods provide the correct asymptotic behavior for short- and long-range correlations. The latter, however, inevitably lead to certain types of nonlinearities which make these methods considerably more complicated than standard many-body perturbation theory (MBPT). Concerning computational complexity, the CC method appears to be better tractable, however, for the price of a rather special ansatz for the correlation operator. This excludes, e.g., the Jastrow ansatz,

$$\mathcal{F}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\exp\left[\sum_i u^{(1)}(\mathbf{r}_i)+\sum_{i<j} u^{(2)}(\mathbf{r}_i,\mathbf{r}_j)\cdots\right], \tag{2}$$

where the correlation operator simply consists of a symmetric function of the spatial electron coordinates. In this context, we have to mention the generalized CC method of Noga and Kutzelnigg,[6] which incorporates a spatial function which depends explicitly on the interelectron distance. Such kind of term describes the wave function near the interelectron cusps and improves convergence with respect to the size of the basis set.

Jastrow factors provide the starting point for the FHNC method and are particularly interesting, concerning possible applications in quantum Monte Carlo (QMC) calculations.[7] Within variational Monte Carlo (VMC), the expectation value of the energy is calculated for Jastrow-type wave functions using various variants of the Metropolis algorithm. The diffusion Monte Carlo (DMC) method enables an exact solution of Schrödinger's equation within the fixed-node approximation. This method requires Jastrow factors as accurate trial wave functions for an efficient reduction of the statistical variance of the energy. Herewith, it is the short-range behavior of the Jastrow factor near the coalescence points of particles that gives the dominant contribution. QMC methods enable a compact representation of the k-particle correlation functions $u^{(k)}$ in terms of rational functions of the interparticle distances.[8,9] Because of the computational complexity of the FHNC method, it became common practice to use stochastic approaches for the optimization of these Jastrow factors.[8–13] Either variance-minimization techniques[8–11] or methods for a direct minimization of the energy[12,13] were employed. These optimization techniques yield wave functions which typically recover between 70% and 95% of the correlation energy with amazingly small numbers of parameters compared to other many-particle methods of similar accuracy. A potential drawback of stochastic approaches, however, is the multitude of local minima that are encountered during the optimization. The resulting Jastrow factors, therefore, typically correspond to local minima which might depend on the initial guess for the parameters. Such kind of ambiguity has only minor effects concerning the total energy of a system; however, it hampers an unbiased calculation of energy differences.

An alternative representation for Jastrow factors can be obtained from wavelet-based multiresolution analysis. This approach takes into account the multiscale character of many-particle systems and provides sparse approximations for correlation functions $u^{(k)}$ in terms of hierarchical tensor product wavelets,[14–17] which can be adapted to the specific length and energy scales of the system under consideration. Multiscale representations are also of potential interest for QMC calculations because of the local character of wavelet bases. In a previous paper,[16] we have studied the computational complexity of wavelet approximations for the local ansatz of Stollhoff and Fulde,[18] cf. Ref. 19, using diagrammatic techniques from FHNC theory. Within the present work, we consider a more general approach based on standard perturbation theory. It turns out that our approach is closely related to the coupled cluster perturbation theory (CCPT) presented in Ref. 2. Furthermore, we have to mention the huge amount of work devoted to linked-cluster expansions for Jastrow-type wave functions in nuclear physics during the late 1960s and early 1970s of the last century, which finally culminated into the development of FHNC theory (see, e.g., Ref. 20 for a comprehensive discussion of this subject). We just want to refer to Talman's approximate variational treatment of Jastrow factors[21,22] that agrees in lowest order with our approach. Except for homogeneous systems, these methods become very costly from the computational point of view. Therefore, standard perturbation theory turns out to be an interesting alternative at the expense of an accurate treatment of long-range correlations. For our envisaged applications in solid state physics, such as electrons or multiexcitons confined to a quantum dot and quantum chemistry, this is perfectly justified. Otherwise, it is possible to combine our perturbative approach with a recently developed random phase approximation (RPA) for inhomogeneous systems by Gaudoin *et al.*[23] that provides an accurate description of the long-range behavior of Jastrow factors.

The paper is organized as follows. In Sec. II, we present a perturbation analysis of Jastrow factors, where linear and exponential perturbation expansions for correlation factors are derived in Secs. II A and II B, respectively. Applications to a screened Fermi gas model with periodic boundary conditions are discussed in Sec. III. A qualitative study of perturbative Jastrow factors through comparison with FHNC calculations is presented in Sec. III A. The second- and third-order correlation energies are compared with results from QMC calculations in Sec.III B. Finally, in Sec. IV we make some concluding remarks.

II. PERTURBATION ANALYSIS OF JASTROW FACTORS

We consider a general product ansatz for the wave function

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \mathcal{F}(\mathbf{x}_1,\ldots,\mathbf{x}_N)\Phi(\mathbf{x}_1,\ldots,\mathbf{x}_N), \tag{3}$$

where the correlation factor $\mathcal{F}$ is a symmetric function of the electron coordinates. The corresponding variational problem consists of minimizing the expectation value of the energy,

$$E = \min_{\mathcal{F}} \frac{\int d^3x_1,\ldots,d^3x_N \mathcal{F}\Phi^*(\mathbf{x}_1,\ldots,\mathbf{x}_N) H \mathcal{F}\Phi(\mathbf{x}_1,\ldots,\mathbf{x}_N)}{\int d^3x_1,\ldots,d^3x_N \mathcal{F}\Phi^*(\mathbf{x}_1,\ldots,\mathbf{x}_N) \mathcal{F}\Phi(\mathbf{x}_1,\ldots,\mathbf{x}_N)}, \tag{4}$$

with respect to the correlation factor $\mathcal{F}$ for a fixed reference wave function Φ. Two different perturbation schemes for this variational problem are discussed below. The first scheme utilizes a linear representation for the correlation factor, whereas the second scheme is based on the exponential Jastrow-type ansatz [Eq. (2)]. Both schemes employ symmetric many-particle basis functions of the form

$$\mathcal{U}^{(0)}(\mathbf{X}) = 1, \quad \mathcal{U}^{(1)}_{\alpha}(\mathbf{X}) = \sum_i u^{(1)}_{\alpha}(\mathbf{x}_i),$$

$$\mathcal{U}^{(2)}_{\beta}(\mathbf{X}) = \frac{1}{2}\sum_{i\neq j} u^{(2)}_{\beta}(\mathbf{x}_i,\mathbf{x}_j),$$

$$\ldots, \tag{5}$$

where $u^{(k)}_{\alpha}(\mathbf{x}_{i_1},\mathbf{x}_{i_2},\ldots,\mathbf{x}_{i_k})$ denote symmetric k-particle basis functions with indices $\alpha \in \Lambda_k$ taken from conveniently defined index sets. In the following, we refer to k as the *degree* of the basis functions. For notational convenience, we have introduced the short-hand notation $\mathbf{X} := (\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)$ to represent the combined vector of all electron coordinates. The computational complexity increases substantially with the degree of the basis functions. Therefore, it is essential to truncate the basis at a certain degree. It turns out that both perturbation schemes discussed below provide such truncations in a natural way.

