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Computational approach for bound states in quantum field theory

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We propose a non-perturbative approach to calculate bound state energies and wave functions for quantum field theoretical models. It is based on the direct diagonalization of the corresponding quantum field theoretical Hamiltonian in an effectively truncated and discretized Hilbert space. We illustrate this approach for a Yukawa-like interaction between fermions and bosons in one spatial dimension and show where it agrees with the traditional method based on the potential picture and where it deviates due to recoil and radiative corrections. This method permits us also to obtain some first insight into the spatial characteristics of the distribution of the fermions in the ground state, such as the bremsstrahlung-induced widening.

To obtain bound state energies and wave functions for general quantum field theoretical interactions with arbitrary coupling strengths is still a fundamental challenge [1]. There is presently no unique procedure for calculating these energies as poles of the S-matrix directly from quantum field theory. The usual Rayleigh-Schrödinger perturbation theory is inapplicable as the radius of convergence of such a power series expansion is zero. This difficulty is illustrated by the non-perturbative Z^2-scaling of the hydrogenic bound states with the nuclear charge Z, or by the fact that many potentials do not even support bound states unless the interaction strength exceeds a non-zero threshold value. In these cases the binding energy is not even a differentiable function of the coupling strength, which would be required for perturbation theory to be applicable.

The most promising method to obtain bound state energies from quantum field theory is the Bethe-Salpeter equation [2,3], which can lead to a description of the interaction in terms of an approximate quantum mechanical potential energy function to describe the dynamics. It is difficult to improve phenomenological treatments of potentials as there are no systematic ways to include various dynamical contributions. While for instance in quantum electrodynamics (QED) or nuclear physics many models provide an excellent match with experimental data, there are still conceptual deficiencies to construct effective many-body forces.

The computational method that we propose here is based on the construction of the Hamiltonian from the quantum field theoretical Lagrangian density and its matrix representation for a suitable set of discretized basis states. The energy eigenstates of the Hamiltonian without any fermion-boson coupling can be used as a basis to diagonalize the matrix numerically. While the required numerical convergence can be controlled rather efficiently by an optimized selection of the basis states, the key limitation of this method is dictated by the available computer memory, which naturally restricts the maximum dimension of the Hilbert space.

We illustrate this approach for a model test theory where two types of fermions (of mass M each) are coupled with each other via mediating bosons (of mass m). Their (1+1)-dimensional interaction is given by the energy $V = \lambda \int dx \, [\Psi_b^\dagger(x) \, \gamma^0 \, \Psi_b(x) + \Psi_d^\dagger(x) \, \gamma^0 \, \Psi_d(x)] \, \phi(x)$, where the parameter λ is the coupling strength, Ψ_b and Ψ_d are the two-component Dirac field operators for the fermions and ϕ denotes the scalar boson operator. For the special case of m=0 this model could also be used to study simplified QED interactions, where the "photon" has spin zero. The three field operators can be expanded in terms of annihilation and creation operators that fulfill the usual anti-commutator and commutator relationships $[b(p), b^\dagger(p')]_+ = [d(p), d^\dagger(p')]_+ = [a(p), a^\dagger(p')]_- =$

$\delta(p-p')$. For couplings λ that are not exceedingly large, fermionic pair-creation processes are not important. The terms in the Hamiltonian that would couple the first fermion to its own antiparticle are proportional to $b^\dagger(p+k)\, B^\dagger(p)\, [a^\dagger(-2p-k)+a(2p+k)]$ and $b(p+k)\, B(p)[a^\dagger(2p+k)+a(-2p-k)]$. Here the anti-particle operators B and $B^\dagger$ fulfill the anticommutator relationships $[b(p), B^\dagger(p')]_+ = 0$ and $[B(p), B^\dagger(p')]_+ = \delta(p-p')$. Similar terms characterize also the second fermion. As very energetic bosons are required in these interactions and the corresponding coupling function decreases rapidly with the boson momentum, we therefore neglect anti-fermions. This leads to the Hamiltonian of the form $H = H_0 + V$ with

$$H_0 = \int dp\, e(p)\, [b^\dagger(p)b(p) + d^\dagger(p)d(p)] + \int dk\, \omega(k)\, a^\dagger(k)a(k) \qquad (1a)$$

$$V = \lambda \int dp \int dk\, \Gamma(p,k)\, [b^\dagger(p+k)b(p) + d^\dagger(p+k)d(p)]\, [a(k) + a^\dagger(-k)] \qquad (1b)$$

