A new Jastrow factor for atoms and molecules, using two-electron systems as a guiding principle

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To get an idea of the qualitative behavior of an optimal Jastrow factor we have considered a Hylleraas-type wave function of very high accuracy for the helium atom. Owing to the lack of nodes this wave function can be easily interpreted as a general type of Jastrow factor. As a result we obtained a simple parameter dependent ansatz for a Jastrow factor, which incorporates the essential features of the observed behavior. We have optimized the parameters with respect to the variance of the local energy, using variational Monte Carlo techniques, for the atoms He through Ne and for the simple molecules H_2, LiH, and Li_2. Finally, we compare our approach with other types of Jastrow factors discussed in the literature. © *1995 American Institute of Physics.*

I. INTRODUCTION

It is long known in many body theory,[1–3] that exponential correlation factors, so-called Jastrow factors, which depend explicitly on interparticle distances, provide a powerful tool to handle particle correlations. For atomic and molecular systems this approach was put forward by Boys and Handy.[4] In recent years there has been increasing interest in finding new forms for Jastrow factors,[5–11] because they show some nice features which distinguish them from other approaches to the electron correlation problem. Through their explicit dependence on electron–electron distances it is easily possible to take care of the electron–electron cusp,[12] which is not feasible for wave functions based on simple linear combinations of Slater determinants like configuration interaction methods. Another, also very appealing advantage is the very compact form of Jastrow factors in contrast to configuration interaction wave functions.[8,10] The main disadvantage which inhibited their broader application to atomic and molecular many body problems for a long time lies in the high dimensionality of the occurring integrals. This can be overcome by application of Monte Carlo methods which are perfectly suited for this kind of wave functions and allow a strictly variational treatment. Furthermore, Monte Carlo techniques offer an efficient way to optimize parameters in Jastrow factors, as could be demonstrated by Umrigar and co-workers.[7,8] The commonly employed ansatz for Jastrow factors based on rational polynomials of the electron–nuclear and electron–electron distances[7,8,10,11] is flexible enough to yield very good results when all coefficients are optimized. Moreover, this ansatz enables the inclusion of electron–electron–nuclear correlation, the significance of which was shown by Schmidt and Moskowitz,[10,11] at least for atoms. We have followed a different course starting with a simple model for which a nearly exact Jastrow factor is known. Such a model is given by the He atom where almost exact solutions of the nonrelativistic Schrödinger equation can be obtained.[13–16] We took the Hylleraas-type wave function of Freund and co-workers[16] which at present is the most accurate solution available. Due to the absence of nodes in the spatial part of the ground state wave function of helium (which can be expressed in terms of the electron–nuclear r_1, r_2 and electron–electron r_{12} distances), we can define a general Jastrow factor by equating the spatial parts of a Jastrow type,

$$\Psi_J = e^{U_G(r_1,r_2,r_{12})}\Psi_{\mathrm{HF}}(r_1,r_2) \quad \langle \Psi_J|\Psi_J\rangle = 1, \tag{1}$$

and a very accurate Hylleraas-type wave function Ψ_{Hyl},

$$U_G = \ln|\Psi_{\mathrm{Hyl}}| - \ln|\Psi_{\mathrm{HF}}| \quad \langle \Psi_{\mathrm{Hyl}}|\Psi_{\mathrm{Hyl}}\rangle = 1. \tag{2}$$

The Hartree–Fock part Ψ_{HF} has been taken from Clementi and Roetti.[17]

