

Pseudopotential approximation in a harmonic trap

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We construct the pseudopotential for two particles subjected to an isotropic harmonic trapping potential while interacting through a hard-sphere potential, and demonstrate that this trap pseudopotential reduces to the standard “zero range” interaction when the ratio of the hard-sphere diameter and the oscillator length is small. We also show that the standard approximation, even when applied to tight traps, is surprisingly accurate.

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The pseudopotential method [1,2] is an important tool for the study of interacting particles. The key idea is to replace the actual, possibly complicated interaction potential by a much simpler pseudopotential operator, such that the exact energy eigenvalues of the interacting system are reproduced at least to the lowest few orders in a suitable expansion parameter. This approach now is of central importance for the theoretical description of Bose-Einstein condensates [3–5], where the approximate pseudopotential mimics the real two-body interaction solely through its s -wave scattering length. However, the condensates are subjected to a trapping potential, and one expects some influence of this external potential on the pseudopotential at least with tight traps, i.e., when the distance over which the trapping potential varies significantly becomes comparable to the scattering length. In this paper we investigate the influence of the trap in detail for a hard-sphere interaction potential, and quantify the accuracy of the standard pseudopotential approximation in an isotropic harmonic trap.

Let us briefly recapitulate the essence of the pseudopotential approach [2] for two identical particles of mass m which interact, in the absence of an additional external trapping potential, via a finite-range potential $V(|\vec{r}|)$ without two-body bound states, so that the Hamiltonian is given by

$$H(\vec{r}_1, \vec{r}_2) = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + V(|\vec{r}_2 - \vec{r}_1|). \quad (1)$$

Introducing center-of-mass coordinates $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ and relative coordinates $\vec{r} = \vec{r}_2 - \vec{r}_1$, and separating off the free center-of-mass motion, the eigenvalue equation for the relative motion becomes

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(|\vec{r}|)\right)\varphi(\vec{r}) = E\varphi(\vec{r}), \quad (2)$$

where $\mu = m/2$ is the reduced mass of the two particles. Writing $E = (\hbar k)^2/(2\mu)$, and denoting the finite range of the interaction potential as a , one encounters the Helmholtz equation in the “outer” range,

$$(\nabla^2 + k^2)\varphi(\vec{r}) = 0 \quad \text{for } r > a. \quad (3)$$

This equation is solved by the familiar linear combination of spherical Bessel functions $j_l(kr)$ and spherical Neumann functions $n_l(kr)$ [6],

$$\varphi(\vec{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l A_{l,m} [j_l(kr) - \tan(\eta_l) n_l(kr)] Y_{l,m}(\vartheta, \varphi) \quad (4)$$

for $r > a$. Here, $\eta_l = \eta_l(k)$ is the phase shift inflicted by the potential on the l th partial wave. Restricting oneself to low energies, $k \rightarrow 0$, so that only s -wave scattering matters, this simplifies to

$$\varphi(\vec{r}) = \frac{A_{0,0}}{\sqrt{4\pi}} \left[\frac{\sin(kr)}{kr} + \tan(\eta_0) \frac{\cos(kr)}{kr} \right] \quad (5)$$

for $r > a$, where we have inserted $j_0(kr) = \sin(kr)/(kr)$ and $n_0(kr) = -\cos(kr)/(kr)$.

The decisive step of the pseudopotential method [1,2] now consists of taking this “outer” wave function (5) for *all* r , even though the actual wave function is affected by the potential, and therefore differs from the function (5) for $r < a$. When extending the outer function (5) to $r < a$, the term proportional to $\tan(\eta_0)$, that is, the term which actually “feels” the potential, becomes singular. It is this singularity which gives rise to the pseudopotential: Since the outer function solves the Helmholtz equation for all $r > 0$, and $r = 0$ is dealt with by the relation $\nabla^2(1/r) = -4\pi\delta(\vec{r})$, the extended wave function obeys the operator equation

$$(\nabla^2 + k^2)\varphi(\vec{r}) = -4\pi \frac{A_{0,0}}{\sqrt{4\pi}} \frac{\tan[\eta_0(k)]}{k} \delta(\vec{r}). \quad (6)$$