The coupling function $\Gamma(p,k) \equiv [e(p+k)e(p)+M^2c^4-p(p+k)c^2]^{1/2}\, [8\pi\omega(k)e(p+k)e(p)]^{-1/2}$ is the result of the scalar product among the Dirac spinors and acts as a natural cut-off function as it decreases with increasing fermion momenta p and boson momenta k. In atomic units (c=137.036 a.u.) the free energies of the fermions and bosons are given by $e(p) \equiv (M^2c^4+c^2p^2)^{1/2}$ and $\omega(k) \equiv (m^2c^4+c^2k^2)^{1/2}$, respectively.

This model Yukawa-like Hamiltonian has a long tradition and has been proposed to approximate the strong nuclear force between protons and neutrons due to the mesons. It can also predict the time-evolution of two spatially nearby fermions [4]. While the omission of the interaction with the fermionic anti-particles removes the relativistic invariance of H, it leads to the conservation of the two particle number operators $\int dp\, b^\dagger(p)b(p)$ and $\int dp\, d^\dagger(p)d(p)$, in addition to the total momentum operator $\int dp\, p\, [b^\dagger(p)b(p) + d^\dagger(p)d(p) + a^\dagger(p)a(p)]$, which also commutes with H. As the result of these invariances a suitable basis can be chosen in which the matrix for H is block-diagonal, which reduces the required computer memory significantly.

In order to represent the operator H by a matrix, the creation and annihilation operators need to be expressed on a spatial grid of total length L. This discretization should not be confused with lattice gauge theory. Unless we are interested in describing a system with a spatial constraint (such as in cavity QED), the finite parameter L is purely computational and could be viewed as a spatial

regulator. In order to preserve the operator algebra, we have defined the dimensionless discretized operators $b_p \equiv (2\pi/L)^{1/2}\, b(p)$, which satisfy $[b_p, b_{p'}^\dagger]_+ = [d_p, d_{p'}^\dagger]_+ = [a_p, a_{p'}^\dagger]_- = \delta_{p,p'}$. As basis states for the Hamiltonian matrix we have chosen the single fermion states $|p\rangle \equiv b_p^\dagger |0\rangle$ and $|p;k\rangle \equiv b_p^\dagger a_k^\dagger |0\rangle$ and for the two-fermion sector the states $|p,q\rangle \equiv b_p^\dagger d_q^\dagger |0\rangle$ and $|p,q;k\rangle \equiv b_p^\dagger d_q^\dagger a_k^\dagger |0\rangle$, where $|0\rangle$ denotes the vacuum state. For the range of coupling strengths λ discussed in this paper it turns out that the restriction to the one-boson exchange case [5,6] is sufficient. For example, for our largest coupling strength (λ=9000 a.u.) the ground state energy is changed by less than 0.37% if the two-boson states are included. Taking a higher number of bosons into account is feasible but would increase the required computer memory.

The matrix elements for the Hamiltonian in the chosen basis for the zero and one-boson sector are given by

$$\langle p,q \mid H \mid p',q' \rangle = e(p)\, \delta_{p,p'} + e(q)\, \delta_{q,q'} \tag{2a}$$

$$\langle p,q;k \mid H \mid p',q';k' \rangle = e(p)\, \delta_{p,p'} + e(q)\, \delta_{q,q'} + \omega(k)\, \delta_{k,k'} \tag{2b}$$

$$\langle p,q \mid H \mid p',q';k' \rangle = \lambda\, (2\pi/L)^{1/2} \left[\Gamma(p',k')\ \delta_{p,p'+k'}\, \delta_{q,q'} + \Gamma(q',k')\ \delta_{q,q'+k'}\, \delta_{p,p'}\right] \tag{2c}$$

where the $\lambda\, (2\pi/L)^{1/2}$ acts as an effective "charged renormalized" coupling constant used in the simulations.