II. NEARLY EXACT JASTROW FACTOR FOR HELIUM

From Eq. (2) it is easy to calculate U_G at every point in space. On the other hand we can expect to be faced with a rather complex behavior of U_G in three dimensions. It would then be a cumbersome task to extract qualitative principles which can be generalized to more complicated systems. Therefore we have inserted an intermediate step in order to reduce the complexity of the problem. We have based our approach on the assumption that Jastrow factors are especially suited for the description of short range correlations. To be more precise, we have tried to describe the short range behavior, which characterizes Jastrow factors in the case of small interparticle distances, as accurate as possible. In order to treat this problem, let us consider the conventional ansatz for the Jastrow factor[18] in the case of the He atom,

$$e^{U_2(r_{12})} \quad U_2 = \frac{1}{2}\,\frac{r_{12}}{1+br_{12}} - \frac{1}{2b}, \tag{3}$$

where we have subtracted the asymptotic value for $r_{12} \rightarrow \infty$ in order to get

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$$\lim_{r_{12}\to\infty} U_2(r_{12})=0. \tag{4}$$

This makes it meaningful to compare the absolute values of different Jastrow factors at the electron–electron cusp. For $b=\text{const.}$ the action of the Jastrow factor on the electrons is not changed. If we generalize ansatz (3) to allow for a position dependent behavior at the electron–electron cusp we have to introduce the function $U_{20}(r_1,r_2)$, which determines the value of U_2 at $r_{12}=0$, by substituting

$$-\frac{1}{2b}\to U_{20}(r_1,r_2), \tag{5}$$

which applied to Eq. (3) yields

$$U_2(r_{12},r_1,r_2)=\frac{U_{20}(r_1,r_2)}{1-r_{12}/[2U_{20}(r_1,r_2)]}. \tag{6}$$

It is interesting to note, that we have obtained in a natural way a coupling between the electrons and the nucleus through the denominator in Eq. (6), which resembles the averaged backflow correlation of Schmidt and Moskowitz.[10]

Turning back to Eq. (2), we are now able to refine our ansatz for the Jastrow factor so that the short range behavior can be separated. This can be achieved by the general ansatz

$$\begin{gathered}\exp\{U_G[U_{G0}(r_1,r_2,r_{12}),r_{12}]\}\\ U_G=\frac{U_{G0}+c_1r_{12}}{1+[(c_1-\frac{1}{2})/U_{G0}]r_{12}+c_2r_{12}^2}+N_G,\end{gathered} \tag{7}$$

which is a modified version of Eq. (6). In Eq. (7) we have assumed that U_{G0} depends additionally on r_{12}, which is necessary for U_G to satisfy Eq. (2). We will analyze in the following the effect of eliminating this dependence. We thus try to have a situation analogous to Eq. (6). However, we now refine the dependence of U_G on r_{12} by introducing two supplementary terms depending on r_{12} [with arbitrary coefficients c_1 and c_2; for $c_1=c_2=0$ we have Eq. (6)]. For reasons discussed below, it is also appropriate to introduce the normalization constant N_G. Next we have to solve Eq. (2) with respect to U_{G0},

$$\begin{gathered}U_{G0}(U_G,r_{12})=\tfrac{1}{2}P-[\tfrac{1}{4}P^2+(c_1-\tfrac{1}{2})\bar{U}_Gr_{12}]^{1/2},\\ P=\bar{U}_G(1+c_2r_{12}^2)-c_1r_{12},\\ \bar{U}_G=U_G(r_1,r_2,r_{12})-N_G,\\ c_1\leqslant\tfrac{1}{2},\ \ 0\leqslant c_2,\ \ 0\leqslant N_G.\end{gathered} \tag{8}$$

The Jastrow factor lowers the probability for electrons to occupy the same part of space, which means that U_G must be negative for small interparticle distances [U_G is uniquely determined through Eq. (2) and the normalization conditions in Eqs. (1) and (2)]. This circumstance enables us to fix the sign in Eq. (8), which is the solution of a quadratic polynomial in U_{G0}. The value of N_G is, of course, immaterial for the calculation of the energy. In order to evaluate the effect of approximations on U_G, we will make comparisons with the exact U_G. Thus, the specific value of N_G is needed.