Obviously, there are certain redundancies in our many-particle basis. According to definition (5), one-particle basis functions can be expressed, e.g., in terms of two-particle functions, etc., which means that the basis is overcomplete without further restrictions. Such kind of restrictions can be imposed in various ways. For example, it is possible to derive a suitable basis from multiresolution analysis. Neglecting spin degrees of freedom, a many-particle basis can be defined via wavelet tensor products,

$$u_\alpha^{(1)}(\mathbf{r}_i) = \gamma_\alpha(\mathbf{r}_i),$$

$$u_{\alpha,\beta}^{(2)}(\mathbf{r}_i,\mathbf{r}_j) = \gamma_\alpha(\mathbf{r}_i)\gamma_\beta(\mathbf{r}_j) + \gamma_\alpha(\mathbf{r}_j)\gamma_\beta(\mathbf{r}_i),$$

$$\ldots, \tag{6}$$

where a k-particle basis function corresponds to a k-fold tensor product of $3d$ wavelets γ_α. The multivariate wavelets γ_α themselves consist of threefold mixed tensor products of univariate wavelets and scaling functions, at which each tensor product contains at least one univariate wavelet. For further details and applications, we refer to our previous publication.[14,16] By definition, these $3d$ wavelets span the so-called homogeneous function spaces[24] that do not contain constant functions. Thereby, this ansatz largely avoids possible redundancies within the many-particle basis. Wavelet tensor products enable an adaptive approximation of electron correlations,[14] where the size of the k-particle basis increases almost linearly, i.e., $O[M\log(M)^{k-1}]$, with the number M of $3d$ wavelets. Furthermore, tensor product structures considerably simplify the evaluation of matrix elements.[16,25]

Second quantization provides another possibility to impose further restrictions on the many-particle basis [Eq. (5)]. Stollhoff and Fulde,[18] cf. Ref. 19, have suggested taking only the normal ordered part of the basis functions [Eq. (5)] which removes all contributions with degree $<k$ from $\mathcal{U}_\alpha^{(k)}$. Furthermore, second quantization introduces additional flexibility into the perturbation analysis. This can be used to reduce the computational complexity which is essential for practical applications. In order to illustrate our assertion, we consider an arbitrary two-particle basis function as an operator in second quantization,

$$\mathcal{U}_\alpha^{(2)} \equiv \hat{U}_\alpha^{(2)} = \frac{1}{2}\sum_{pqrs} \langle pq|u_\alpha^{(2)}|rs\rangle c_p^\dagger c_q^\dagger c_s c_r, \tag{7}$$

where $c_p^\dagger$ and c_s denote the creation and anihilation operators for the corresponding orbitals φ_p and φ_s of a single-particle Hamiltonian H_0. In the following, we denote virtual orbitals by $a,b,\ldots$, occupied orbitals by $i,j,\ldots$, and arbitrary orbitals by $p,q,\ldots$. Using standard diagrammatic notation,[26] we can express two-particle operators in terms of Goldstone diagrams. These diagrams are depicted in Fig. 1, where horizontal dashed lines represent two-particle integrals $\langle pq|u_\alpha^{(2)}|rs\rangle$ and upward and downward pointing solid lines denote "particle" (virtual orbitals) and "hole" states (occupied orbitals), respectively. We want to mention that virtual orbitals $\{\varphi_a\}$ are introduced for purely formal reasons and that for diagrammatic calculations only occupied orbitals $\{\varphi_i\}$ are required. This is due to the fact that the underlying basis [Eq. (5)] consists of simple functions which allows us to use the identity

$$\sum_a \varphi_a(\mathbf{x}_1)\varphi_a^*(\mathbf{x}_2) = \delta(\mathbf{r}_1-\mathbf{r}_2)\delta_{\sigma_1,\sigma_2} - \sum_i \varphi_i(\mathbf{x}_1)\varphi_i^*(\mathbf{x}_2). \tag{8}$$

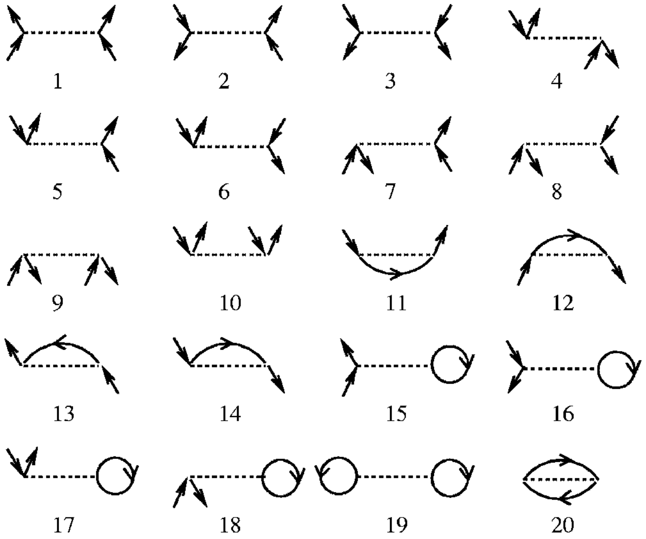

FIG. 1. Goldstone diagrams representing a symmetric two-particle basis function $\mathcal{U}_\alpha^{(2)}$.

We refer to Ref. 16 for further details. The normal ordered part of the operator [Eq. (7)] comprises diagrams 1–10. According to the original suggestion of Stollhoff and Fulde,[18] only these diagrams should be taken into account. The remaining diagrams 11–18 represent one-particle operators; however, diagrams 11–14 are intrinsically nonlocal and are therefore not represented by basis functions of degree <2. To keep all nonlocal diagrams preserves commutativity of the many-particle basis, which turns out to be essential for the exponential perturbation scheme. Furthermore, it has the advantage of being directly applicable in QMC calculations where only local functions can be used to represent the Jastrow factor. The new local basis functions, corresponding to diagrams 1–14, are given by

$$\tilde{\mathcal{U}}_\alpha^{(2)}(\mathbf{X}) = \mathcal{U}_\alpha^{(2)}(\mathbf{X}) - \sum_i \int d^3x'\, u_\alpha^{(2)}(\mathbf{x}_i,\mathbf{x}')\rho(\mathbf{x}') - \frac{1}{2}\sum_{i,j}(\langle ij|u_\alpha^{(2)}|ij\rangle - \langle ij|u_\alpha^{(2)}|ji\rangle), \tag{9}$$

where $\rho(\mathbf{x})$ is the spin density of the reference wave function Φ. A more radical approach in the spirit of CC theory is to keep only the tenth diagram, where the corresponding cluster-type operator,

$$\hat{U}_\alpha^{(2,c)} \coloneqq \frac{1}{2}\sum_{abij}\langle ab|u_\alpha^{(2)}|ij\rangle c_a^\dagger c_b^\dagger c_j c_i, \tag{10}$$

is of nonlocal character and cannot be immediately applied in QMC calculations. It turns out that cluster operators significantly reduce the computational complexity at higher orders of perturbation theory.