In order to guarantee that the spectrum of the single-fermion sector remains invariant under the interaction V and the fermion mass remains M for all orders in λ, we have added an appropriate (finite) λ-dependent counter-term to the original Hamiltonian. It can be determined as a function of the annihilation and creation operators directly from the (numerical) energy spectrum of the single-fermion sector [7]. In the special case of a relativistically invariant Hamiltonian, this counter-term would reduce to a simpler form, where a single λ-dependent bare mass parameter $M(\lambda)$ ensures the mass-renormalization and the invariance of the physical mass M with λ.

We propose here to compute the (positive) binding energy $E_g(\lambda)$ from the difference between the (renormalized) lowest energy of the two-fermion sector and $2\,Mc^2$. Alternatively, it could also be defined as $|E_2(\lambda) - 2E_1(\lambda)|$, where $E_1(\lambda)$ and $E_2(\lambda)$ are the ground states of the single- and two-fermion sectors of the original Hamiltonian. This second procedure would also remove the

need for energy renormalization as any energy shifts in E_1 and E_2 are naturally cancelled out. While both definitions seem to give similar binding energies, it remains an open question to us, which of the two definitions matches actual experimental data better.

In Figure 1 we display the binding energy $E_g(\lambda)$ between the two fermions as a function of a wide range of the coupling strength λ. We choose here M=1 a.u. and m=0.1 a.u., which leads to a similar mass ratio as the one for real nucleons and pi-mesons (about 939/139). For a coupling strength around λ=9000 a.u. the binding energy to rest mass ratio computed from our model is comparable to the real ratio for the three-dimensional deuteron, which has a binding energy of E_g=2.2 MeV.

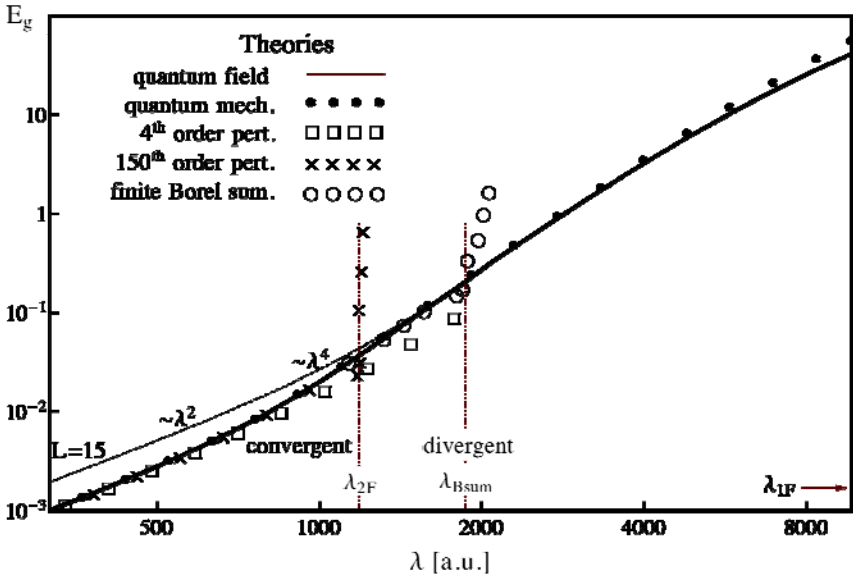

Figure 1. The bound state energy $E_g(\lambda)$ for two fermions as a function of the coupling constant λ. The discrete markers show the predictions according to several approximate theories as discussed in the text. The parameters λ_{2F}, λ_{Bsum} are for L=30 a.u. and λ_{1F} is larger than the displayed range. The number of maximum momentum states for the fermions and bosons (P_{max}=200 2π/L corresponding to 22454 states in the Hilbert space) was chosen large enough to have converged data.

In order to better visualize the different scaling of the energy with the coupling strength λ, we have used doubly logarithmic axis notations. There are (at least) two distinct regions where the nearly straight-line behavior suggests a simple power-law scaling of E_g in λ. In the very weak coupling regime the binding energy grows quadratically with λ. Here the spatial extension of the corresponding weakly coupled bound state is comparable to the computational box length L and as

a result the binding energy itself depends on L, as the second curve for L=15 a.u. (dashed line) shows deviations from L= 30 a.u. With increasing L, the size of this λ^2-region (in terms of λ) decreases and it vanishes for infinitely extended systems, $L \to \infty$.