The short range behavior of U_{G0} is strongly influenced by the electron–electron cusp condition for electrons with antiparallel spin,[12,18]

$$\left.\frac{\partial U_G}{\partial r_{12}}\right|_{r_{12}=0}=\frac{1}{2}. \tag{9}$$

Therefore U_{G0} has a vanishing first derivative with respect to r_{12},

$$\left.\frac{\partial U_{G0}}{\partial r_{12}}\right|_{r_{12}=0}=0. \tag{10}$$

As a consequence, for small interparticle distances we get at most a second order dependence on r_{12}. This leads to a significant simplification for our analysis of the function U_{G0} which can be treated in the important regions of configuration space, at least in a first approximation as independent of r_{12}.

III. A SIMPLE MODEL FOR U_{G0}

In the following section we will try to find an explicit parameter dependent model for U_{G0} which exhibits most of the significant features. Obviously the optimal choice of the remaining free parameters c_1, c_2, and N_G depend on it. Fortunately, the qualitative behavior of U_{G0} is rather insensitive with respect to the choice of the parameters in Eq. (8). Figures 1(a) and 1(c) show the behavior of U_{G0} with appropriately chosen parameters (Table I) for two opposite situations. Both electrons are on a straight line through the nucleus. In Fig. 1(a), the electrons are at the same side whereas in Fig. 1(c) they are on opposite sides with respect to the nucleus. Both contour maps exhibit a rather similar behavior not only qualitatively but also quantitatively. To complete our considerations Fig. 1(b) shows the behavior of U_{G0} when the electrons are situated on perpendicular straight lines through the nucleus. The function U_{G0} is nearly constant when both electrons are in the inner region around the nucleus and falls off increasingly fast when one or both electrons depart from the nucleus. We thus conclude that U_{G0} is not only nearly independent of r_{12} for $r_{12}\to 0$ [cf. Eq. (10)], but also, within a good approximation, for all r_{12}.

As a basic approximation we have neclected the r_{12} dependence of U_{G0} which seems justifiable due to the observed behavior. As we can see, this has an important consequence on the contour maps of Fig. 1. Because of the electron–nuclear cusp condition,[12]

$$\left.\frac{1}{\Psi_J}\frac{\partial\Psi_J}{\partial r_i}\right|_{r_i=0}=-Z\quad i=1,2\quad \Psi_J=e^{U_G}\Psi_{\text{HF}} \tag{11}$$

for the total wave function Ψ_J, which is already satisfied by the Hartree–Fock part Ψ_{HF}, we must have

$$\left.\frac{\partial U_{G0}(r_1,r_2,r_{12})}{\partial r_i}\right|_{r_i=0}=0\quad i=1,2. \tag{12}$$

Considering the situation depicted in Fig. 1(a), the total derivative along a straight line with $r_1=\text{const.}$ and $r_{12}=|r_1-r_2|$ at the point $r_2=0$ is