A. Linear perturbation expansion of the correlation factor

It is instructive to consider first a linear expansion of the correlation factor in second quantization,

$$\hat{\mathcal{F}} = \sum_{k=0}^{N} \sum_{\alpha \in \Lambda_k} a_{k\alpha} \hat{U}_\alpha^{(k)}, \tag{11}$$

where, e.g., $\hat{U}_\alpha^{(2)}$ can be represented by any subset of the diagrams in Fig. 1. A variation of the Rayleigh quotient [Eq. (4)] with respect to the coefficients $a_{k\alpha}$ leads to a generalized eigenvalue problem,

$$\langle \hat{U}_\alpha^{(k)\dagger} \hat{H} \hat{\mathcal{F}} \rangle = E \langle \hat{U}_\alpha^{(k)\dagger} \hat{\mathcal{F}} \rangle, \tag{12}$$

in which we use here and in the following $\langle \hat{O} \rangle$ to denote $\int d^3x_1, \ldots, d^3x_N \Phi^*(\mathbf{x}_1, \ldots, \mathbf{x}_N) \hat{O} \Phi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$. The eigenvalue problem [Eq. (12)] determines the correlated wave function $\hat{\mathcal{F}}\Phi$ up to a normalization constant. In order to fix this constant, we have chosen the intermediate normalization condition

$$\langle \hat{\mathcal{F}} \rangle = 1, \tag{13}$$

which is frequently used in standard MBPT.[27]

A basic drawback of the variational treatment of the linear ansatz [Eq. (11)] is that there exists no simple size-consistent truncation scheme with respect to the degree of the basis functions [Eq. (5)]. However, such a scheme exists for a perturbative treatment of Eq. (12). According to a standard procedure in perturbation theory, we split up the Hamiltonian,

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{W}, \tag{14}$$

into a one-particle operator $\hat{H}_0$ and a two-particle operator $\hat{W}$ times the coupling constant λ, where the reference wave function Φ solves the ground-state eigenvalue problem,

$$\hat{H}_0 \Phi = E_0 \Phi. \tag{15}$$

Furthermore, we assume that there exist power-series expansions with respect to the coupling constant λ for the energy

$$E(\lambda) = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots, \tag{16}$$

and the correlation factor

$$\hat{\mathcal{F}}(\lambda) = \hat{F}_0 + \lambda \hat{F}_1 + \lambda^2 \hat{F}_2 + \cdots. \tag{17}$$

It follows immediately from the intermediate normalization condition [Eq. (13)] that

$$\hat{F}_0 = 1 \text{ and } \langle \hat{F}_m \rangle = 0 \quad \text{for } m \geqslant 1. \tag{18}$$

Actually, $\hat{\mathcal{F}}$ depends on λ, according to Eq. (11), via its coefficients $a_{k\alpha}(\lambda)$. These coefficients have formal expansions,

$$a_{k\alpha}(\lambda) = \sum_m a_{k\alpha}^{(m)} \lambda^m, \tag{19}$$

so that the mth-order correlation factor $\hat{F}_m$ in Eq. (17) can be written as

$$\hat{F}_m = \sum_{k=0}^{N} \sum_{\alpha \in \Lambda_k} a_{k\alpha}^{(m)} \hat{U}_\alpha^{(k)}. \tag{20}$$

Inserting Eqs. (14) and (16) into Eq. (12) and comparing different powers of λ, we obtain perturbation equations for the correlation factor,

$$\begin{aligned} &\langle \hat{U}_\alpha^{(k)\dagger} (\hat{H}_0 - E_0) \hat{F}_m \rangle \\ &\quad = - \langle \hat{U}_\alpha^{(k)\dagger} \hat{W} \hat{F}_{m-1} \rangle + \sum_{p=1}^{m} E_p \langle \hat{U}_\alpha^{(k)\dagger} \hat{F}_{m-p} \rangle, \quad m = 1, 2, \ldots . \end{aligned} \tag{21}$$

These equations resemble Galerkin discretizations of continuous perturbation equations already mentioned by Møller and Plesset.[28] However, we want to remind the reader that our test basis $\mathcal{U}_\alpha(\mathbf{X})\Phi$ is generically incomplete in the space of many-particle wave functions. To a certain extent, our approach resembles the fixed-node approximation in QMC calculations because all of our test basis functions in the Galerkin scheme share the nodes of the reference wave function Φ. We should bear in mind this important aspect in the following, when we obtain expressions which appear similar to standard perturbation theory. In this respect, our approach differs from the Gaussian geminal method described in Refs. 29 and 30, where highly accurate solutions of the continuous perturbation equations have been considered following Sinanoğlu's work.[31,32]

The underlying variational formulation for correlation factors [Eq. (4)] is obviously size consistent. Therefore, size consistency is satisfied for each order of perturbation theory separately. Furthermore, the sequence of perturbation equations [Eq. (21)] implies a truncation scheme with respect to the degree of the many-particle basis [Eq. (5)], which has already been recognized by Sinanoğlu.[32] For example, a first-order correlation factor $\hat{F}_1$ contains contributions only from one- and two-particle normal ordered or cluster-type operators $\hat{U}_\alpha^{(k)}$.

B. Perturbation expansion of the Jastrow ansatz

The linear expansion of the correlation factor is not convenient for further usage in QMC calculations. Although the perturbation energies are size consistent, this is not the case anymore for a variational treatment of the perturbative wave function. It is therefore natural to consider a perturbation theory for the exponential Jastrow ansatz,

$$\hat{\mathcal{F}} = e^{\hat{\tau}} \quad \text{with } \hat{\tau} = \sum_{k=0}^{K} \sum_{\alpha \in \Lambda_k} a_{k\alpha} \hat{U}_\alpha^{(k)}, \tag{22}$$

where we can truncate the expansion with respect to k at any order $K \leqslant N$ without violating size consistency for the variational energy [Eq. (4)]. It is well known that the two-particle terms $\hat{U}_\alpha^{(2)}$ give the dominant contribution to the correlation energy (cf. Ref. 33 for a discussion of higher-order terms). The exponential ansatz incorporates already a lot of essential physics and therefore considerably reduces the number of degrees of freedom that have to be taken into account. Variation with respect to the coefficients $a_{k\alpha}$ leads to a nonlinear eigenvalue problem,

$$\langle \hat{U}_\alpha^{(k)\dagger} e^{\hat{\tau}^\dagger} \hat{H} e^{\hat{\tau}} \rangle = E \langle \hat{U}_\alpha^{(k)\dagger} e^{\hat{\tau}^\dagger} e^{\hat{\tau}} \rangle, \tag{23}$$

where we have assumed that the operators $\hat{U}_\alpha^{(k)}$ commute with each other. This is the case for simple functions as well as for cluster-type operators. According to our previous discussion, cluster-type operators are much more favorable concerning the diagrammatic evaluation of matrix elements. At first glance, the exponential Jastrow ansatz [Eq. (22)] closely resembles the CC approach.[3] There is, however, an essential difference inasmuch as the underlying function basis $\mathcal{U}_\alpha^{(k)}$ does not guaranty the convergence of the product ansatz [Eq. (3)] to the exact wave function in the complete basis-set limit. Here, completeness has to be considered in an appropriate function space to which the $\mathcal{U}_\alpha^{(k)}$ belong. This shortcoming of the Jastrow ansatz manifests itself in the fixed-node error of DMC calculations. For that reason, we take the variational energy [Eq. (4)] as the starting point for our perturbation analysis instead of the CC energy and projection equations. The latter assume an exact ansatz for the wave function and provide the basis for the CCPT presented in Ref. 2.