The physically more interesting region is the one for larger coupling strength λ where the ground state is so deeply bound that its spatial extension is much less than L and the energy becomes independent of L. Here the binding energy grows with a power in λ higher than quadratic and the results for L=15 a.u. and L=30 a.u. merge.

As the energies are converged numerically they should agree in principle with the predictions of the exact scattering operator and therefore be equivalent to the summation of the Feynman diagrams to all orders in the relevant Hilbert space. However, the computational approach can be used in regions where traditional methods (Feynman-Dyson expansions, etc.) are difficult to apply and non-perturbative approaches are necessary.

In the second part of this work the validity domains of approximate theories such as the Rayleigh-Schrödinger perturbation theory in V (Eq. 1) and the effective potential picture are established.

As the operators are available as finite matrices, it is possible to compute the perturbative predictions for the energy E_g to nearly arbitrary orders in λ. In this finite dimensional Hilbert space we need to construct the corresponding matrices for the interaction potential V and the truncated resolvent G in the unperturbed basis. It is related to the usual resolvent $G(H_0,z) \equiv 1/(z-H_0)$, but evaluated at the unperturbed energy $z=\omega^{(0)}$ and acts only on the complementary space, such that $G\,|\omega^{(0)}\rangle = 0$, where $H_0\,|\omega^{(0)}\rangle = \omega^{(0)}\,|\omega^{(0)}\rangle$. The expansion coefficients in the energy $E_g(\lambda) = \Sigma_{n=0}\,\omega^{(n)}\,\lambda^n$ can then be obtained iteratively from the usual scheme of the Raleigh-Schrödinger perturbation theory [8,9] as

$$\omega^{(n)} = \langle\omega^{(0)}|\, V\,|\omega^{(n-1)}\rangle \qquad (3a)$$

$$|\omega^{(n)}\rangle = G\,V|\omega^{(n-1)}\rangle - \Sigma_{j=1}^{j=n-1}\ \omega^{(j)}\,G\,|\omega^{(n-j)}\rangle \qquad (3b)$$

The squares (crosses) in Figure 1 denote the perturbative predictions up to 4^{th} (150^{th}) order for $E_g(\lambda)$. It is interesting to note that while the Hamiltonian is the same for the single- and

two-fermion sectors, the radii of convergence as well as their scaling with the spatial regulator L are quite different. The power series expansion in the two-fermion sector for $E_g(\lambda)$ in λ is convergent for $\lambda<\lambda_{2F}$ (with $\lambda_{2F} \approx 6.3 \times 10^3 \ L^{-1/2}$) while the corresponding radius for the one-fermion sector does not even depend on the spatial cut-off L and is given by λ_{1F} ($\approx 2.9 \times 10^4$ a.u., outside the plot range of Fig. 1). In the limited region of convergence ($\lambda<\lambda_{2F}$), perturbation theory predicts the true binding energy $E_g(\lambda)$ accurately. For example, for λ=600 a.u. the error of 150th order perturbation theory is less than 3×10^{-7} % compared to the exact value.

For larger couplings $\lambda_{2F}<\lambda<\lambda_{Bsum}$, we enter a very interesting intermediate regime that is independent of the regulator L, but the perturbative expansion diverges. This is consistent with the expectation that bound states are intrinsically non-perturbative for any dynamics that are spatially not constrained (L=∞). However, quite surprisingly, the terms can still be summed up if the normal Borel procedure for infinite sums [10,11] is generalized to a finite number of terms with diverging trend. This shows that, contrary to common belief, the information contained in a (diverging) perturbation theory can still be used to predict bound state energies. However, this is possible only for a *finite* L [12], as each individual expansion coefficient approaches infinity for L$\rightarrow\infty$. The numerically obtained predictions by this summation technique are indicated by the open circles in Fig. 1. For example, while for λ = 1380 a.u. the sum of the first 150 perturbative terms $E_g(\lambda) = \Sigma_{n=0}^{150} \omega^{(n)} \lambda^n$ amounts to 6.9×10^8 a.u. (reflecting the diverging nature of its partial sums), applying the Borel-like technique predicts $E_g(\lambda) = 6.575 \times 10^{-2}$ a.u., which differs from the exact numerical energy by less than 0.45%.

