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Conditions for bound states of the pseudopotential with harmonic confinement in arbitrary dimensions

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Abstract

We determine the conditions for bound states ($E < 0$) for arbitrary Cartesian dimension d using a shape-independent regularized pseudopotential with scattering length a for two cold particles in a harmonic trap. It is known for $d \leqslant 3$ that the regularized pseudopotential supports one bound state for positive scattering length but does not support bound states for negative scattering length. We find that the usual ($d \leqslant 3$) positive scattering length bound states rule holds for certain higher odd dimensions $d = 4n + 3$ ($n = 0, 1, \ldots$), but the existence of pseudopotential bound states at other odd dimensions requires a negative scattering length. Specifically, bound states are allowed in higher dimensions $d = 4n + 1$ ($n = 1, 2, \ldots$) but they require a negative scattering length, which suggests a universe in these dimensions might lead to different chemistry than $d = 3$. We derive analytical approximations for bound state ($E < 0$) and scattering ($E > 0$) energies for a harmonic trap perturbed by the pseudopotential in arbitrary dimensions.

1. Introduction

A perennial question in physics and philosophy was investigated by Ehrenfest who asked, 'Why has our space just three dimensions? [1]' A related question, motivated by string theory, asks why did three of the nine compactified spatial dimensions expand? A constraint that is often considered for spatial dimensions, based on anthropic principles, is the existence of bound states or stable orbits. For example, the analysis by Ehrenfest determined that circular orbits are not stable for $d > 3$, and [2] used a Virial theorem derivation to argue that atomic bound states are not possible for $d > 3$. However, [3] concluded that the Hydrogen atom has stable states for $d > 3$, albeit using $1/r$ as the electrostatic potential rather than $1/r^{d-2}$. In the current study, we investigate the effect of spatial dimension on bound states for two cold atoms in a harmonic trap perturbed by a regularized Fermi pseudopotential interaction.

While the main motivation of this study is to understand the conditions for bound states of ultracold atoms in higher dimensional universes, the results also apply to higher synthetic dimensions [4, 5] and dimensional crossover from three to lower dimensions [6]. Energies for confined systems in three and one dimension have been calculated with the pseudopotential interaction [7], in two dimensions with a delta function [8], and in d dimensions with multiple delta function interactions [9]. The Gross–Pitaevskii equation (GPE) has been used to study potential synthetic 4d Bose–Einstein Condensate (BEC) gases with vortices [10], and d-dimensional ultracold BEC gases with vortices have been studied with dimensional perturbation theory of the GPE [11].

For the interaction between ultracold atoms, we use the d-dimensional pseudopotential,

$$ {}_{C_0}V_k^{(d)} = \frac{\Omega(d)\bar{a}^{d-2}}{\Gamma(d-2)} T(d, k\bar{a})\, \delta^{(d)}(r)\ {}_{C_0}D_r^{d-2} r^{d-2}, \tag{1} $$

where $\bar{a}$ is the s-wave scattering length in oscillator units $\sqrt{\hbar/m\omega}$ in d dimensions and ${}_{C_0}D_r^{d-2}$ is the $(d-2)$-order Caputo fractional derivative when d is non-integer. Fractional derivatives generalize integer-order derivatives (i.e., d^n/dx^n) to arbitrary order, which arose in our derivation when analytically continuing the dimension to arbitrary values, including non-integer (see appendix A of [12]). The Caputo fractional derivative ensures that the fractional derivative of a constants is zero. When d is integer, which is mostly considered in the current study, the fractional derivative reduces to the usual derivative (d^{d-2}/dr^{d-2}). Previously, we derived the above general-dimension pseudopotential with wavenumber k using a fractional calculus Frobenius series solution to the d-dimensional relative-motion Schrödinger free-wave equation with a hard-sphere boundary condition [12]. The derivative and r^{d-2} operator in the pseudopotential removes the leading singularity of the form $1/r^{d-2}$ from the wave function series solution and removes other lower-order singularities in powers of $1/r$. The strength of the exact interatomic potential is parameterized by the scattering length and the exact shape is replaced by a d-dimensional contact/zero-range delta function. The quantity $\Omega(d) = 2\pi^{d/2}/\Gamma(d/2)$ is the d-dimensional solid angle, and we defined T as an s-wave scattering phase shift function in d dimensions in terms of hypergeometric functions:

$$T(d,\, k\bar{a}) = \frac{{}_0F_1\left(;\frac{d}{2};\, -\frac{k^2\bar{a}^2}{4}\right)}{{}_0F_1\left(;2-\frac{d}{2};\, -\frac{k^2\bar{a}^2}{4}\right)}, \tag{2}$$

or in terms of Bessel functions:

$$T(d,\, k\bar{a}) = \left(\frac{k\bar{a}}{2}\right)^{2-d} \frac{\Gamma\left(\frac{d}{2}\right) J_{\frac{d-2}{2}}(k\bar{a})}{\Gamma\left(2-\frac{d}{2}\right) J_{\frac{2-d}{2}}(k\bar{a})}. \tag{3}$$

For reference, when $d = 3$, $T(3,\, k\bar{a}) = \tan(k\bar{a})/k\bar{a}$, which is the s-wave scattering phase shift for a hard sphere with radius $\bar{a}$ in $d = 3$.

