High-fidelity pseudopotentials for the contact interaction

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The contact interaction is often used in modeling ultracold atomic gases, although it leads to pathological behavior arising from the divergence of the many-body wave function when two particles coalesce. This makes it difficult to use this model interaction in quantum Monte Carlo and other popular numerical methods. Researchers therefore model the contact interaction with pseudopotentials, such as the square well potential, whose scattering properties deviate markedly from those of the contact potential. In this article, we propose a family of pseudopotentials that reproduce the scattering phase shifts of the contact interaction up to a hundred times more accurately than the square well potential. Moreover, the pseudopotentials are smooth, resulting in significant improvements in efficiency when used in numerical calculations.

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I. INTRODUCTION

Interactions between particles are central to our understanding of correlated phenomena. The contact potential is often used to model interactions in ultracold atomic gases but, despite its widespread use, it displays pathological behavior: both the potential and wave function diverge when two particles coalesce. These divergences impede numerical methods and are commonly handled by replacing the contact potential by a pseudopotential, such as a hard sphere or a square well potential. However, these approximations to the contact potential display incorrect variations in the scattering phase shift with incident particle energy [1–6]. In this article, we adapt methods commonly used for the development of electron-ion pseudopotentials in the electronic structure community to propose an atom-atom pseudopotential whose scattering properties agree closely with those of the contact interaction.

Ultracold atomic gases have delivered many important insights into strongly correlated systems. They can both provide clean model Hamiltonians and introduce the ability to tune the strength of the contact interactions. Ultracold atoms interact through an underlying attractive van der Waals interaction. An external magnetic field can be used to tune the energy of the bound molecular state to approach the energy of the scattering state, causing the states to couple resonantly. The effect of the resonance on the scattering state can be modeled by an effective interparticle potential [7]. In the case of broad Feshbach resonances, the scattering can be described by a single universal scattering length \( a \) which describes the scattering phase shift arising from a contact interaction. There are three types of contact interaction: sufficiently deep to trap a two-body bound state \((a > 0)\), weakly attractive with no bound state \((a < 0)\), and repulsive (excited state of the \( a > 0 \) potential).

Contemporary numerical simulations of the first two types, the bound state \((a > 0)\) and weak attractive interactions \((a < 0)\), normally adopt a finite-ranged square well or Pöschl-Teller interaction. Such simulations have delivered crucial insights into Bose gases [2] and the crossover from a gas of weakly coupled Bardeen-Cooper-Schrieffer pairs to a strongly interacting Bose-Einstein condensate [1,8], as well as few-atom physics [9–11]. However, the finite range imbues the potential with incorrect scattering properties. Reducing the range of the potential alleviates this problem, but slows numerical calculations.

The third type of contact potential gives repulsive interactions that drive itinerant ferromagnetism in Fermi gases [4,5,12], a Tonks-Girardeau gas [1], and a Bose gas [6]. The repulsive interaction emerges from the first excited state of the bound-state potential. Both the repulsive contact potential and the bound-state potential therefore have \( a > 0 \). In ultracold atomic gas experiments [13] the excited state (also called the upper branch) is protected from decay to the ground state by a slow three-body loss process, allowing the study of repulsive interactions. To simulate these repulsive interactions, one can adopt a finite-ranged attractive potential and study the first excited eigenstate [4,5]. However, studying excited states in quantum Monte Carlo (QMC) methods often requires restricting the excited-state wave function to be orthogonal to the lower energy states. Variational estimates of excited-state energies calculated within the widely used diffusion quantum Monte Carlo (DMC) method [14–16] are discussed in Ref. [17]. The fixed node constraint used in the DMC method prevents collapse into the ground state, but it is still difficult to calculate reliable excited-state energies within the framework of DMC. An alternative approach is to use a repulsive top-hat potential [12] whose ground state resembles the first excited state of the contact potential. However, this potential has a finite range greater than the scattering length, resulting in an incorrect scattering phase shift.

The difficulty in simulating repulsive interactions means that there are important open questions about fermionic gases: Is the ground state of a strongly interacting fermionic system ferromagnetic [3,12,18–23]? Is the ferromagnetic transition first or second order? And do exotic phases emerge around the quantum criticality such as spin spirals [12], nematic phases [21,24,25], and a counterintuitive \( p \)-wave superconducting state [26–32]? The development of a pseudopotential that is better able to reproduce the scattering properties of the contact interaction will help resolve these open questions.