Another approximate approach frequently used to obtain binding energies is based on a quantum mechanical potential energy V(r) that can be constructed from an effective Hamiltonian H_d. Here the Hamiltonian H_d is constructed in such a way that it leads to the same scattering operator up to $O(\lambda^2)$ in the relevant subspace as the one for H. It can be obtained from a general Ansatz for the interaction energy that obeys all required symmetries as a multiple integral over hexa-linear products of the fermionic and bosonic annihilation and creation operators with unknown expansion coefficients. By comparing the scattering operators to the same order, these coefficients can be determined. It also turns out that the first-order term in λ vanishes. For the specific system in Eq. (1) this procedure would lead to the effective Hamiltonian [13,14] as

$$H_d = H_0 + \lambda^2 \int dp \int dp' \int dk\, S(p,p',k)\, b^\dagger(p+k)\, b(p)\, d^\dagger(p'-k)\, d(p)\, a(k)\, a^\dagger(k) \qquad (4)$$

where the coupling function is given by $S(p,p',k) \equiv 2\Gamma(p,k)\,\Gamma(p',-k)\,/(E_{p'+k} - E_{p'} - \omega_k)$. In order to relate H_d to an effective single-particle quantum mechanical problem, we have to assume that the recoil of the bosons on the fermions is negligible. We can then approximate the energy $e(p) \rightarrow Mc^2 + p^2/(2M)$, the coupling function $\Gamma(p,k) \rightarrow [4\pi\,\omega(k)]^{-1/2}$ and therefore $S(p,p',k) \rightarrow -[2\pi\,\omega(k)^2]^{-1}$. In the two-fermion sector for zero total momentum, the resulting Hamiltonian matrix takes the form $\langle -p_i,p_i|\, H_d\, |-p_j,p_j\rangle = p_i^2/M\, \delta(p_i-p_j) + W(p_i-p_j)$, where $W(k) \equiv -\gamma^2/[2\pi\omega(k)^2]$. This matrix is mathematically identical to the one for a quantum mechanical Hamiltonian $H_{qm} = p^2/(2M_{red}) + V(r)$ for an effective particle with reduced mass $M_{red} \equiv M/2$ in an attractive (Yukawa-like) binding potential $V(r) = (2\pi)^{-1/2} \int dk\, \exp(ikr)\, W(k) = -\lambda^2/(2mc^3)\, \exp(-m\,c\,|r|)$. Solving the Schrödinger equation for the ground state energy $E_{qm}(\lambda)$ we find that $E_{qm}(\lambda)$ for small λ grows quadratically (finite L) or quartically ($L=\infty$).

The quantum mechanical ground state energies $E_{qm}(\lambda)$ are indicated in Fig. 1 by the solid circles. For interactions up to λ=3000 a.u., the omission of the fermion-boson recoil and other potentially relevant processes (used to derive H_d) seems to be justified. In fact, for the entire displayed range $0<\lambda<9000$ a.u. recoil would only decrease the binding energy by at most 0.17%. As the effective Hamiltonian [and therefore V(r)] was constructed from only the lowest-order term in the Feynman-Dyson expansion, it cannot take higher order radiative processes such as the Bremstrahlung or other non-photon number conserving mechanisms into account. The figure shows that these radiative corrections become rather relevant for $\lambda>3500$ a.u. where they begin to lower the binding energy. For λ=9000 a.u. (corresponding to the real deuteron system), the higher-order processes lower the energy [predicted by V(r)] by 37%. It is in this regime where the proposed computational approach will be most valuable to provide us with new insights into the various dominant contributions to the binding energy and to guide the construction of effective many-body forces.

In addition to providing us with data about the binding energy, the computational approach can be used to study for the first time the spatial distribution of the particles in the bound state beyond the potential picture.