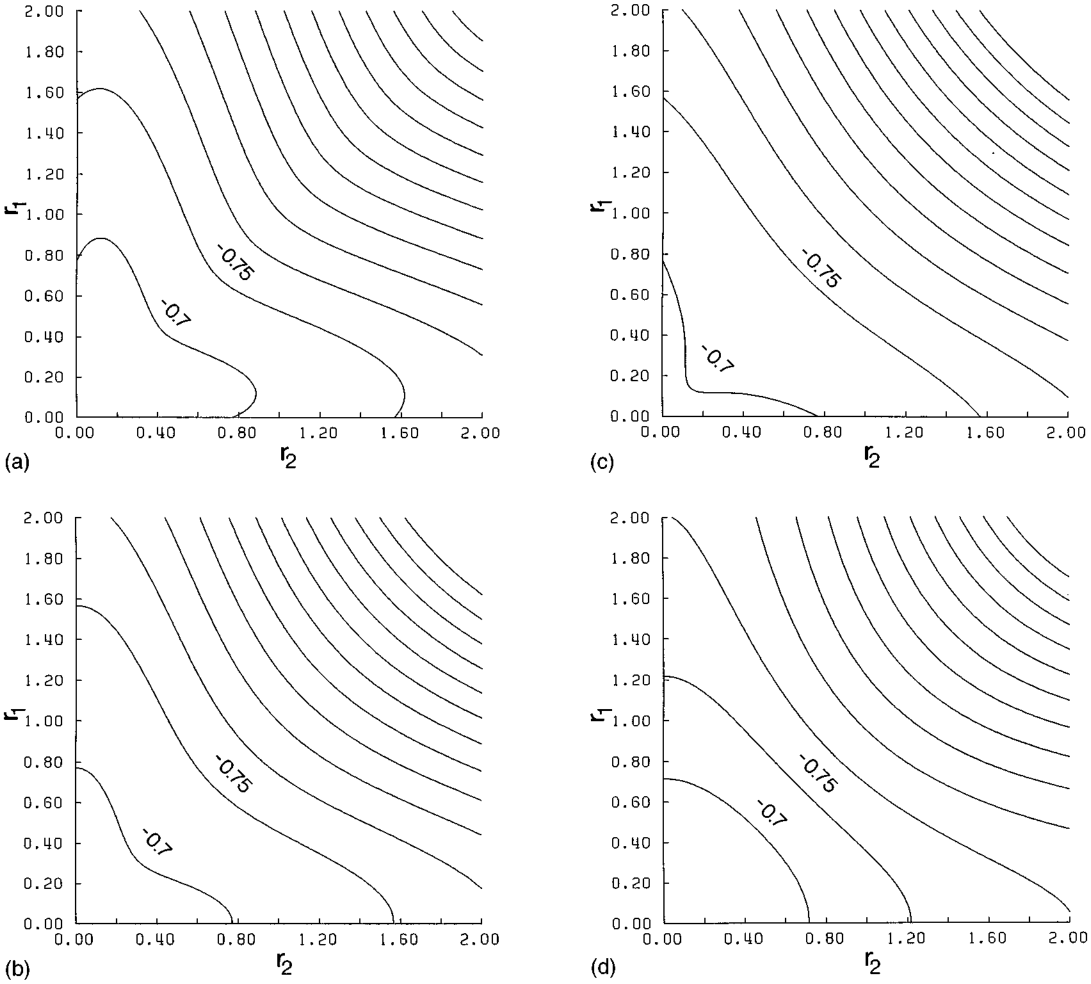

FIG. 1. (a), (b), (c) show contour maps of the function U_{G0} for He calculated from a Hylleraas-type wave function (Ref. 16) through Eq. (8). (a), (b), (c) correspond to fixed electron–nucleus–electron angles of 0°, 90°, 180°. The parameters c_1, c_2, and N_G are in agreement with the optimized parameters of Table I. (d) shows the contour map of our model $\tilde{U}_{G0}$ for He defined through Eq. (17). The parameter values are listed in Table I. The contour lines are calculated for equidistant values starting with -0.7, -0.75, -0.8, ...

$$\left.\frac{dU_{G0}(r_1,r_2,r_{12})}{dr_2}\right|_{\substack{r_1=\text{const.}\\ r_2=0}}=-\left.\frac{\partial U_{G0}(r_1,r_2,r_{12})}{\partial r_{12}}\right|_{\substack{r_1=\text{const.}\\ r_2=0}}. \tag{13}$$

In the case of our intended approximation, this means, that the contour lines should approach at right angles to the axes. A similar situation with reversed sign occurs in Fig. 1(c). We have found a strong bending of the contour lines near the axes in Fig. 1(a) and a much weaker one in Fig. 1(c). The angles deviate considerably from 90° in both cases. Despite of these discrepancies we maintained the approximation for our model, because we were interested mainly in the short range behavior near the electron–electron cusp and in this case the approximation rests on Eq. (10). Moreover, our model for U_{G0} will satisfy the electron–nuclear cusp condition (12) and therefore it provides a reasonable behavior near the axes.