In Sec. II, we present two pseudopotentials for the interatomic interaction in a cold atom gas. We first adapt norm-conserving pseudopotentials [33–35], developed by the electronic structure community for electron-ion interactions, to deal effectively with scattering states. We then present a pseudopotential constructed to minimize the scattering phase...
shift error for all wave vectors in a Fermi gas. In Sec. III, we test the accuracy of the proposed formalism using the exactly soluble system of two trapped atoms. In Sec. IV, we investigate how the pseudopotential performs in a many-body setting by calculating the equation of state of the weakly repulsive Fermi gas and comparing results to a perturbation expansion.

II. DERIVATION OF THE PSEUDOPOTENTIALS

To construct the pseudopotential we study the two-body problem: two identical fermions in their center-of-mass frame with wave vector \( k \geq 0 \). The Hamiltonian in atomic units (\( \hbar = m = 1 \)) in the center of mass frame is

\[
-\frac{\nabla^2}{2\mu} \psi + V(r)\psi = \frac{k^2}{2\mu} \psi ,
\]

where \( V(r) = 4\pi a_0 \delta(r)(\partial/\partial r)r \) is the contact potential for scattering length \( a_0 \) and interparticle separation \( r \) \([36]\), and \( \mu = 1/2 \) is the reduced mass.

The scattering states for the contact potential are \( \psi_{k,\ell}^{\text{cont}} = \sin(kr - \ell \pi/2 + \delta_{\ell}^{\text{cont}}(k))/kr \), where

\[
\delta_{\ell}^{\text{cont}}(k) = \begin{cases} \arctan(-ka_0), & \ell = 0, \\ 0, & \ell > 0, \end{cases}
\]

is the scattering phase shift in the angular momentum channel \( \ell \). We seek a pseudopotential that

1. reproduces the correct phase shifts over the range of wave vectors \( 0 \leq k \leq k_F \) present in a Fermi gas with Fermi wave vector \( k_F \),

2. supports no superfluous bound states to be compatible with ground state methods, and

3. is smooth to accelerate numerical calculations.

We start by developing pseudopotentials for the repulsive branch, then the attractive branch, and finally the bound state. When developing pseudopotentials, we benchmark their quality by looking at how closely the phase shift of the wave function for the relative motion of two particles interacting via the pseudopotential reproduces the phase shift of the contact interaction for all wave vectors \( 0 \leq k \leq k_F \) present in a Fermi gas, as shown in Figs. 2 and 3.

A. Repulsive branch

We first focus on developing a pseudopotential for the repulsive branch of the contact interaction. This branch offers a particular challenge. The bare potential is strongly attractive, harboring a single bound state. The scattering states incident on the potential incur a positive phase shift with respect to the noninteracting scattering wave function (dotted line). \( r_n \) denotes the first node of the scattering wave function and \( r_c \) denotes the first antinode, which we use as the cutoff radius when constructing pseudopotentials, as described in Sec. II A. (b) The pseudopotentials at \( k_F a = 1/2 \) on the repulsive branch. The potential labeled “Troullier” denotes the pseudopotential derived using the Troullier-Martins formalism. The line labeled “UTP” denotes the pseudopotential derived using the UTP formalism. These formalisms are described in Sec. II. (c) The wave functions for the relative motion of two particles interacting with a contact potential, the hard sphere, Troullier-Martins pseudopotential, and UTP, at \( k = k_F \).

used as approximations to the contact potential in numerical calculations \([3–5,11,12]\).

The usual approach \([4,12]\) to the construction of pseudopotentials for the contact interaction starts from the low-energy expansion for the \( s \)-wave scattering phase shift,

\[
\cot \delta_0(k) = -\frac{1}{ka_0} + \frac{1}{2}k_{\text{eff}}^2 - Pr\frac{\hbar^2}{\mu}k^2 + O(k^4) ,
\]

where \( r_{\text{eff}} \) is the “effective range” of the potential and \( P \) is the “shape parameter.” For a contact potential, \( r_{\text{eff}} \) and all higher
order terms are zero. Perhaps the simplest pseudopotential is a hard-sphere potential with radius $a$. This reproduces the correct scattering length $a$, thereby delivering the correct phase shift for $k = 0$. However, the hard sphere has an effective range $r_{\text{eff}} = 2a/3$. To study the impact of the pseudopotential on the scattering states, we calculate the phase shifts at $ka = 1/2$ for all wave vectors between 0 and $k_F$ and compare them to the contact phase shifts. Figure 2 shows that the finite effective range of the hard-sphere potential causes significant deviations in the scattering phase shift for $k > 0$.

To reduce the error in the scattering phase shift, Ref. [12] adopted a soft-sphere potential: $V(r) = V_0 \delta(r - R)$, with $V_0$ and $R$ chosen to reproduce the contact scattering length $a = R(1 - \tanh \gamma/\gamma)$ and effective range $r_{\text{eff}} = R[1 + \tanh \gamma/(3\tanh \gamma)] = 0$, where $\gamma = R \sqrt{2} \mu V_0$. The first two terms in the low-energy expansion of the phase shift are now correct, leading to a small reduction in phase-shift error as shown in Fig. 2.