The further observation that Eq. (5) implies

$$\frac{A_{0,0}}{\sqrt{4\pi}} = \frac{\partial}{\partial r} [r\varphi(\vec{r})] \Big|_{r \rightarrow 0} \quad (7)$$

allows one to eliminate the amplitude $A_{0,0}$ from Eq. (6) by reintroducing the wave function itself, leading to

$$(\nabla^2 + k^2)\varphi(\vec{r}) = -4\pi \frac{\tan[\eta_0(k)]}{k} \delta(\vec{r}) \frac{\partial}{\partial r} [r\varphi(\vec{r})] \Big|_{r \rightarrow 0}; \quad (8)$$

this equation now holds for all r . In effect, the actual interaction potential has thus been replaced, for s -wave scattering, by the pseudopotential operator

$$U_{\text{pp}}(\vec{r}) = -\frac{4\pi\hbar^2}{m} \frac{\tan[\eta_0(k)]}{k} \delta(\vec{r}) \frac{\partial}{\partial r} r, \quad (9)$$

where we have reinserted the actual particle mass $m = 2\mu$. In the special case of a hard-sphere interaction of diameter a ,

$$V(|\vec{r}|) = \begin{cases} 0 & \text{for } |\vec{r}| > a \\ \infty & \text{for } |\vec{r}| \leq a, \end{cases} \quad (10)$$

one has $\eta_0(k) = -ka$ [6]. Therefore, neglecting terms of the order $O[(ka)^3]$, and observing that the differential operator $(\partial/\partial r)r$ may be replaced by unity when acting on functions which are well behaved at $r=0$ [1,2], one obtains from Eq. (9) the commonly quoted effective “zero range” interaction [5]

$$U_{\text{pp}}(\vec{r}) = \frac{4\pi a \hbar^2}{m} \delta(\vec{r}). \quad (11)$$

It should be noted, however, that this delta potential does not lead to a proper self-adjoint Hamiltonian [7]; it is rather to be used as a starting point for perturbative analysis. In the case of a general interaction potential, the hard-sphere diameter a has to be replaced by the corresponding s -wave scattering length.

When considering, instead of free particles which scatter from each other, cold atoms confined by some trapping potential, the above reasoning is in jeopardy. The trapped two-particle states then do no longer conform to the scattering solutions (4) with a continuous wave-number k , but rather to bound states with discrete energy E . Therefore, the proper pseudopotential for trapped particles has to be constructed from the two-particle eigenstates provided by the trapping potential, and some effect of the trap should make itself felt when the two relevant length scales, the interaction range a and the trap size L , are of the same order of magnitude. In order to assess the accuracy of the standard approximation (11) in the presence of a trapping potential, and to study the influence of the trap on the proper pseudopotential, we now treat two particles stored in an isotropic harmonic trap with angular frequency ω . The particles are assumed to interact through the hard-sphere potential (10), and thus are described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) + \frac{1}{2} m \omega^2 (\vec{r}_1^2 + \vec{r}_2^2) + V(|\vec{r}_2 - \vec{r}_1|). \quad (12)$$

Again introducing center-of-mass coordinates \vec{R} and relative coordinates \vec{r} , this Hamiltonian takes the form

$$H = -\frac{\hbar^2}{2M} \nabla_{\vec{R}}^2 + \frac{1}{2} M \omega^2 \vec{R}^2 - \frac{\hbar^2}{2\mu} \nabla_{\vec{r}}^2 + \frac{1}{2} \mu \omega^2 \vec{r}^2 + V(|\vec{r}|), \quad (13)$$

with the reduced mass $\mu = m/2$, and the total mass $M = 2m$. Therefore, writing the wave function as a product $\psi(\vec{r}_1, \vec{r}_2) = \varphi(\vec{r})\chi(\vec{R})$, the center-of-mass motion separates from the

relative motion even in the presence of the harmonic trapping potential. The Schrödinger equation for the center-of-mass wave function $\chi(\vec{R})$ simply is an equation for an unperturbed harmonic oscillator with particle mass M , whereas the relative motion is governed by

$$\left(-\frac{\hbar^2}{2\mu} \nabla^2 + \frac{1}{2} \mu \omega^2 \vec{r}^2 + V(|\vec{r}|) \right) \varphi(\vec{r}) = E \varphi(\vec{r}). \quad (14)$$