For the perturbation analysis, we assume again a λ-dependent Hamiltonian [Eq. (14)] which leads to power-series expansions for the energy [Eq. (16)] and correlation operator,

$$\hat{\tau}(\lambda) = \hat{\tau}_0 + \hat{\tau}_1\lambda + \hat{\tau}_2\lambda^2 + \cdots + \hat{\tau}_m\lambda^m + \cdots. \tag{24}$$

Analogous to Eq. (11), different orders of the correlation operator are represented through expansions in the operator basis,

$$\hat{\tau}_m = \sum_{k=0}^{K} \sum_{\alpha\in\Lambda_k} a_{k\alpha}^{(m)} \hat{U}_\alpha^{(k)}, \tag{25}$$

which can be truncated at any order $K \leqslant N$. In order to derive the perturbation equations for $\hat{\tau}_m$, we expand the exponential ansatz in powers of λ.

$$e^{\hat{\tau}(\lambda)} = \hat{F}_0 + \hat{F}_1\lambda + \hat{F}_2\lambda^2 + \cdots + \hat{F}_m\lambda^m + \cdots, \tag{26}$$

where the constant term $\hat{F}_0 = 1\,(\hat{\tau}_0 = 0)$ is fixed by the intermediate normalization condition [Eq. (13)] and the next lowest-order terms are given by

$$\hat{F}_1 = \hat{\tau}_1, \quad \hat{F}_2 = \hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2,$$

$$\hat{F}_3 = \hat{\tau}_3 + \hat{\tau}_2\hat{\tau}_1 + \frac{1}{3!}\hat{\tau}_1^3,$$

$$\hat{F}_4 = \hat{\tau}_4 + \hat{\tau}_3\hat{\tau}_1 + \frac{1}{2}\hat{\tau}_2^2 + \frac{1}{2}\hat{\tau}_2\hat{\tau}_1^2 + \frac{1}{4!}\hat{\tau}_1^4,$$

$$\ldots .$$

Perturbation equations for the Jastrow ansatz can be obtained by inserting Eqs. (16) and (26) into the eigenvalue problem [Eq. (23)] and comparing the coefficients for fixed powers of λ. In the following, we refer to this method as Jastrow perturbation theory (JPT). The first-order equation for the correlation operator $\hat{\tau}_1$ is given by

$$\langle \hat{U}_\alpha^{(k)\dagger} (\hat{H}_0 - E_0)\hat{\tau}_1 \rangle = -\langle \hat{U}_\alpha^{(k)\dagger} (\hat{W} - E_1) \rangle, \tag{27}$$

from which we obtain the second-order energy (JPT2),

$$E_2 = \langle \hat{W}\hat{\tau}_1 \rangle, \tag{28}$$

with $E_1 = \langle \hat{W} \rangle$ and $\langle \hat{\tau}_1 \rangle = \langle \hat{F}_1 \rangle = 0$ as before. For higher orders, we have the following general equation:

$$\begin{aligned} \langle \hat{U}_\alpha^{(k)\dagger} (\hat{H}_0 - E_0)\hat{F}_m \rangle = & -\sum_{p=1}^{m-1} \langle \hat{U}_\alpha^{(k)\dagger} \hat{F}_p^\dagger (\hat{H}_0 - E_0)\hat{F}_{m-p} \rangle \\ & - \sum_{p=0}^{m-1} \langle \hat{U}_\alpha^{(k)\dagger} \hat{F}_p^\dagger \hat{W} \hat{F}_{m-p-1} \rangle \\ & + \sum_{p=1}^{m} E_p \sum_{q=0}^{m-p} \langle \hat{U}_\alpha^{(k)\dagger} \hat{F}_q^\dagger \hat{F}_{m-p-q} \rangle. \end{aligned} \tag{29}$$

From this, we get the second-order equation,

$$\begin{aligned} & \langle \hat{U}_\alpha^{(k)\dagger} (\hat{H}_0 - E_0)\hat{\tau}_2 \rangle \\ & \quad = -\langle \hat{U}_\alpha^{(k)\dagger} (\hat{W} - E_1)\hat{\tau}_1 \rangle - \frac{1}{2}\langle \hat{U}_\alpha^{(k)\dagger} (\hat{H}_0 - E_0)\hat{\tau}_1^2 \rangle \\ & \qquad - \langle \hat{U}_\alpha^{(k)\dagger} \hat{\tau}_1^\dagger (\hat{H}_0 - E_0)\hat{\tau}_1 \rangle - \langle \hat{U}_\alpha^{(k)\dagger} \hat{\tau}_1^\dagger (\hat{W} - E_1) \rangle + E_2 \langle \hat{U}_\alpha^{(k)\dagger} \rangle, \end{aligned} \tag{30}$$

and the third-order energy (JPT3),

$$\begin{aligned} E_3 & = \frac{1}{2}\langle \hat{\tau}_1^\dagger (\hat{W} - E_1)\hat{\tau}_1 \rangle + \left\langle \hat{\tau}_1^\dagger (\hat{H}_0 - E_0)\left(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\right) \right\rangle \\ & \quad + \left\langle (\hat{W} - E_1)\left(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\right) \right\rangle + \text{c.c.} \\ & = \frac{1}{2}\langle \hat{\tau}_1^\dagger (\hat{W} - E_1)\hat{\tau}_1 \rangle + \frac{1}{2}\langle \hat{\tau}_1^\dagger (\hat{H}_0 - E_0)\hat{\tau}_1^2 \rangle \\ & \quad + \frac{1}{2}\langle (\hat{W} - E_1)\hat{\tau}_1^2 \rangle + \text{c.c.}, \end{aligned} \tag{31}$$

where we have used the relation

$$\langle \hat{\tau}_1^\dagger (\hat{H}_0 - E_0)\hat{\tau}_2 \rangle = -\langle (\hat{W} - E_1)\hat{\tau}_2 \rangle, \tag{32}$$

which can be easily derived from Eq. (27). In accordance with Wigner's $2m+1$ rule,[2] the third-order energy requires only the first-order correction of the wave function. Furthermore, with the second-order wave function, we obtain an expression for the fourth-order energy (JPT4),

$$\begin{aligned}E_4 = \frac{1}{2}\Big\langle \Big(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\Big)^\dagger (\hat{H}_0 - E_0)\Big(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\Big)\Big\rangle \\ + \Big\langle \hat{\tau}_1^\dagger (\hat{W} - E_1)\Big(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\Big)\Big\rangle - E_2\frac{1}{2}\langle \hat{\tau}_1^\dagger \hat{\tau}_1\rangle \\ + \Big\langle \hat{\tau}_1^\dagger (\hat{H}_0 - E_0)\Big(\hat{\tau}_2\hat{\tau}_1 + \frac{1}{3!}\hat{\tau}_1^3\Big)\Big\rangle \\ + \Big\langle (\hat{W} - E_1)\Big(\hat{\tau}_2\hat{\tau}_1 + \frac{1}{3!}\hat{\tau}_1^3\Big)\Big\rangle + \text{c.c.}\end{aligned} \tag{33}$$