The two potentials considered so far display incorrect behavior at large wave vectors due to the focus on reproducing the correct $k = 0$ scattering behavior. To improve the accuracy we turn to the Troullier-Martins [37] formalism developed for constructing attractive-electron pseudopotentials [33–35,38–40]. These pseudopotentials reproduce both the correct phase shift and its derivative with respect to energy at a prescribed calibration energy. The Troullier-Martins form of norm-conserving pseudopotential can readily be applied to the construction of a pseudopotential for the contact interaction. We choose a calibration energy and cutoff radius as follows:

**Calibration energy.** The pseudopotential will have scattering properties identical to the contact potential at the calibration energy. For electron-ion pseudopotentials, the bound-state energy in an isolated ion is a natural choice.

For example, in a homogeneous fermionic gas the scattering of states with incident momenta less than $\sim k_F$ is particularly important, and therefore we choose a calibration energy equal to the median energy of the occupied states, $(3/5)E_F$.

**Cutoff radius.** The Troullier-Martins pseudo-wave-function is identical to the contact wave function outside of the cutoff radius, but has no nodes inside the cutoff radius, as shown in Fig. 1(c). We can therefore choose the cutoff radius to eliminate the bound state: by selecting a radius $r_c > r_n$, where $r_n$ is the position of the first node in the wave function, we construct a pseudopotential that does not have a bound state, as shown in Fig. 1(b). We choose the first antinode of the wave function at the calibration energy as the cutoff radius for the pseudopotential.

Having chosen a suitable calibration energy and cutoff radius, we construct the pseudo-wave-function. The contact potential exhibits a nonzero phase shift only when the particles are incident with angular momentum quantum number $\ell = 0$. We therefore concentrate on reproducing the correct $\ell = 0$ behavior in this section. We demonstrate how to eliminate scattering in higher angular momentum channels in Sec. IID.

The functional form of the pseudo-wave-function in the $\ell = 0$ channel at the calibration energy is

$$\psi_{\text{PP}}(r) = \begin{cases} \exp \left( \sum_{i=0}^6 c_i r_i^2 \right) Y_0(\theta, \phi), & r < r_c, \\ \psi_{\text{cont}}^{\text{rel}}(r), & r \geq r_c, \end{cases}$$

where $k = \sqrt{(3/5)E_F}$ is the wave vector at the calibration energy and $r = (r, \theta, \phi)$ is the relative position of the interacting particles. The coefficients $c_i$ are calculated by demanding continuity of the pseudo-wave-function and its first four derivatives at the cutoff radius, and requiring that the derivative of the phase shift with respect to energy, $\delta(\cot \delta)/\delta E \big|_{(3/5)E_F}$, be the same as that of the contact interaction at the calibration energy. This last condition, called the norm-conservation condition, is equivalent to demanding that the total density enclosed by $r < r_c$ for the pseudo-wave-function matches that of the contact wave function,

$$\int_{|r|<r_c} |\psi_{\text{PP}}(r)|^2 \, dr = \int_{|r|<r_c} |\psi_{\text{cont}}^{\text{rel}}(r)|^2 \, dr.$$

Finally, we demand that $c_2^2 = -5c_4$, to guarantee that the pseudopotential has zero curvature at the origin. Having constructed the pseudo-wave-function at the calibration energy, we invert the Schrödinger equation to obtain the pseudopotential $V_{\text{PP}}(r)$. The formalism for the contact interaction is detailed in the Appendix. We also provide a computer program to generate the pseudopotential [41].

By calibrating the pseudopotential at the median incident scattering energy $E = (3/5)E_F$, we reduce the error in the scattering phase shift over a broad range of wave vectors. This generates the pseudopotential shown in Fig. 1(b), whose smoothness leads to improved numerical stability and efficiency. Figure 2 demonstrates that this potential is exact at the calibration energy $E = (3/5)E_F$ and delivers a hundredfold decrease in phase-shift error across all wave vectors, compared to the soft-sphere pseudopotential.
The Troullier-Martins formalism yields a pseudopotential that reproduces the contact behavior exactly at the calibration energy, but deviates at other energies. One approach for reducing the deviation is to ensure that higher order derivatives of the phase shift with respect to energy are equal to those of the contact interaction. A second option is to impose accurate scattering at multiple energies through additional parameters.