Employing the dimensionless radial coordinate $\xi = r/L$, where

$$L = \sqrt{\hbar/(\mu\omega)} \quad (15)$$

is the “oscillator length” associated with the reduced mass μ , and again focusing on s waves (states with relative angular momentum $l=0$) only, the ansatz $\varphi(\vec{\xi}) = u(\xi)/\xi$ immediately leads to the radial equation

$$\left(-\frac{1}{2} \frac{d^2}{d\xi^2} + \frac{1}{2} \xi^2 - \varepsilon \right) u(\xi) = 0 \quad \text{for } \xi > \alpha, \quad (16)$$

with $\alpha = a/L$, and scaled energy $\varepsilon = E/(\hbar\omega)$. The hard-sphere interaction then translates into the boundary-condition $u(\xi) = 0$ for $\xi \leq \alpha$.

A set of fundamental solutions to this equation is provided by the parabolic cylinder functions $U(-\varepsilon, \sqrt{2}\xi)$ and $V(-\varepsilon, \sqrt{2}\xi)$, using the notation of Ref. [8]. Since the latter function increases exponentially with increasing particle distance ξ [8], it has to be discarded; the relative wave function thus has to be constructed from the former solution alone. Therefore, the hard-sphere boundary condition leads to the quantization condition

$$U(-\varepsilon_n, \sqrt{2}\alpha) = 0 \quad (17)$$

for the discrete energies ε_n of the relative motion, and the corresponding eigenfunctions take the form

$$\varphi_n(\vec{\xi}) = \frac{N_n}{\xi} U(-\varepsilon_n, \sqrt{2}\xi) \quad \text{for } \xi > \alpha, \quad (18)$$

with normalization constants N_n . Figure 1 shows a plot of the lowest three eigenvalues ε_n , as functions of the scaled hard-sphere diameter α . We remark that only for particular numerical values of ε_n , namely, when $\varepsilon_n = n + 1/2$ ($n=0,1,2, \dots$) coincides with an eigenvalue of a usual one-dimensional harmonic oscillator, the above solutions become elementary and can also be obtained from a Sommerfeld polynomial ansatz [9].

We now exploit the knowledge of the exact relative wave functions (18) for constructing the associated pseudopotential. To this end, we again extend these functions to the regime $\xi < \alpha$. Since the parabolic cylinder function $U(-\varepsilon, x)$ can be represented in the form [8]

$$U(-\varepsilon, x) = \cos(\pi\beta_\varepsilon) Y_1(-\varepsilon, x) - \sin(\pi\beta_\varepsilon) Y_2(-\varepsilon, x), \quad (19)$$

with $\beta_\varepsilon = 1/4 - \varepsilon/2$, and (see Ref. [8] for higher-order terms)

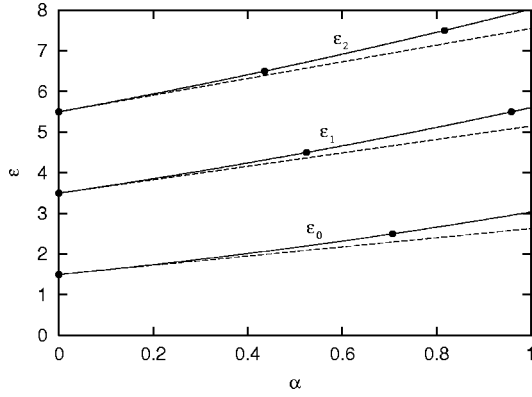


FIG. 1. Lowest three exact s -wave energy eigenvalues $\varepsilon_n = E_n/(\hbar\omega)$ (full lines) compared to the first-order perturbative pseudopotential approximations (29) (dashed lines), as functions of the dimensionless hard-sphere diameter $\alpha = a/L$. The full circles indicate parameters for which the exact solutions (18) become elementary [9].