In the current study, we explore conditions for bound states in arbitrary dimensions for two cold harmonically trapped atoms interacting via the d-dimensional pseudopotential. In the ultracold limit ($k \to 0$), $T \to 1$ for non-even d and the generalized pseudopotential (equation (1)) simplifies to

$$ {}_{C_0}V^{(d)}_{k\to 0} = \frac{\Omega(d)\bar{a}^{d-2}}{\Gamma(d-2)} \delta^{(d)}(r)\ {}_{C_0}D_r^{d-2} r^{d-2}. \tag{4}$$

We used this generalized pseudopotential as the interaction in the following d-dimensional relative-motion Schrödinger equation for two cold atoms in a harmonic trap:

$$(H^{(d)}_{osc} + {}_{C_0}V^{(d)}_{k\to 0}(r))\Psi(r) = E^{(d)}\Psi(r), \tag{5}$$

where $H^{(d)}_{osc}$ is the d-dimensional harmonic oscillator Hamiltonian. To solve equation (5) in [12], we used a harmonic oscillator basis similar to the approach by Busch *et al* [13], and the solution for the relative-motion energy $E^{(d)}$ takes the form of an implicit equation parameterized by d:

$$\frac{\Gamma\left(-\frac{E^{(d)}}{2} + \frac{d}{4}\right)}{\Gamma\left(-\frac{E^{(d)}}{2} + \frac{4-d}{4}\right)} = \frac{2^{\frac{d-2}{2}}\Gamma^2\left(\frac{d}{2}\right)}{\bar{a}_o^{d-2}} \frac{\sin\left(\frac{\pi}{2}(d-2)\right)}{\frac{\pi}{2}(d-2)}, \tag{6}$$

where $\bar{a}_o$ is the scattering length in relative-motion oscillator units. We modified the sine term in equation (6) from the version found in [12] using the identity $\sin(\frac{\pi}{2}(d-2)) = -\sin\left(\frac{d\pi}{2}\right)$ in order to emphasize the $d \to 2$ limit. The $2^{d/2}$ factor comes from using the relative motion coordinates defined in [13]. They chose values for the center of mass coordinate $\left(\mathbf{R} = \frac{1}{\sqrt{2}}(\mathbf{r}_1 + \mathbf{r}_2)\right)$ and the relative motion coordinate $\left(\mathbf{r} = \frac{1}{\sqrt{2}}(\mathbf{r}_1 - \mathbf{r}_2)\right)$ so that the effective masses of the center-of-mass motion and the relative motion are the same. This choice introduces an unconventional factor of $\frac{1}{\sqrt{2}}$ and so $1/\text{length}^d$ terms lead to $2^{d/2}$ in equation (6).

The paper is organized in the following way to determine conditions for bound states of the trapped pseudopotential in arbitrary dimension. In section 2, we derive an analytical approximation for the bound state energy ($E < 0$) in arbitrary dimension, resulting in equations (10) and (12). In section 3, we calculate $E < 0$ exact numerical solutions of the functional (equation (6)) and compare with the analytical approximation. It is known for $d = 3$ that the pseudopotential supports a single bound state for positive scattering length and no bound state for negative scattering length [7, 13, 14]. We show that bound states can exist in higher dimensions ($d > 3$) for the pseudopotential, but the scattering length would need to be negative when $d = 4n + 1$, $n \geqslant 1$. In section 4, for completeness we derive d-dimensional analytical approximations for positive energies (equations (15) and (23)), which represent harmonic oscillator energies perturbed by the pseudopotential. Finally, we discuss implications and limitations of these results.

2. $\bar{E} \to -\infty$ analytical approximations of equation (6) for pseudopotential bound state energies in a trap