\[
\frac{V(r)}{E_F} = \begin{cases} 
1 - \left(\frac{r}{r_c}\right)^2, & 0 \leq r \leq r_c, \\
0, & r > r_c,
\end{cases}
\]

with \(N_c = 9\). The term \((1 - r/r_c)^2\) ensures that the potential goes smoothly to zero at \(r = r_c\), and the term \(v_1(1/2 + r/r_c)\) constrains the potential to have zero gradient at \(r = 0\) to allow the pseudo-wave-function to be as smooth as possible. This is advantageous in quantum chemistry methods in which the absence of a cusp improves convergence with respect to the basis set size. As with the Troullier-Martins pseudopotential, we choose a cutoff radius that corresponds to the first antinode of the true wave function, removing the node at \(r = r_n\) and therefore eliminating the bound state. To calculate the coefficients \(\{v_i\}\), we minimize the total squared error in the phase shift over all wave vectors between 0 and \(k_F\),

\[
\left(\delta^\text{PP} - \delta^\text{cont}\right)^2 = \int_0^{k_F} \left(\delta^\text{PP}(k) - \delta^\text{cont}(k)\right)^2 w(k) \, dk
\]

where the phase shift \(\delta^\text{PP}(k)\) is determined from a numerical calculation of the scattering solution of the pseudopotential and \(w(k) = k^2\) is a positive weighting function. We include a computer program to generate the UTP in the supplemental material [41]. The computer program starts with coefficients determined from the Troullier-Martins pseudopotential, but we verified that the optimization was not stuck in a local minimum by repeating the process with different initial coefficients.

As demonstrated in Fig. 2, this potential gives an error in \(\delta_0\) of less than \(10^{-2}\) for all wave vectors \(0 \leq k \leq k_F\) found in a Fermi gas, corresponding to an improvement of two orders of magnitude over previously used pseudopotentials, and an approximate twofold improvement over the Troullier-Martins pseudopotential.

We test the robustness of the UTP construction by generating additional variants of the formalism. The first, inspired by the Troullier-Martins pseudopotential, contains only even terms in the polynomial functional form of the potential. For the second variant, rather than minimizing the total squared phase-shift error \(\int_0^{k_F} \left(\delta^\text{PP}(k) - \delta^\text{cont}(k)\right)^2 w(k) \, dk\), we instead minimize the maximum phase-shift error \(\max_{0 \leq k \leq k_F} (\delta^\text{PP}(k) - \delta^\text{cont}(k))\). Including only even terms in the polynomial functional form of the pseudopotential delivers a 1% poorer quality pseudopotential for the same number of variational parameters. Minimizing the maximum phase-shift error leads to a similar pseudopotential, with a slightly smaller peak error, but the phase shifts deviate more from those of the contact interaction elsewhere. Ultimately the selection of the optimization strategy depends on the physics of the system: for density waves one should minimize the error around \(k = 0\), while for \(s\)-wave superconductivity one should minimize the error around \(k = k_F\). However, having verified that different optimization procedures lead to similar high-quality pseudopotentials, we continue with the optimization of the total squared phase-shift error.

B. Attractive branch

We can use a similar procedure to derive Troullier-Martins and ultratransferable pseudopotentials for the attractive branch, \(a < 0\). The main difference from the repulsive branch lies in the choice of cutoff: for the repulsive branch, the cutoff must lie beyond the first node of the wave function, while for the attractive branch there is no lower bound on the cutoff.

The smaller the cutoff, the closer the scattering properties of the pseudopotential approach those of the contact potential. However, reducing the cutoff comes at the cost of computational efficiency. For example, in quantum Monte Carlo simulations, the sampling efficiency of a potential is proportional to the fraction of configuration space volume in which the potential is finite, \(r_c^3/\Omega\), where \(\Omega\) is the simulation cell volume.

In Fig. 3(a) we adopt a cutoff \(r_c = 1/2k_F\), and compare the results to the square well potential with cutoff \(r_c = 0.01\sqrt{3}\pi^2/k_F\) used in Ref. [1]. Both the Troullier-Martins pseudopotential and the UTP have an average error approximately 10 times smaller than the square well potential, but their larger cutoff allows them to be sampled 4000 times more efficiently in QMC. Reducing the cutoff used for the Troullier-Martins pseudopotential or the UTP would further increase their accuracy, at the cost of a reduction in sampling efficiency.