$$Y_1(-\varepsilon, x) = \frac{1}{\sqrt{\pi}} \frac{\Gamma(1/4 + \varepsilon/2)}{2^{1/4 - \varepsilon/2}} \left[1 - \varepsilon \frac{x^2}{2} + O(x^4) \right] \quad (20)$$

and

$$Y_2(-\varepsilon, x) = \frac{1}{\sqrt{\pi}} \frac{\Gamma(3/4 + \varepsilon/2)}{2^{-1/4 - \varepsilon/2}} \left[x - \varepsilon \frac{x^3}{3!} + O(x^5) \right], \quad (21)$$

the behavior of the relative wave functions for small distances ξ is given by

$$\varphi_n(\vec{\xi}) = A_n \left[1 - \cot(\pi\beta_{\varepsilon_n}) \frac{\Gamma(1/4 + \varepsilon_n/2)}{\Gamma(3/4 + \varepsilon_n/2)} \frac{1}{2\xi} \right] + O(\xi). \quad (22)$$

In analogy to the previous Eq. (7), the overall amplitudes A_n are related to the wave functions at small ξ through

$$A_n = -N_n \sin(\pi\beta_{\varepsilon_n}) \frac{\Gamma(3/4 + \varepsilon_n/2)}{2^{-3/4 - \varepsilon_n/2} \sqrt{\pi}} = \frac{\partial}{\partial \xi} [\xi \varphi_n(\vec{\xi})] \Big|_{\xi \rightarrow 0}. \quad (23)$$

Thus, the wave functions (18) exhibit the same type of singularity for $\xi \rightarrow 0$ as their free-space counterpart (5). This fact, which stems from the occurrence of the Laplacian in both Eq. (2) for the free case, and Eq. (14) for the trapped motion, now allows us to directly determine the desired (dimensionless) trap pseudopotential

$$v_{\text{pp}}(\vec{\xi}) = \pi \cot(\pi\beta_{\varepsilon_n}) \frac{\Gamma(1/4 + \varepsilon_n/2)}{\Gamma(3/4 + \varepsilon_n/2)} \delta(\vec{\xi}) \frac{\partial}{\partial \xi} \xi. \quad (24)$$

Taken in this form, the usefulness of the pseudopotential is limited: It depends explicitly on the still unknown eigenvalues ε_n , so that the corresponding Schrödinger equation has to be solved self-consistently. However, the quantization condition (17) and the representations (20) and (21) combine to yield

$$\begin{aligned} \cot(\pi\beta_{\varepsilon_n}) &= \frac{Y_2(-\varepsilon_n, \sqrt{2}\alpha)}{Y_1(-\varepsilon_n, \sqrt{2}\alpha)} \\ &= \frac{\Gamma(3/4 + \varepsilon_n/2)}{\Gamma(1/4 + \varepsilon_n/2)} \left[2\alpha + \frac{4}{3} \varepsilon_n \alpha^3 + O(\alpha^5) \right], \end{aligned} \quad (25)$$

so that, to the lowest order in $\alpha = a/L$, the s -wave pseudopotential (24) pertaining to the harmonic trap is independent of the energy ε_n :

$$v_{\text{pp}}(\vec{\xi}) = 2\pi\alpha \delta(\vec{\xi}) \frac{\partial}{\partial \xi} \xi + O(\alpha^3). \quad (26)$$

Moreover, replacing the dimensionless variable ξ by the physical distance $r = L\xi$, re-installing the unit of energy $\hbar\omega$, and omitting terms of order $O[(a/L)^3]$, we find

$$\hbar\omega v_{\text{pp}}(\vec{r}) = \frac{2\pi a \hbar^2}{\mu} \delta(\vec{r}) \frac{\partial}{\partial r} r. \quad (27)$$

Hence, recalling $\mu = m/2$, to leading order the proper trap pseudopotential (24) equals its free-space precursor (11). As seen in the derivation, this is a consequence of the fact that in both cases the leading-order term of the pseudopotential is determined by the singular solution of the Laplace equation $\nabla^2 \varphi = 0$.