If a cluster-type basis is used, further simplifications of the second-order [Eq. (30)] as well as of third- and fourth-order energies [Eqs. (31) and (33)] can be achieved, provided that the operator basis is closed with respect to multiplication up to degree of 2 i.e.,

$$\hat{U}_\alpha^{(1)}\hat{U}_\beta^{(1)} = \sum_\gamma c_\gamma \hat{U}_\gamma^{(2)}. \tag{34}$$

Under this assumption, we can make use of the relation

$$\begin{aligned}\langle \hat{U}_\alpha^{(k_1)\dagger}\hat{U}_\beta^{(k_2)\dagger}\hat{U}_\lambda^{(k_3)\dagger}(\hat{H}_0 - E_0)\hat{\tau}_1\rangle \\ = -\langle \hat{U}_\alpha^{(k_1)\dagger}\hat{U}_\beta^{(k_2)\dagger}\hat{U}_\lambda^{(k_3)\dagger}(\hat{W} - E_1)\rangle.\end{aligned} \tag{35}$$

For an operator product $\hat{U}_\alpha^{(k_1)\dagger}\hat{U}_\beta^{(k_2)\dagger}\hat{U}_\lambda^{(k_3)\dagger}$ of degree $k_1 + k_2 + k_3 > 2$, both sides of the relation vanish since it cannot be fully contracted by $(\hat{H}_0 - E_0)\hat{\tau}_1$ and $\hat{W}$, respectively. In the remaining cases, relation (35) either directly corresponds to the first-order equation [Eq. (27)] or can be reduced to it by applying the closedness assumption [Eq. (34)]. Using relation (35) for a cluster-type operator basis which satisfies the closedness condition [Eq. (34)], Eqs. (30), (31), and (33) reduce to

$$\begin{aligned}\langle \hat{U}_\alpha^{(k)\dagger}(\hat{H}_0 - E_0)\hat{\tau}_2\rangle = -\langle \hat{U}_\alpha^{(k)\dagger}(\hat{W} - E_1)\hat{\tau}_1\rangle \\ - \frac{1}{2}\langle \hat{U}_\alpha^{(k)\dagger}(\hat{H}_0 - E_0)\hat{\tau}_1^2\rangle + E_2\langle \hat{U}_\alpha^{(k)\dagger}\rangle\end{aligned} \tag{36}$$

$$E_3 = \langle \hat{\tau}_1^\dagger (\hat{W} - E_1)\hat{\tau}_1\rangle, \tag{37}$$

$$\begin{aligned}E_4 = \frac{1}{2}\Big\langle \Big(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\Big)^\dagger (\hat{H}_0 - E_0)\Big(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\Big)\Big\rangle \\ + \Big\langle \hat{\tau}_1^\dagger (\hat{W} - E_1)\Big(\hat{\tau}_2 + \frac{1}{2}\hat{\tau}_1^2\Big)\Big\rangle - \frac{1}{2}E_2\langle \hat{\tau}_1^\dagger \hat{\tau}_1\rangle + \text{c.c.}\end{aligned} \tag{38}$$

We want to close this section with a remark concerning the intimate relation between JPT3 and the local ansatz of Stollhoff and Fulde.[18] In Ref. 16, we have discussed the local ansatz in its simplest variant, namely, for two-particle normal-ordered operators only. Concerning the local ansatz, these operators are equivalent to cluster-type operators [Eq. (10)]. In our present notation, the local ansatz corresponds to the linear equation,

$$\langle \hat{U}_\alpha^{(2)\dagger}(\hat{H}_0 + \hat{W})\hat{\tau}\rangle - (E_0 + E_1)\langle \hat{U}_\alpha^{(2)\dagger}\hat{\tau}\rangle = -\langle \hat{U}_\alpha^{(2)\dagger}\hat{W}\rangle, \tag{39}$$

where the correlation energy is given by

$$E_{\text{corr}} = \langle \hat{W}\hat{\tau}\rangle. \tag{40}$$

It is easy to see that a perturbative treatment of the local ansatz using Eqs. (14), (16), and (24) reproduces the first- and second-order equations [Eqs. (27) and (36)] as well as the second- and third-order energy expressions [Eqs. (28) and (37)].

III. PERTURBATIVE JASTROW FACTORS FOR A HOMOGENEOUS FERMI GAS

In order to test the accuracy of the JPT approach for short-range correlations, we have studied a homogeneous spin-unpolarized Fermi gas at various densities. Because of the well-known shortcoming of finite order perturbation theory for the homogeneous electron gas, we have chosen, instead of the bare Coulomb potential, a Yukawa potential,

$$v(\mathbf{r}) = \frac{e^{-\mu|\mathbf{r}|}}{|\mathbf{r}|}, \tag{41}$$

with screening parameter μ. To be consistent with QMC methods, the calculations have been performed for supercell models with periodic boundary conditions.[7,34] The supercell Hamiltonian is of the form

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\Delta_i + \frac{1}{2}\sum_{\mathbf{R}}\sum_{i\neq j} v(\mathbf{r}_i - \mathbf{r}_j + \mathbf{R}), \tag{42}$$

where the periodic interaction potential has been taken as a sum over all lattice vectors **R** of the supercell. We have considered two different decompositions of the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{W}$, where $\hat{H}_0$ corresponds either to the bare kinetic energy or to the Fock operator. For homogeneous systems this makes only a minor difference because the zeroth-order wavefunction Φ is already fixed by translational symmetry. For small values of the screening parameter ($\mu \leqslant 1$ bohr^{-1}), the Fock operator yields more accurate correlation energies and pair-correlation functions. It turns out, however, that with increasing μ, this difference becomes marginal. In the following, we present results only for the Fock operator.

Because of translational symmetry, the first-order Jastrow factor requires only two-particle basis functions. Adapted to periodic boundary conditions and translational symmetry, we have chosen two-particle basis functions of the form

$$u_\alpha^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{R}} g_\alpha(\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{R}) \quad \text{with } g_\alpha(\mathbf{r}) = \exp(-\xi_\alpha \mathbf{r}^2), \tag{43}$$

where the exponents of the Gaussian basis set have been taken from an even-tempered sequence $\xi_\alpha = a_0 b^{\alpha-1}$, $\alpha = 1, \ldots, n$, with appropriately chosen parameters $a_0 = 0.03$, $b = 3$, and $n = 6$. Expressed in second quantization, this basis can be modified by removing the constant diagrams 19 and

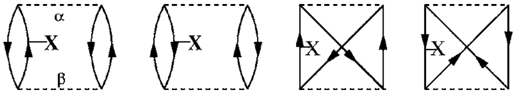

FIG. 2. Diagrams required for the calculation of matrix elements $\langle \hat{U}_{\alpha}^{(2)\dagger}(\hat{H}_0 - E_0)\hat{U}_{\beta}^{(2)}\rangle$.