In Fig. 3(b), we compare the phase-shift accuracy of the pseudopotentials as a function of cutoff. Both the Troullier-Martins and ultratransferable formalisms result in pseudopotentials whose scattering phase shifts converge to those of the contact interaction considerably faster than the square well potential. We find that the average error in phase shift of both the Troullier-Martins pseudopotential and UTP tends to zero as \(r_c^3\). By contrast, the square well converges as \(r_c\). The improved convergence can be understood as a consequence of imposing norm-conservation, which guarantees the correctness of \(\partial |\psi(\delta)\rangle/\partial E|_{E = E_F}\) around the calibration energy \((3/5)E_F\). Equation (1) then shows that the leading error in the phase shifts is approximately proportional to
Nonlocal pseudopotentials have been used effectively in quantum Monte Carlo calculations for the electron-ion interaction [45]. Adapting the formalism to interparticle pseudopotentials is straightforward. The total contribution to the local energy from the nonlocal pseudopotential can be written as a double sum over particles in each spin channel,

$$\int PP/cont k \delta k \biggl| \delta k - \delta k_{0} \biggr|^{2} d \delta k,$$

where $\Psi$ is the many-body wave function. To calculate the contribution $\hat{V}_{nl}/\Psi /\Psi$ that arises from the interaction between an up-spin particle at $r_{ij}$ and a down-spin particle at $r_{j}$, it is convenient to translate all particle positions by $-r_{i}$, such that particle $i$ is located at the origin. Then,

$$\hat{V}_{nl}/\Psi /\Psi = \sum_{i \in \uparrow} \sum_{j \in \downarrow} \hat{V}_{nl}/\psi /\psi ,$$

where $r_{ij} = |r_{ij}|$, $V(r_{ij})$ is the value of the pseudopotential at $r_{ij}$, and $R_{ij}^{1}$ denotes all of the up-spin particles, and the integration runs over all solid angles on a sphere or radius $r_{j}$ centered at the origin. We note that, inasmuch as the proposed pseudopotentials are short-ranged, we need only carry out the spherical integration for a small number of pairs of atoms: all those with $|r_{i} - r_{j}| < r_{c}$.

Additional accuracy could be gained by using different projectors for different energy ranges [46,47]. Nonlocal pseudopotentials have been used successfully to describe electron-ion interactions in numerical calculations. The formalism necessary to implement the projectors is therefore already in place.

## III. ATOMS IN A TRAP

We have developed a pseudopotential that delivers the correct scattering phase shift for an isolated system. To test the pseudopotential we turn to an experimentally realizable configuration [48,49]: two atoms in a spherical harmonic trap with frequency $\omega$ and characteristic width $d = 1/\sqrt{\omega}$. For all three types of contact interaction, this system has an analytical solution plotted in Fig. 4(a) [36] that we can benchmark against. Moreover, the exact solution extends to excited states, allowing us to test the performance of the pseudopotential across a wide range of energy levels to provide a firm foundation from which to study the many-body system.

### A. Ground state

We first compare the pseudopotential estimates of the ground-state energy to the exact analytical solution [36]. For the repulsive and attractive branches, both the hard- and soft-sphere potentials deliver a $\sim 1\%$ error in the energy, while both
Both the square well and Troullier-Martins formalism give the exact ground-state energy for two atoms in a vacuum. However, the trapping potential introduces inhomogeneity, and the square well potential gives a $\sim 10\%$ error in the ground-state energy, whereas the Troullier-Martins pseudopotential delivers errors of less than $\sim 0.01\%$. This affirms the benefits of using a pseudopotential that is robust against changes in the local environment. The success of the Troullier-Martins and ultratransferable formalisms in describing the ground state is all the more significant considering that these pseudopotentials aim to describe the correct scattering properties over a range of energies. We would therefore expect them to perform even better when modeling the excited states of the trap.

**B. Excited states**

We now examine the predictions for the excited states in the repulsive and attractive branches. Due to the shell structure, the excited states of a few-body system are related to the ground state of a many-body system [9], allowing us to probe the performance expected from the pseudopotential in a many-body setting. We consider states up to a maximum energy of $E_{\text{max}} = 7.5\hbar\omega$, corresponding to 112 noninteracting atoms in the trap. In Figs. 4(b) and 4(c) the Troullier-Martins pseudopotential has a mean-squared error averaged over all bands below $E_{\text{max}}$ between 10 and 100 times lower than the hard sphere and square well pseudopotentials. The UTP is a further factor of 2 more accurate. Additionally, when modeling the attractive branch, the Troullier-Martins and ultratransferable formalisms produce pseudopotentials that converge to the contact limit more rapidly than the attractive square well, resulting in improved efficiency when used in a QMC simulation. For the cutoff radii used in Fig. 4(c), using the Troullier-Martins pseudopotentials or the UTP results in QMC calculations that are 4000 times more efficient than the equivalent calculation with the square well.