Writing the exact relative s -wave eigenfunctions for non-interacting, harmonically trapped particles in terms of Laguerre polynomials $L_n^{(1/2)}(\xi^2)$ [10],

$$\varphi_n(\vec{\xi}) = \frac{1}{\sqrt{2\pi^{3/4}}} [L_n^{(1/2)}(0)]^{-1/2} e^{-\xi^2/2} L_n^{(1/2)}(\xi^2), \quad (28)$$

corresponding to scaled energy eigenvalues $\varepsilon_n = 2n + 3/2$ with $n = 0, 1, 2, \dots$, the approximate pseudopotential (27) allows one to calculate the effect of the hard-sphere interaction perturbatively; to lowest order in α , one immediately finds the energy shifts

$$\Delta \varepsilon_n = \frac{\alpha}{\sqrt{\pi}} L_n^{(1/2)}(0) = \frac{\alpha}{\sqrt{\pi}} \frac{(2n+1)!}{(2^n n!)^2}. \quad (29)$$

In particular, $\Delta \varepsilon_0 = \alpha/\sqrt{\pi}$ for the ground-state $n=0$. As witnessed by Fig. 1, this approximation, which is tantamount to simply employing the familiar free-space pseudopotential (11), yields a quite good description of the true eigenvalues: The error is only of order $O(\alpha^3)$, so that even for $\alpha = 0.2$, that is, when the hard-sphere diameter a already amounts to 20% of the oscillator length L , the actual ground-state shift is underestimated by less than 1%. The relative error of the lowest-order pseudopotential approximation to the ground-state energy ε_0 is depicted in detail in Fig. 2, as a function of α .

If the pseudopotential (27) is taken at face value, i.e., if it is not taken as a substitute for a hard-sphere potential and employed as the starting point for a perturbative calculation, but if instead the Schrödinger equation for the relative mo-

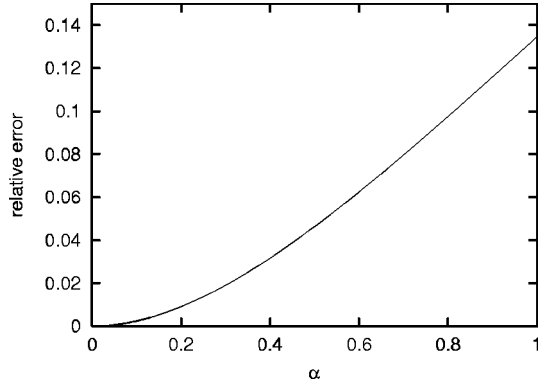


FIG. 2. Relative error of the lowest-order pseudopotential approximation, based on the standard pseudopotential (27), to the exact ground-state energy ε_0 for two harmonically trapped particles with hard-sphere interaction.

tion is solved *exactly* with this potential, an interesting observation is made. In that case, the quantization condition takes the form [10]

$$\frac{\Gamma(3/4 - \varepsilon_n/2)}{\Gamma(1/4 - \varepsilon_n/2)} = \frac{1}{\alpha}, \quad (30)$$

to be contrasted to the condition (17) or (25) for the hard-sphere interaction eigenvalues. Under the assumption that a small diameter α leads to an energy that differs only by a small amount $\Delta\varepsilon_n$ from an unperturbed eigenvalue, so that $\varepsilon_n = 2n + 3/2 + \Delta\varepsilon_n$, the Gamma function in the numerator of Eq. (30) is evaluated close to a pole,

$$\Gamma\left(-n - \frac{\Delta\varepsilon_n}{2}\right) \approx \frac{(-1)^{n+1}}{n!} \frac{2}{\Delta\varepsilon_n}, \quad (31)$$

whereas the denominator is smooth and can therefore be approximated by neglecting the shift $\Delta\varepsilon_n$, yielding

$$\Gamma\left(-n - \frac{1}{2}\right) = (-1)^{n+1} \frac{2^{2n+1} n! \sqrt{\pi}}{(2n+1)!}. \quad (32)$$