The dimensionality of the problem can be further reduced by considering situations where the electrons occupy the same part of space. As we have already mentioned, this part of configuration space is of special interest with respect to electron correlation. In an earlier paper[19] we have investigated the behavior of Jastrow factors near the electron–electron cusp for the homogeneous electron gas, where we got for U_{G0} an approximately linear dependence on r_s,

$$r_s=\frac{1}{a_0}\left(\frac{4}{3}\,\pi\rho\right)^{-(1/3)} \tag{14}$$

(a_0 is the Bohr radius, ρ is the electron density) from Fermi-hypernetted chain calculations.[20] Therefore we treated the problem in a similar manner as discussed above. We define a new function g_0 through the following relation:

$$U_{G0}(r,r)=-[\tfrac{4}{3}\pi g_0(r)]^{-(1/3)} \tag{15}$$

for which we can easily obtain numerical values from the Hylleraas-type wave function,

$$g_0^{\mathrm{Hyl}}(r)=-\frac{3}{4\pi\bar{U}_{G0}(r,r,0)^3}. \tag{16}$$

Figure 2 shows the function g_0^{Hyl} for the He atom. In view of the strong resemblance to a Gaussian function it seemed reasonable to look for a model which is based on such functions. Summarizing, we have looked for a model which

TABLE I. Parameters of the Jastrow factors for the atoms He to Ne together with variational energies (a.u.) (statistical errors are given in parentheses) and standard deviations of the local energy $\sigma(E_l)$. The parameters where optimized with respect to $\sigma^2(E_l)$.

	He[a]	Li	Be	B	C
E	−2.902 4(2)	−7.473 1(6)	−14.631 1(8)	−24.609 5(10)	−37.793 0(16)
$\sigma(E_l)$	0.111	0.208	0.348	0.528	0.686
c_1	0.111	0.254	0.243	0.032	0.083
c_2	0.001	0.253	0.366	0.003	0.010
α_1	1.719	8.724	11.59	9.297	18.41
α_2	0.447 0	2.293	2.951	1.415	2.136
α_3	⋯	0.087 15	0.254 0	0.271 0	0.398 0
d_1	0.910 7	1.593	1.974	0.218 9	0.153 2
d_2	9.030	16.69	19.84	17.04	25.99
d_3	⋯	192.9	156.4	132.1	154.0

	N	O	F	Ne
E	−54.535(2)	−74.988(2)	−99.648(2)	−128.835(2)
$\sigma(E_l)$	0.864	1.078	1.333	1.578
c_1	0.073	0.142	0.129	0.163
c_2	0.000 4	0.723	0.001	0.679
α_1	23.14	38.12	28.43	12.68
α_2	2.912	4.183	4.386	3.476
α_3	0.727 1	1.090	1.033	1.149
α_4	0.020 08	0.020 78	0.034 01	0.030 75
d_1	0.127 7	0.407 4	0.477 2	12.89
d_2	16.63	50.96	41.72	74.01
d_3	129.9	118.1	160.9	105.6
d_4	581.9	243.6	278.3	124.9

[a] $N_G=0.4228$.

shows the general behavior of Figs. 1(a), 1(b), 1(c), and is especially close to the exact behavior in the vincinity of the electron–electron cusp. Both conditions can be fulfilled by an ansatz termed $\tilde{U}_{G0}$ of the general form,

$$\tilde{U}_{G0}(r_1,r_2) = -\left[\frac{2}{3}\pi\sum_l d_l\left(\frac{\alpha_l}{\pi}\right)^{3/2}\left(e^{-\alpha_l r_1^2}+e^{-\alpha_l r_2^2}\right)\right]^{-(1/3)}, \tag{17}$$

where we have the variational parameters α_l and d_l.