20 from Fig. 1 in order to satisfy the intermediate normalization condition $\langle \tau_1 \rangle = 0$. Actually, only diagram 10 in Fig. 1 contributes to the first-order equation [Eq. (27)]. It makes no difference with respect to the coefficients $a_{2\alpha}^{(1)}$ and therefore for the JPT2 and JPT3 correlation energies, cf. Eqs. (28) and (31), whether local basis functions [Eq. (9)] or cluster-type operators [Eq. (10)] have been chosen as a basis set. For higher orders in perturbation theory, the two basis sets are not equivalent anymore.

The matrix elements of the first-order equation [Eq. (27)] require the calculation of the Goldstone diagrams shown in Fig. 2, where the symbol $-X$ denotes insertion of the Fock operator. With the first-order Jastrow factor in hand, one can also calculate the second- and third-order contributions to the correlation energy. These contributions are expressed in terms of Goldstone diagrams in Figs. 3 and 4, where dashed lines represent the first-order correlation operator τ_1 and wavy lines represent the interaction potential [Eq. (41)]. For the third-order contribution, we have assumed that $\hat{W} - E_1$ is normal ordered, which is actually the case if H_0 corresponds to the Fock operator. The computational complexity of third-order diagrams for wavelet bases has been discussed in detail in Ref. 16.

A. Comparison with Fermi hypernetted chain Jastrow factors

In order to judge the quality of first-order Jastrow factors, we have performed FHNC//0 calculations[4,5] for the homogeneous Fermi gas model [Eq. (41)]. The FHNC//0 calculations represent the thermodynamic limit of an infinitely large supercell. Due to the finite size of the supercell in our JPT calculations, Jastrow factors possess a periodic structure with a small anisotropy due to the lattice sum [Eq. (43)] over neighboring supercells. In Fig. 5, we present first-order pair-correlation functions along the (100) direction for different supercell sizes at density $r_s = 2$ and $\mu = 1\ \text{bohr}^{-1}$, together with the corresponding FHNC//0 result. For short-range correlations, good agreement between first-order approximations and the FHNC//0 Jastrow factor can be observed already for rather small supercells. With increasing size of the supercell, first-order JPT converges amazingly well toward the FHNC//0 result even at intermediate distances where good agreement cannot be taken for granted.

Since our focus is on short-range correlations, we have chosen in the following a fixed supercell with $N = 54$ particles. Different values of the screening parameter μ, at fixed density $r_s = 2$, have been considered in Fig. 6(a). It turns out that there is close agreement between first-order JPT and FHNC//0 pair-correlation functions for the whole range of parameters. To avoid computational artifacts, we have plotted the JPT pair-correlation functions only up to 0.1 bohr because our Gaussian approximation [Eq. (43)] does not provide a resolution of the cusp beyond this scale. For comparison, Fig. 6(b) shows the behavior at different densities and fixed $\mu = 1\ \text{bohr}^{-1}$. From this figure, we observe a discrepancy between first-order JPT and FHNC//0 pair-correlation functions at low densities and intermediate interparticle distances $\geqslant 1$ bohr. This is because in the low-density regime, correlations are getting stronger and perturbation theory, in general, becomes less accurate.

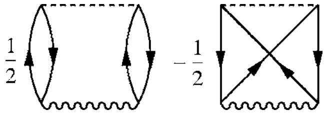

FIG. 3. Diagrammatic representation of $E_2 = \langle \hat{W}\hat{\tau}_1 \rangle$.

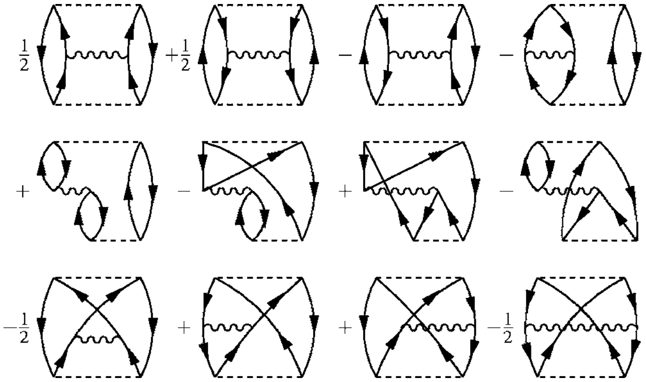

FIG. 4. Diagrammatic representation of $E_3 = \langle \hat{\tau}_1^{\dagger}(\hat{W} - E_1)\hat{\tau}_1 \rangle$.

In our previous calculations, we have not distinguished between pairs with parallel and antiparallel spins. By a slight modification of the formalism, however, it is possible to calculate spin dependent Jastrow factors. The resulting first-order pair-correlation functions for $\mu = 1\ \text{bohr}^{-1}$, $r_s = 2$, and $N = 54$ are shown in Fig. 7. It is interesting to compare the slopes at short interparticle distances with Kato's cusp condition.[35,36] For this, we have used a slightly enlarged basis containing 14 even-tempered Gaussians. The value of the

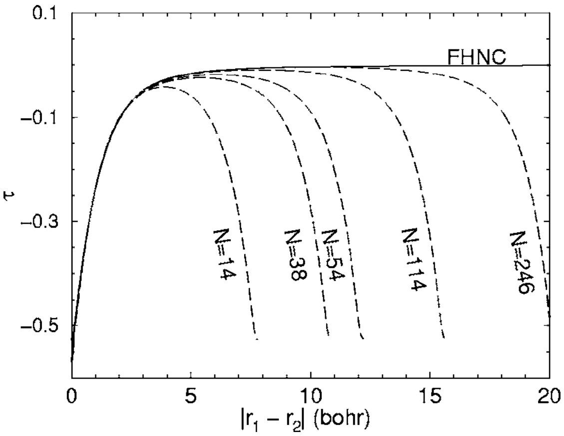

FIG. 5. First-order JPT pair-correlation functions (dashed lines) for a homogeneous Fermi gas at density $r_s = 2$ and screening parameter $\mu = 1\ \text{bohr}^{-1}$ for different sizes of the supercell. For comparison, the FHNC//0 result for the infinite system (solid line) is shown.