With these approximations, which capture those states which evolve continuously with α from the unperturbed states (28), the exact quantization condition (30) for the pseudopotential (27) reduces precisely to the result (29) of the perturbative calculation, as it should. There is, however, an additional possibility to satisfy Eq. (30): Since, by Stirling's formula, $\Gamma(z+1/2)/\Gamma(z) \sim \sqrt{z}$ for large, *positive* z , the condition (30) also admits a solution ε that decreases without bound when

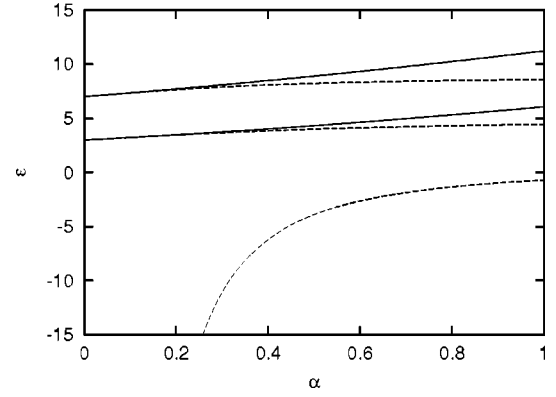


FIG. 3. Exact lowest three eigenvalues of relative motion for the pseudopotential (27) (dashed), compared to the exact eigenvalues pertaining to the hard-sphere potential (10) (full lines). Note that the pseudopotential, when diagonalized exactly, gives rise to an additional bound state which is not met in the original hard-sphere problem.

the (positive) value of α approaches zero, $\varepsilon \rightarrow -\infty$ for $\alpha \rightarrow 0+$, as plotted in Fig. 3. It is clear that this additional state, which is not present in the original hard-sphere problem and which cannot be obtained from the perturbative treatment, is required for mathematical consistency: After the boundary condition has been shifted from $r=a$ to $r=0$ through the introduction of the pseudopotential (27), the extended scattering solutions no longer form a complete set, and therefore have to be supplemented by the additional bound state. However, when the pseudopotential is regarded as a convenient substitute for an actual hard-sphere potential, the additional state is redundant.

To summarize, we have constructed the pseudopotential for two particles which are subjected to an external harmonic trapping potential and interact through a hard-sphere potential. When the ratio α of the hard-sphere diameter and the oscillator length is small, this trap pseudopotential (24) properly reduces to the familiar free-space pseudopotential (11). Exact diagonalization of this approximate pseudopotential produces a bound state not connected to an eigenstate of the noninteracting system. Nonetheless, the approach works reliably, and with surprising accuracy, within lowest-order perturbation theory: For the lowest-lying state, the relative error then exceeds 5% only when $\alpha > 0.53$, and 10% only when $\alpha > 0.82$.

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- [1] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).
- [2] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).
- [3] A. S. Parkins and D. F. Walls, Phys. Rep. **303**, 1 (1998).
- [4] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).
- [5] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
- [6] J. J. Sakurai, *Modern Quantum Mechanics* (Addison Wesley, Reading, MA, 1994).
- [7] S. Albeverio, F. Gesztesy, R. Hoegh-Krohn, and H. Holden,

Solvable Models in Quantum Mechanics (Springer, Heidelberg, 1988).

- [8] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972), Chap. 19.
- [9] M. Taut, Phys. Rev. A **48**, 3561 (1993).
- [10] Th. Busch, B.-G. Englert, K. Rzażewski, and M. Wilkens, Found. Phys. **28**, 549 (1998).