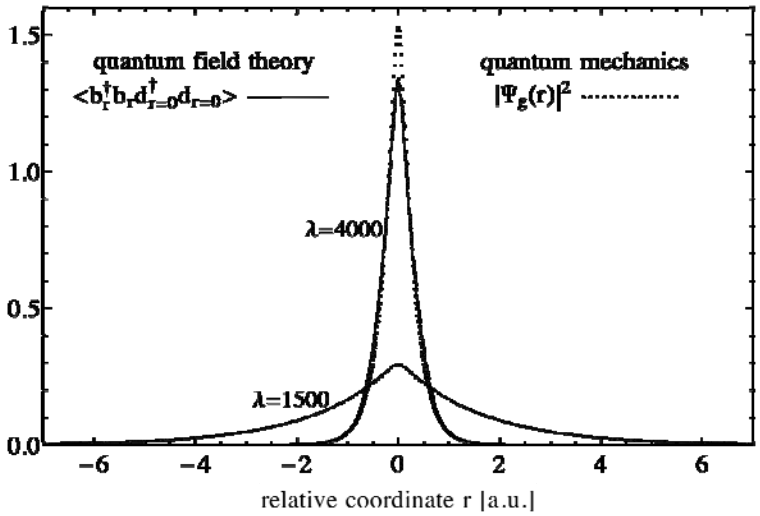

Figure 2. The spatial distribution of the two fermions in the ground state as a function of the relative coordinate r. For comparison, the dotted line is the quantum mechanical ground state obtained from the Schrödinger equation for the Yukawa potential V(r). [Parameters as in Fig. 1]

The spatial probability distribution of the fermions can be obtained from the expectation value $\langle b^\dagger(r)b(r)d^\dagger(r=0)d(r=0)\rangle$, where the position-dependent operators are obtained from the Fourier transform of the corresponding momentum creation and annihilation operators. In Figure 2 we display this distribution together with the quantum mechanical ground state probability $|\Psi_g(r)|^2$, obtained from the Schrödinger equation $[p^2/(2M_{red}) + V(r)]\Psi_g(r) = E_g\Psi_g(r)$. For small λ the match is fairly good, which is unexpected as the Hamiltonians H and H_d are only unitarily equivalent and thus do not necessarily guarantee identical wave functions.

Again, a direct comparison of the two states shows that the omission of the fermions' recoil is insignificant for the spatial distribution. However, for larger λ the quantum mechanical Yukawa potential-based description fails to account for the wider spatial distribution of quantum field theory. Higher-order radiative processes apparently lead to a decrease in localization. This increase of the average separation between the two fermions in the ground state is also consistent with the decreased binding energy as discussed in Fig. 1.

In addition to predicting the spatial distribution of the two fermions, we can also examine the joint boson-fermion spatial distribution in the ground state $|g\rangle$ of the single-fermion sector given by the expectation value $\rho_{f,b}(x,y) \equiv \langle g|\, b^\dagger(x)b(x)\, a^\dagger(y)a(y)\,|g\rangle$. Due to the overall translation invariance under a shift s, $\rho_{f,b}(x+s,y+s) = \rho_{f,b}(x,y)$, this distribution is only a function of the relative

coordinate r = x-y. Even though this distribution is for virtual bosons, it might still provide us with a possible connection to the classical force field that surrounds each fermion. If the fermion-boson mass ratio M/m is very large, $\rho_{f,b}(x,y)$ falls off monotonically on the scale given by the Compton wavelength of the boson. This is similar to spatial decay of the (Yukawa) force field associated with the potential picture discussed above. We will defer it to future studies to examine if there is a more quantitative relationship between these quantum field theoretical densities of the bosons and the force fields predicted from quantum mechanics. We can speculate that these bosonic spatial distributions might also guide a better construction of effective force-fields.

In order for the proposed approach to become an effective tool for future investigations (for example in QED), several challenges have to be addressed. As mentioned above, the main bottleneck of this tool is the restriction of the accessible Hilbert space due to the available computer memory. However, it should be possible to optimize the set of basis states, as we need to describe only specific energy regions within the spectrum, such as bound states. While for our illustrative model system the fermion sectors were decoupled, in a real QED system the number of electrons and positrons are not conserved and for example, bound state energy corrections due to the vacuum polarization could be studied by the current approach.

In summary, we have proposed a computational method to determine the bound state energies and wave functions for general quantum field theoretical interactions between fermions and bosons. For systems that are computationally accessible (meaning that the data do not depend on the spatial and momentum regularization or any truncation to the Hilbert space) this approach is in principle exact. This was illustrated for a Yukawa-like system and demonstrated how it can be used to evaluate the accuracy of approximate methods, including perturbation theory (in its converging and diverging regimes) or methods that can lead to quantum mechanical potentials. For example, Bremsstrahlung as the leading radiative correction to the potential picture decreases the binding energy and widens the spatial distribution of the two fermions in the ground state.

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