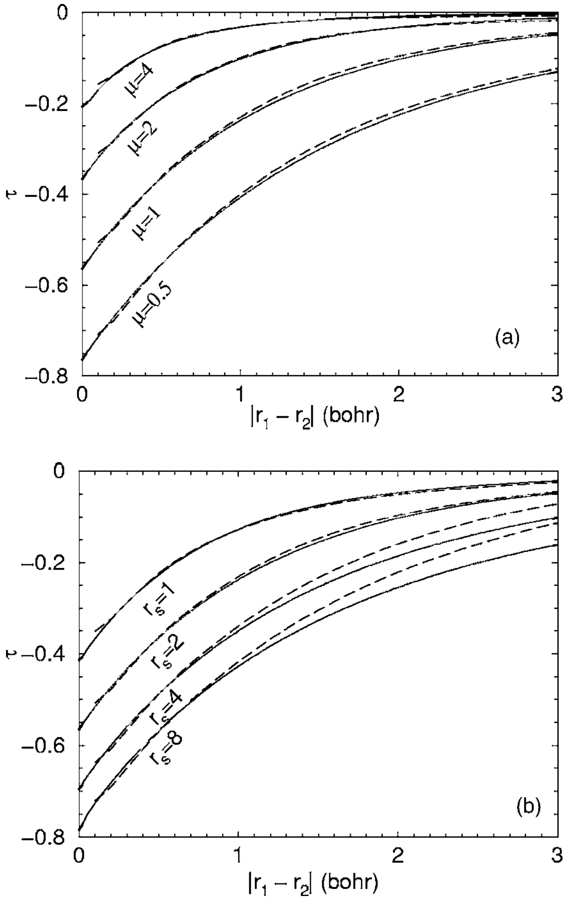

FIG. 6. Comparison of first-order JPT (dashed lines) and FHNC//0 (solid lines) pair-correlation functions for various screening parameters and densities. (a) Fixed density $r_s=2$ and different screening parameters ranging from $\mu=0.5$ to 4 bohr^{-1}. (b) Fixed screening parameter $\mu=1$ bohr^{-1} and different densities ranging from $r_s=1$ to 8. The JPT results have been calculated for a supercell containing $N=54$ particles.

averaged slope in the interval (0.1, 0.2) is 0.23 and 0.46 for parallel and antiparallel spins, respectively. This compares favorably with Kato's cusp condition which requires spherically averaged derivatives of 0.25 and 0.5 at the interparticle cusp.

B. Correlation energies

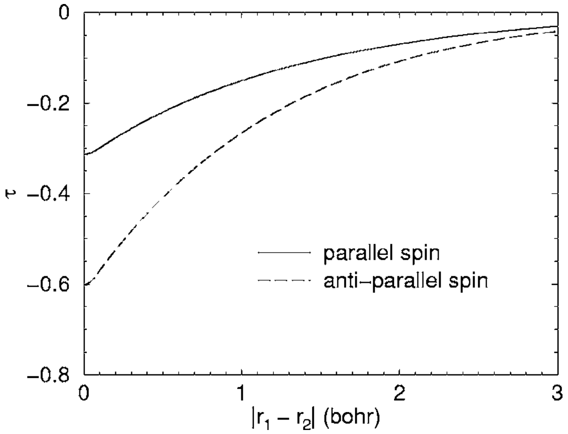

FIG. 7. First-order JPT pair-correlation functions for parallel and antiparallel spins. The homogeneous Fermi gas has been considered at density $r_s=2$ and $\mu=1$ bohr^{-1} for a supercell with $N=54$ particles.

With first-order Jastrow factors at hand, we have calculated JPT2 and JPT3 correlation energies for the homogeneous Fermi gas model. Due to momentum conservation, the diagrams with two external lines in Fig. 1 do not contribute to Eq. (27). Therefore, we can immediately identify correlation operators $\hat{\tau}_1$ with ordinary two-particle correlation functions in Jastrow factors. In order to judge the quality of our results, we have performed VMC and pure diffusion quantum Monte Carlo (PDMC) calculations[37,38] for the Hamiltonian [Eq. (42)] using these Jastrow factors as trial wave functions. The VMC method directly calculates the energy expectation value [Eq. (4)] for a given trial wave function and therefore provides a measure for the quality of the Jastrow factors. Despite small fixed node errors, PDMC provides fairly accurate benchmark values for the correlation energy of a homogeneous Fermi gas. Furthermore, we compare it with standard second-order Møller-Plesset (MP2) perturbation theory,[27] which can be expressed as a sum over momentum vectors $\mathbf{k}_p$ and corresponding eigenvalues ϵ_p of spatial Hartree-Fock (HF) orbitals,

$$E^{(2)} = \sum_{ijab} \frac{2\langle ij\|ab\rangle\langle ab\|ij\rangle - \langle ij\|ab\rangle\langle ab\|ji\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}, \tag{44}$$

$$\langle ij\|ab\rangle = \frac{1}{\Omega_s}\frac{4\pi}{(\mathbf{k}_a-\mathbf{k}_i)^2+\mu^2}\delta_{\mathbf{k}_i+\mathbf{k}_j,\mathbf{k}_a+\mathbf{k}_b}, \tag{45}$$

where Ω_s denotes the volume of the supercell and indices i, j, a, and b have the same meaning as in Sec. II.

According to our discussion in Sec. III A, we first consider the size dependence of JPT2, MP2, VMC, and PDMC correlation energies. These are shown in Fig. 8 for different

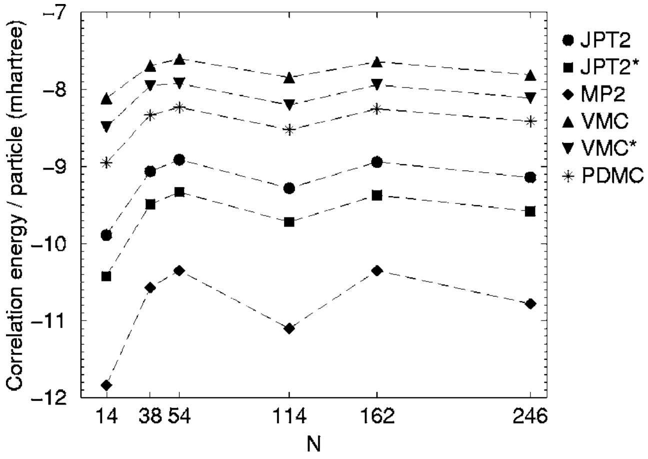

FIG. 8. Correlation energy per particle (mhartree) of a homogeneous Fermi gas at density $r_s=2$ and $\mu=1$ bohr^{-1} for different sizes of the supercell.

TABLE I. Correlation energy per particle (mhartree) of a homogeneous Fermi gas at density $r_s=2$ and different screening parameters μ. JPT2, JPT3, and VMC results have been obtained from first-order spin-independent and spin-dependent (*) Jastrow factors. The VMC method corresponds to a direct evaluation of the energy expectation value for first-order wave functions, whereas PDMC provides almost exact energies within the fixed-node approximation which do not depend on the Jastrow factor. For comparison, MP2 correlation energies have been stated. A supercell containing $N=54$ particles has been used in all calculations.