The pseudopotentials deliver energies with better than $\sim 0.01\%$ accuracy, a significant improvement over existing pseudopotentials. This means that they are no longer the limiting factor in studies of ultracold atomic gases with state-of-the-art computational methods. For example, exact diagonalization calculations have been performed at a similar $\sim 0.01\%$ accuracy [11], and high-fidelity many-body QMC can also achieve $\sim 0.01\%$ stochastic error [3–5]. We are therefore well positioned to test the pseudopotential in a many-body setting.

**IV. CASE STUDY: FERMI GAS**

Having demonstrated the efficacy of the Troullier-Martins and UTP formalisms for an inhomogeneous two-body system, we now test the pseudopotentials using quantum Monte Carlo methods. We calculate the equation of state of a Fermi gas with weak interactions. Fermi gases serve as models for free electrons in a conductor, for nucleons inside a large nucleus, and for liquid He$_3$ [50].

For the attractive Fermi gas, the quality of a pseudopotential can be systematically improved by reducing the cutoff radius. We therefore concentrate on the repulsive branch of the Feshbach resonance, for which the top-hat pseudopotential cannot be systematically improved. We compare the energies...
predicted by DMC calculations with exact perturbation expansions calculated with the contact potential. The main result is shown in Fig. 5: energies calculated using the UTP and top hat differ significantly for $k_Fa \gtrsim 0.3$. The equation of state calculated using the UTP formalism agrees well with third-order perturbation theory, confirming the accuracy of the formalism.

**A. Formalism**

We use the DMC method [14–16], as implemented in the CASINO code [51] with a Slater-Jastrow trial wave function and a backflow transformation [52]. The wave function takes the form $\Psi = e^J D_U D_D$, where $D_U$ and $D_D$ are Slater determinants of plane-wave orbitals for each of the spin channels. The Jastrow factor $e^J$ describes the interparticle correlation

$$J = \sum_{j \neq i} \left(1 - \frac{|\mathbf{r}_j - \mathbf{r}_i|}{L_{u\alpha\beta}}\right)^2 u_{\alpha\beta}(|\mathbf{r}_i - \mathbf{r}_j|) \times \Theta(L_{u\alpha\beta} - |\mathbf{r}_i - \mathbf{r}_j|),$$

where $u_{\alpha\beta}$ is a polynomial whose parameters we optimize in a variational Monte Carlo (VMC) calculation, $L_{u\alpha\beta}$ is a cutoff length that we also optimize variationally, and $\Theta$ is the Heaviside step function [53]. The backflow transformation shifts electron positions in the Slater determinant as

$$\mathbf{r}_i \rightarrow \mathbf{r}_i + \sum_{j \neq i} \left(\mathbf{r}_i - \mathbf{r}_j\right) \eta_{ij}(|\mathbf{r}_i - \mathbf{r}_j|),$$

where

$$\eta_{ij}(r) = \left(1 - \frac{r}{L_{a\alpha\beta}}\right)^2 \Theta(|L_{a\alpha\beta} - r|) p_{a\alpha\beta}(r),$$

$p_{a\alpha\beta}$ is a polynomial whose parameters are optimized in VMC, and $L_{a\alpha\beta}$ is a cutoff length that we also optimize. The backflow transformation allows the description of further correlation, reducing the final DMC energy [5,52].

We calculate the equation of state of the Fermi gas with 81 up-spin and 81 down-spin particles. We use twist averaging [54–56] and correct the noninteracting kinetic energy with that of the corresponding infinite system [4] to reduce finite-size effects. We use a control variate method to reduce the stochastic error resulting from the twist-averaging procedure [57]. We find that the control variate method leads to a fivefold reduction in stochastic error for this system at no additional computational cost.

**B. Results**

We compare the equations of state of the UTP and soft-sphere pseudopotential in Fig. 5. The two differ significantly for $k_Fa \gtrsim 0.3$, highlighting the importance of using an accurate pseudopotential. To establish which potential reproduces the equation of state of the contact potential more closely, we compare the results to a third-order perturbation theory calculation of the equation of state [50,58],

$$E^{(3)} = \frac{3}{5} E_\Psi \left[1 + \frac{10}{9\pi} k_Fa + \frac{4(11 - 2\ln 2)}{21\pi^2} (k_Fa)^2 \right. + \left. \left(0.076 \pm 0.005 - 1/3\pi\right)(k_Fa)^3\right].$$

Figure 5(a) shows that the equation of state calculated using the UTP remains within the stochastic error of $E^{(3)}$ up to $k_Fa \sim 0.6$. In contrast, the equation of state for the soft-sphere system deviates significantly from the perturbation result for $k_Fa \gtrsim 0.3$. The energy $E^{(2)}$ obtained using second-order perturbation theory [59], which is used frequently in the literature [18,23], differs markedly from both the UTP and soft-sphere pseudopotential energy. These significant differences in energy affirm the importance of using a pseudopotential whose scattering properties accurately replicate those of the contact interaction.