In order to get an idea of the correctness of our arguments we have optimized the parameters in the ansatz (17) together with c_1 and c_2 for the He atom. This can be done in a very efficient way by the method of Umrigar and co-workers[7,8] which is based on the minimization of the variance of the local energy. The resulting parameters together with the expectation value of the energy and the standard deviation of the local energy are listed in Table I. After having fixed all free parameters it is easy to calculate the normalization constant N_G from the normalization condition in Eq. (1). This has been done numerically as described in Ref. 19. Before we discuss the properties of our model it is worth mentioning that we have recovered 97% of the correlation energy. First we will look at the behavior near the electron cusp. Figure 2 shows the function g_0 for the ansatz (17) with optimized parameters together with g_0^{Hyl} and the functions g_{90}^{Hyl}, g_{180}^{Hyl},

$$g_{90}^{\text{Hyl}}(r) = -\frac{3}{4\pi\bar{U}_G(r,r,\sqrt{2}r)^3}, \qquad g_{180}^{\text{Hyl}}(r) = -\frac{3}{4\pi\bar{U}_G(r,r,2r)^3}, \tag{18}$$

where the electrons are separated with fixed electron–nuclear–electron angle. In accordance with our assumption Fig. 2 shows a close agreement between the curves at least for distances above 0.5 bohr. The small discrepancies close to the nucleus are probably due to the three body cusp which

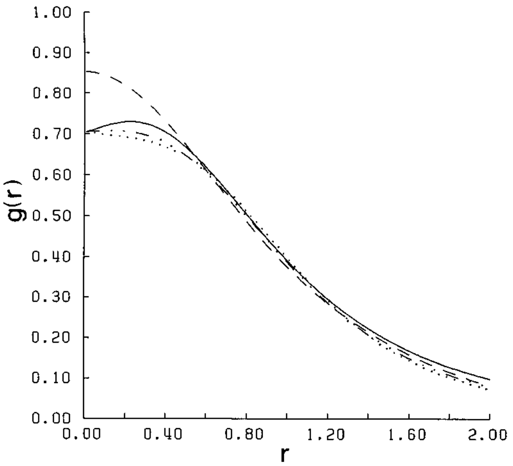

FIG. 2. Function g_0 (– – –) for the He atom calculated with the optimized parameters of Table I, together with the functions g_0^{Hyl} (—), g_{90}^{Hyl} (–···–) and g_{180}^{Hyl} (···) obtained from the Hylleraas-type wave function (Ref. 16) through Eqs. (16) and (18).

is insufficiently described within our model. The general behavior of our model $\tilde{U}_{G0}$ is shown in Fig. 1(d) which exhibits a reasonably close agreement to results obtained from the nearly exact Hylleraas-type wave function.

IV. APPLICATION TO ATOMS AND MOLECULES

We have applied our ansatz given by Eqs. (7) and (17) to systems with more than two electrons in a straightforward manner, by neglecting three-electron and higher correlations as well as spatial anisotropy due to a nonvanishing total angular momentum of the wave function. The total wave function Ψ_J is composed of a Jastrow factor and a HF wave function,

$$\Psi_J = \prod_{i<j} e^{\tilde{U}_G(r_i, r_j, r_{ij})} \Psi_{\mathrm{HF}}. \tag{19}$$

At first we have considered the ground states of the atoms Li to Ne. For the HF part we used the very accurate wave functions of Clementi and Roetti.[17] The parameters c_1, c_2, α_l, d_l were optimized as already mentioned with respect to the variance of the local energy. Results are listed in Table I. Computational details concerning the course of the optimization will be discussed in the next section. It is now interesting to compare the correlation energies obtained for our ansatz with those obtained for other forms of Jastrow factors reported in the literature. Of special interest are the Jastrow factors of Schmidt and Moskowitz[10] due to their partitioning of different contributions to electron correlation.