μ	JPT2	JPT3	VMC	JPT2*	JPT3*	VMC*	MP2	PDMC
0.5	−21.52	−15.66	−17.69(2)	−22.12	−16.19	−18.12(2)	−24.20	−18.70(3)
1	−8.91	−7.22	−7.63(2)	−9.33	−7.55	−7.94(2)	−10.35	−8.23(3)
2	−2.36	−2.03	−2.08(1)	−2.53	−2.15	−2.20(1)	−2.79	−2.31(2)
4	−0.450	−0.407	−0.415(4)	−0.480	−0.431	−0.435(4)	−0.525	−0.461(6)

sizes of the supercell in the case of a homogeneous Fermi gas at density $r_s=2$ and $\mu=1$ bohr^{-1}. The JPT2 and VMC calculations have been performed for spin-independent and spin-dependent (JPT2* and VMC*) Jastrow factors. It can be seen that the different methods yield almost parallel curves, where the correlation energies turned out to be fairly stable already for a small number of particles ($N \geqslant 54$). Both JPT2 and JPT2* overestimate the correlation energy by roughly 9% and 14%, respectively. By comparison with the corresponding VMC calculations, we observed that the first-order perturbative Jastrow factors are actually significantly better and recover 93% and 96% of the PDMC correlation energy, respectively. These results have to be compared with standard MP2 calculations which overestimate the correlation energy by about 28%.

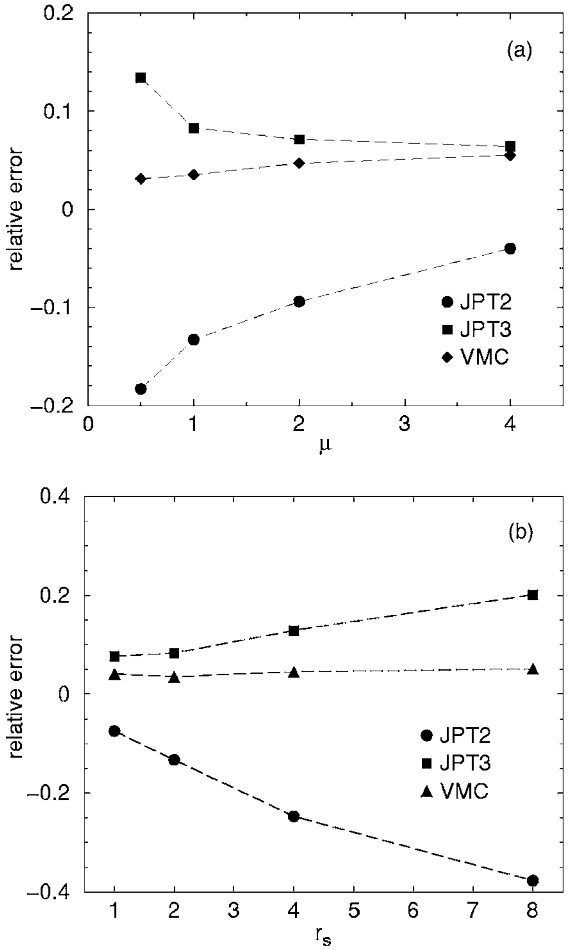

FIG. 9. Relative errors $(E_{\text{corr}}-E_{\text{corr}}^{\text{PDMC}})/|E_{\text{corr}}^{\text{PDMC}}|$ of JPT2, JPT3, and VMC correlation energies for different densities and screening parameters. The results are for spin-dependent Jastrow factors and supercells with $N=54$ particles. (a) Fixed density $r_s=2$. (b) Fixed screening parameter $\mu=1$ bohr^{-1}.

In order to study the homogeneous Fermi gas model for a larger range of densities and screening parameters, we restricted ourselves to a fixed supercell size with $N=54$ particles. Since we compare our results with PDMC benchmark calculations for the same supercell size, possible finite-size errors can be ignored. Correlation energies for a homogeneous Fermi gas at density $r_s=2$ and different screening parameters μ are listed in Table I. It can be seen that JPT2 overestimates, whereas JPT3 underestimates the correlation energy. The JPT3 results are in better agreement with VMC calculations than the corresponding JPT2 energies. Except for very small values $\mu<1$ bohr^{-1}, the relative errors of JPT3 and VMC calculations remain almost constant with respect to variations of the screening parameter, as it is shown in Fig. 9(a) for spin-dependent Jastrow factors. In contrast to this, the JPT2 relative errors decrease with increasing values for the screening parameter, which has to be expected because short-range correlations become increasingly important. These observations once again suggest that the first-order Jastrow factor is more accurate than the corresponding perturbative correlation energies. A similar behavior has been observed for a fixed screening parameter $\mu=1$ bohr^{-1} and different densities which can be seen from Table II and Fig. 9(b).

It turns out that the second-order correlation energies for $r_s=2$ and $\mu=0.5$, 1, 2, and 4 bohr^{-1} are quite close to those for $\mu=1$ bohr^{-1} and $r_s=1$, 2, 4, and 8, respectively. Actually they should be exactly the same if $\hat{H}_0$ contains only the kinetic energy. By rescaling the electron coordinates $\mathbf{r}_i'=\mathbf{r}_i/r_s$ for $i=1,\ldots,N$, it can be seen that r_s serves as a coupling constant in the Schrödinger equation,

$$\left[-\frac{1}{2}\sum_{i=1}^{N}\Delta_i' + r_s\sum_{i<j}\frac{e^{-\mu r_s|\mathbf{r}_i'-\mathbf{r}_j'|}}{|\mathbf{r}_i'-\mathbf{r}_j'|}\right]\Psi = r_s^2 E\Psi = E'\Psi. \quad (46)$$

It follows from the perturbation series for the energy

TABLE II. Same as Table I but for fixed screening parameter μ=1 bohr^{-1} and different densities.

r_s	JPT2	JPT3	VMC	JPT2*	JPT3*	VMC*	MP2	PDMC
1	−22.46	−19.26	−20.03(3)	−23.11	−19.87	−20.61(3)	−25.39	−21.5(1)
2	−8.91	−7.22	−7.63(2)	−9.33	−7.55	−7.94(2)	−10.35	−8.23(3)
4	−2.36	−1.68	−1.84(1)	−2.52	−1.76	−1.93(1)	−2.78	−2.02(1)
8	−0.457	−0.274	−0.322(2)	−0.486	−0.282	−0.335(2)	−0.524	−0.353(2)

$$E' = E'_0 + r_s E'_1 + r_s^2 E'_2 + \cdots \rightarrow E = E'_0/r_s^2 + E'_1/r_s + E'_2 + \cdots \tag{47}$$

that the second-order correlation energy depends only on the product μr_s.

IV. CONCLUSIONS

We have presented a perturbation scheme for Jastrow-type correlation functions. From a computational point of view, this scheme is simple enough to be of practical significance for the determination of accurate trial wave functions to be used in QMC calculations. Although essentially limited to short-range correlations, JPT can be applied to the model Hamiltonian of the inhomogeneous RPA method in Ref. 23 in order to obtain Jastrow factors for metalic systems, where long-range correlations become important. Our applications to a screened homogeneous Fermi gas suggest that first-order Jastrow factors are fairly accurate for short-range correlations and provide significantly better results in VMC calculations than it could be expected on the basis of second- and third-order correlation energies. It remains to develop an efficient implementation for inhomogeneous systems. For this, we have proposed multiscale bases,[16] such as wavelets, which provide sparse representations for two-particle correlation functions and a favorable computational complexity concerning the evaluation of Goldstone diagrams.

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