In Fig. 5(b), we compare the variance in the local energy $E_\Psi = \langle H \Psi / \Psi \rangle$ of the ground-state wave function for different pseudopotentials. The stochastic error for a quantum Monte Carlo calculation is proportional to $\sqrt{\text{Var}(E_\Psi)}$. A smoother local energy will therefore result in more accurate results for the same computational expense. By virtue of its smoothness, we find that the UTP leads to smoother local energies than the soft-sphere pseudopotential. In particular, the variance of the local energy at small $k_Fa$ diverges for the zero-range soft-sphere pseudopotential. Even at $k_Fa = 0.6$, we find that
the standard deviation of the UTP ground state is about five
times smaller than that of the soft-sphere ground state, resulting
in a 25-fold improvement in efficiency in quantum Monte
Carlo calculations.

The computational expense, for a fixed number of VMC or
DMC samples, of all the pseudopotentials considered in this
article scales as \( O(N^2) \) with particle number \( N \). This quadratic
dependence arises from the need to check the separation of all
pairs of particles to decide whether the particles are close
enough to interact. The prefactor of this term is therefore
identical for all pseudopotentials. We must therefore consider
the prefactor of the \( O(N) \) term to discern a difference in the
computational expense of using the pseudopotentials. The square
well or top hat potential scales more favorably, both
because it is easier to compute the value of the pseudopotential
and because, by virtue of its smaller cutoff radius, fewer
pairs of particles interact. In practice, we find that for the
162-particle system considered in this section at \( k_F a = 0.6 \), it
takes approximately 25% less CPU time to acquire the same
number of VMC samples with a top-hat potential than with a
UTP. This difference is far outweighed by the lower variance
in local energy of the UTP: QMC calculations with a top-hat
pseudopotential are approximately 19 times more costly than
calculations with a UTP, to obtain the same level of accuracy.

V. DISCUSSION

We have developed a high-fidelity pseudopotential for the
contact interaction inspired by pseudopotentials common in the
electronic structure community. We tested the pseudopotential
by examining the scattering phase shifts, the energy of
two trapped particles, and the ground-state energy of a Fermi
gas, finding the new pseudopotentials to be approximately 100
times more accurate for the repulsive branch, and 10 times
more accurate for the attractive and bound-state branches of the
Feshbach resonance, while also 4000 times more efficient than
temporary approximations. The pseudopotential delivers
accurate scattering properties over all wave vectors \( 0 \leq k \lesssim
k_F \) in a Fermi gas. Its smoothness also greatly accelerates
computation: for instance, for the repulsive branch of the
Feshbach resonance, calculations are accelerated by a factor
of at least 19.

The performance and transferability of the pseudopotential
makes it widely applicable across first-principles methods
including VMC, DMC, coupled cluster, and configuration
interaction methods. The formalism developed can also be
applied more widely to generate pseudopotentials for narrow
Feshbach resonances, the repulsive Coulomb interaction, or
the dipolar interaction. The formalism could also be extended
by using more projectors or the ultrasoft \cite{ultrasoft} or augmented
plane-wave \cite{augmented} formalisms popular in the electronic structure
community.

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APPENDIX: CONSTRUCTION OF THE TROUILLIER-MARTINS PSEUDOPOTENTIAL

The equations in the Troullier-Martins paper pertain to
electron-ion pseudopotentials in the context of the Born-
Oppenheimer approximation \cite{BO}. They therefore consider the
interaction of an electron with a much heavier nucleus. By
contrast, in this paper, we are interested in the interaction
between two particles of equal mass. This corresponds to
using a reduced mass \( \mu = 1/2 \) in the center-of-mass frame,
rather than \( \mu \lesssim 1 \) for electron-ion pseudopotentials. We adapt
the Troullier-Martins formalism to the construction of a
pseudopotential for two particles of equal mass interacting
with a contact interaction.

The Schrödinger equation for relative motion with reduced
mass of 1/2 and a spherically symmetric interparticle potential is

\[
[-\nabla^2 + V(r)]\psi_{E,\ell}(r) = E\psi_{E,\ell}(r),
\]

where \( r = r_1 - r_2 \) is the relative position of the two particles and
\( \psi_{E,\ell} \) is the relative wave function associated with energy
eigenvalue \( E \) and angular momentum channel \( \ell \). We only
consider particles with relative angular momentum quantum number \( \ell = 0 \), since the contact interaction only scatters in this
channel.