They considered three different types of correlations, that is electron–electron ($e-e$), electron–nuclear ($e-n$), and electron–electron–nuclear ($e-e-n$) correlation. The $e-n$ correlation is needed to restore the density which is disturbed by that part of the Jastrow factor which describes the $e-e$ correlation.[21] With increasing nuclear charge the $e-e-n$ correlation becomes more and more significant. This is of particular importance because we have not taken it into account explicitly when constructing our ansatz. Nevertheless $e-e-n$ correlation occurs in a natural way in Eq. (7) through the coupling of U_{G0} and r_{ij}. Schmidt and Moskowitz discussed three different types of Jastrow factors. Their 7-term Jastrow factor includes only $e-e$ and $e-n$ correlation, whereas the 9-term and 17-term Jastrow factors additively contain $e-e-n$ correlation in an increasingly complex manner. In Table II we have compared our results with correlation energies reported for these Jastrow factors. For He to N we obtained approximately the same results as Schmidt and Moskowitz's 9-term factor, for O, F, Ne our results are slightly worse. In all cases however our results are significantly better than those for the 7-term factor. This seems to indicate that we have recovered a substantial portion of the $e-e-n$ correlation. It is worth mentioning that the function U_{G0} is responsible for both $e-e-n$ and $e-n$ correlations. These are not separated in our Jastrow factor in contrast to Ref. 10. Besides this we have listed in Table II some results of Umrigar and co-workers.[7,8] Their Jastrow factors probably represent the limit for electron correlation that can be described by this type of wave function. Therefore we can say that our ansatz works satisfactorily also for systems with more than two electrons.

TABLE II. Comparison of correlation energies (%) for the atoms He to Ne obtained with various types of Jastrow factors.

	$\tilde{U}_G$[a]	7-term[b]	9-term[b]	17-term[b]	Pade[c]
He	97	90	98	100	100
Li	89	92	89	97	⋯
Be	62	56	64	68	76
B	64	52	66	69	⋯
C	67	53	68	72	⋯
N	71	54	73	77	⋯
O	69	53	78	80	⋯
F	74	51	80	82	⋯
Ne	74	57	85	85	86

[a] Present work (reference energies from Ref. 26).
[b] Reference 10.
[c] Reference 8.

Next we have applied our Jastrow factor to small molecules like H_2, LiH, Li_2. Before doing this, we have to make a slight modification in the definition of U_{G0} for systems with more than one nucleus. This can be done in a straightforward way by taking into account Gaussian functions at different centers

$$\tilde{U}_{G0}(r_i, r_j) = -\left\{ \frac{2\pi}{3} \left[\sum_k \sum_l d_{kl} \left(\frac{\alpha_{kl}}{\pi} \right)^{3/2} \times \left(e^{-\alpha_{kl} r_{ki}^2} + e^{-\alpha_{kl} r_{kj}^2} \right) \right] \right\}^{-(1/3)}, \tag{20}$$

where k runs over all nuclei. The parameters were optimized in the same way as for the atoms and are listed in Table III, together with total energies and standard deviations of the local energies. HF wave functions for H_2 and LiH were taken from Refs. 22 and 23, respectively. In the case of Li_2 we have used the $(6s)$ Slater-type basis set of Clementi and Roetti[17] supplemented by 2 p polarization functions. All calculations were done for the ground states at equilibrium distances. For Li_2 we obtain a very small exponent in U_{G0}

TABLE III. Parameters of the Jastrow factors for the molecules H_2, LiH, Li_2 together with variational energies (a.u.) (statistical errors are given in parentheses) and standard deviations of the local energy $\sigma(E_l)$. The parameters where optimized with respect to $\sigma^2(E_l)$.