By expanding the relative wave function \( \psi_{E,\ell=0}(r) =
R_{E,\ell=0}(r)Y_0 \), where \( Y_0 = 1/\sqrt{4\pi} \) is the zeroth spherical
harmonic and \( r = |r| \), we can recast the three-dimensional
Schrödinger equation as a radial equation,

\[
\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r)\right] R_{E,\ell=0} = E R_{E,\ell=0}.
\]  

(A1)

We choose a calibration energy \( E_c \), as described in the
main text, and construct the pseudopotential by choosing a
pseudo-wave-function that matches the exact form beyond a
cutoff radius \( r_c \), at the calibration energy. Following
Troullier-Martins, we define the pseudo-wave-function at the
calibration energy as \( \psi_{E,\ell=0}^{\text{PP}} = R_{E,\ell=0}^{\text{PP}} Y_0 \) with the radial component

\[
R_{E,\ell=0}^{\text{PP}}(r) = \begin{cases} R_{E,\ell=0}^{\text{cont}}(r), & r \geq r_c, \\ \exp[p(r)], & r < r_c, \end{cases}
\]

where \( p(r) = \sum_{l=0}^{6} c_l r^{2l} \) is a polynomial and \( R_{E,\ell=0}^{\text{cont}} \) is the
radial wave function for the contact interaction at the calibration
energy \( E_c \). Inserting this form into the radial equation, Eq. (A1), we calculate an expression for the pseudopotential
\( V_{E,\ell=0}^{\text{PP}} \) as a function of \( p(r) \),

\[
V_{E,\ell=0}^{\text{PP}}(r) = \begin{cases} 0, & r \geq r_c, \\ E_c + p'' + p^2 + \frac{3}{2} p', & r < r_c. \end{cases}
\]  

(A2)

where the primes indicate derivatives.

To proceed further, we must consider an explicit functional
form for \( R_{E,\ell=0}^{\text{cont}} \). This depends on whether we are constructing
a pseudopotential for a scattering state or the bound state
of the contact interaction. We consider these two cases in Appendices 1 and 2.

1. Scattering states

The relative wave function for two particles interacting via contact interactions is

\[ R^\text{cont}_{E,\text{cutoff}}(r) = \frac{\sin[kr + \delta_0(k)]}{kr}, \]

where \( \delta_0(k) = \arctan(-ka) \) and \( k = \sqrt{E} \). The continuity equations at the cutoff are

\[
\begin{align*}
p(r_c) &= \ln\left(\frac{\sin[kr_c + \delta_0(k)]}{r_c}\right), \\
p'(r_c) &= \frac{k}{\tan(kr_c + \delta)} - \frac{1}{r_c}, \\
p''(r_c) &= -k^2 - \frac{2}{r_c}p' - p^2, \\
p^{(3)}(r_c) &= \frac{2}{r_c^2}p' - \frac{2}{r_c}p'' - 2p'p'', \\
p^{(4)}(r_c) &= \frac{4}{r_c^2}p' + \frac{4}{r_c}p'' - \frac{2}{r_c}p^{(3)} - 2p'^2 - 2p'p^{(3)},
\end{align*}
\]

where \( p^{(i)} \) denotes the \( i \)th derivative of \( p \) and all derivatives are evaluated at \( r = r_c \). To obtain the pseudo-wave-function at the calibration energy, we solve this system of five equations, as well as the norm-conservation condition and impose \( c_r^2 = -5c_a \) to guarantee \( \partial^2 V^{pp}/\partial r^2 |_{r=a} = 0 \). This uniquely determines the polynomial \( p(r) \), which, in turn, determines the pseudopotential, following Eq. (A2).

2. Bound state

The relative wave function for two particles in the bound state of the contact interaction is

\[ R^\text{cont}_{E,\text{cutoff}}(r) = \left(\frac{k^3}{2\pi}\right)^{1/2} \exp(kr) \frac{1}{kr}, \]

where \( k = \sqrt{E} \) and \( E = -1/a^2 \) for scattering length \( a \). The continuity equations at the cutoff \( r = r_c \) are

\[
\begin{align*}
p(r_c) &= -\frac{k}{r_c} - \ln(r_c), \\
p'(r_c) &= -\frac{1}{r_c}, \\
p''(r_c) &= -k^2 - \frac{2}{r_c}p' - p^2, \\
p^{(3)}(r_c) &= \frac{2}{r_c^2}p' - \frac{2}{r_c}p'' - 2p'p'', \\
p^{(4)}(r_c) &= \frac{4}{r_c^2}p' + \frac{4}{r_c}p'' - \frac{2}{r_c}p^{(3)} - 2p'^2 - 2p'p^{(3)}.
\end{align*}
\]

[41] We provide a Python program to generate the Troullier-Martins, UTP, and square well pseudopotentials at https://pypi.python.org/pypi/contactpp.