	H_2	LiH		Li_2
E	−1.172 3(3)	−8.049 8(10)		−14.961(2)
$\sigma(E_l)$	0.082	0.264		0.327
c_1	0.002	0.305		0.267
c_2	0.000 2	0.282		0.264
		Li	H	
α_1	0.523 0	13.36	3.942	8.255
α_2	0.116 0	3.382	0.289 9	1.732
α_3	⋯	0.522 5	⋯	0.000 04
d_1	0.435 8	1.281	0.012 47	2.355
d_2	3.634	16.10	78.52	25.17
d_3	⋯	58.67	⋯	6978×10^3

TABLE IV. Correlation energies (%) for some small molecules obtained with various types of Jastrow factors.

	$\tilde{U}_G$[a]	Ref. 27[b]	Ref. 29	Ref. 30	Ref. 9
H_2	95	95	⋯	⋯	80
Li_2	72	68	70	⋯	58
LiH	75	⋯	84	77	83

[a] Present work [reference energies for H_2 (Ref. 31), LiH (Ref. 32), Li_2 (Ref. 27)].

[b] See also Ref. 28.

which avoids the occurrence of too negative values for this function when both electrons are far away from the nuclei. This may be important due to the covalent nature of the bond and the rather large bond distance. In Table IV we have compared our results with other Jastrow factors for these molecules described in the literature. For H_2 and Li_2 our results are as good as the best values cited in the literature. Only for LiH we obtained a slightly worse correlation energy.

V. COMPUTATIONAL DETAILS

The variational Monte Carlo calculations were carried out with a generalized Metropolis algorithm, which is equivalent to a diffusion Monte Carlo algorithm without branching.[24] Parameter optimization of the Jastrow factors can be done in an efficient way within the variational Monte Carlo method[7,8] which generates a distribution in configuration space proportional to the square of a given wave function. We have chosen 1000 statistically independent points in configuration space and optimized the parameters in order to minimize the variance of the local energy. This was done by a simplex algorithm.[25] After the optimization we have computed new points in configuration space which were distributed with respect to the optimized set of parameters. Optimization and renewing steps were repeated until we could observe no further improvement.

VI. CONCLUSIONS AND OUTLOOK

We have found a way to reduce the complexity of a nearly exact two-electron wave function by considering the function U_{G0} which can be defined with respect to this wave function through Eqs. (2), (7), and (8). It could be shown that it is possible, at least in an approximate way, to reduce the problem from three to two dimensions. This enabled us to obtain a simple model for U_{G0} which agrees almost quantitatively with the exact behavior in the neighborhood of the electron–electron cusp. The model could be generalized in a straightforward manner to other atoms and molecules. By comparing our results with those of Schmidt and Moskowitz,[10] we found that our model is capable of describing $e-e-n$ correlation to a certain extent. This is of minor significance for the He atom but increasingly important for the heavier systems.

At last we will discuss some possibilities to further improve our ansatz. Here we have to distinguish two lines of investigations. The first is based on a further improvement of the Jastrow factor, while in the second case the HF part is replaced by a multiconfiguration wave function. We have neglected higher order terms in the expansion of U_{G0} with respect to r_{12}. However the necessity of such terms to get a quantitative agreement for points in configuration space, where one electron is close to the nucleus, can be seen from Eq. (13) and Fig. 1(a). This can be achieved by adding a term of the general form,

$$\tilde{U}_{G0}^{(2)}(r_1,r_2)r_{12}^2 \tag{21}$$

to $\tilde{U}_{G0}$ which will improve the description of $e-e-n$ correlation. The behavior of $\tilde{U}_{G0}^{(2)}$ can be analyzed by the methods discussed above. It would also be of interest to repeat the whole procedure for a very accurate H_2 wave function and to compare it with our Jastrow factor for this molecule. This will be the subject of further studies. Another point which is currently under investigation is the combination of multiconfiguration wave functions with Jastrow factors. Umrigar and co-workers[8] obtained impressive results for the Be atom by taking care of near-degeneracy effects. These are also important for the atoms B and C and cannot be described by Jastrow factors.[10]

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