To find an analytical approximation for the bound state energy for two cold trapped atoms with a pseudopotential interaction in d dimensions, we consider the $\bar{E} \to -\infty$ limit in equation (6). We use the known limit of the ratio of gamma functions:

$$\lim_{\nu\to\infty} \frac{\Gamma(\nu+\alpha)}{\Gamma(\nu)\nu^{\alpha}} = 1, \tag{7}$$

where ν is real and α can be complex. We rewrite this as

$$\lim_{\nu\to\infty} \frac{\Gamma(\nu+\alpha)}{\Gamma(\nu)} = \nu^{-\alpha}, \tag{8}$$

and let $\nu = -\bar{E}^{(d)}/2 + d/4$ and $\alpha = 1 - d/2$. In the $\bar{E} \to -\infty$ limit, the ratio of gamma functions in equation (6) becomes

$$\lim_{\bar{E}^{(d)}\to-\infty} \frac{\Gamma\left(-\frac{\bar{E}^{(d)}}{2} + \frac{d}{4}\right)}{\Gamma(-\frac{\bar{E}^{(d)}}{2} + \frac{4-d}{4})} = \left(\frac{-\bar{E}^{(d)}}{2} + \frac{d}{4}\right)^{\frac{d-2}{2}} \to \left(\frac{-\bar{E}^{(d)}}{2}\right)^{\frac{d-2}{2}}, \tag{9}$$

where in the last limit we assume $-\bar{E}^{(d)} \gg d/4$. Substituting this limit in equation (6), the approximate binding energy becomes

$$\bar{E}^{(d)}_{\text{bind}} \approx -\frac{2}{\bar{a}_o^2}\left(2^{\frac{d-2}{2}}\Gamma^2\left(\frac{d}{2}\right)\frac{\sin\left(\frac{\pi}{2}(d-2)\right)}{\frac{\pi}{2}(d-2)}\right)^{\frac{2}{d-2}} \qquad d \neq 2. \tag{10}$$

The $d = 3$ value gives the known $\bar{E}^{(3)}_{\text{bind}} \approx -1/\bar{a}_o^2$. Note that the approximation equation (10) is not valid for odd $d = 4n + 1$ for $\bar{a}_o > 0$ because its corresponding exact equation (Equation (6)) does not have negative energy solutions for these conditions. However, at these dimensions, the negative scattering length with corresponding magnitude does have a binding energy solution to the exact equation (6), and equation (10) would be a valid approximation.

The equation (10) approximate solution has a proper value everywhere except $d = 2$. However, we can find the limit $d \to 2$ by first expanding equation (6) about $d = 2$. To first order in $d - 2$, equation (6) yields

$$\psi\left(\frac{1}{2} - \frac{\bar{E}^{(2)}}{2}\right) = \ln\left(\frac{2}{\bar{a}^2}\right) - 2\gamma, \tag{11}$$

where $\psi(\cdot)$ is the logarithmic derivative of Euler's Γ-function and γ is the Euler-Mascheroni constant. Next, using the known limit $\psi(x) \to \ln(x)$ as $x \to \infty$, the $E \to -\infty$ limit is $\psi\left(\frac{1}{2} - \frac{\bar{E}^{(2)}}{2}\right) \to \ln\left(-\frac{\bar{E}^{(2)}}{2}\right)$ and finally the $d \to 2$ limit of equation (11) is

$$\bar{E}^{(2)}_{\text{bind}} \approx -\frac{4e^{-2\gamma}}{\bar{a}_o^2}. \tag{12}$$

When we let $\bar{a}_o = 1$ in the next section, the value from equation (12) ($\bar{E}^{(2)}_{\text{bind}} = -1.26095$) agrees closely with the value obtained from solving equation (10) with $d = 1.99$ ($\bar{E}^{(1.99)}_{\text{bind}} = -1.26092$).

3. Effect of d on bound state energies for scattering length $\bar{a}_o = 1$

For scattering length $\bar{a}_o = 1$ and real dimensions $d \in (0, 12)$, we compare the exact numerical bound state energy solutions of equation (6) (black circles, figure 1) with the analytical estimates from equation (10) (blue lines, figure 1). Equation (6) also has positive energy solutions, which we discussed and analytically approximated in [12] (also see additional analytical results equations (15) and (23)). The negative energy solutions of equation (6), discussed here, are bound states of the pseudopotential in the presence of the trap. It is known for a positive scattering length that the pseudopotential has a bound state for $d = 3$. There are also bound states for lower dimensions ($d \leqslant 3$), and the minimum energy in the domain $(0, 3]$ occurs at $d = 2$ (figure 1). If we allow d to have arbitrarily large values, there are infinite bound states for $\bar{a}_o > 0$ (figure 1). However, there are also infinite integer dimensions where bound states are forbidden for $\bar{a}_o > 0$ (gray intervals centered at odd $d = 4n + 1, n >= 1$). For $\bar{a}_o > 0$, the sine term in equation (6) causes a sign change when $d = 4n + 1$ ($n >= 1$) so that the equation becomes inconsistent with a negative energy (bound state) solution for these dimensions; however, bound states are supported at these dimensions for $\bar{a}_o < 0$. In other words, bound states oscillate from occurring for positive $\bar{a}_o$ when $d \in \{1, 2, 3, 7, 11, 15, \dots\}$ to occurring for negative $\bar{a}_o$ when $d \in \{5, 9, 13, \dots\}$.

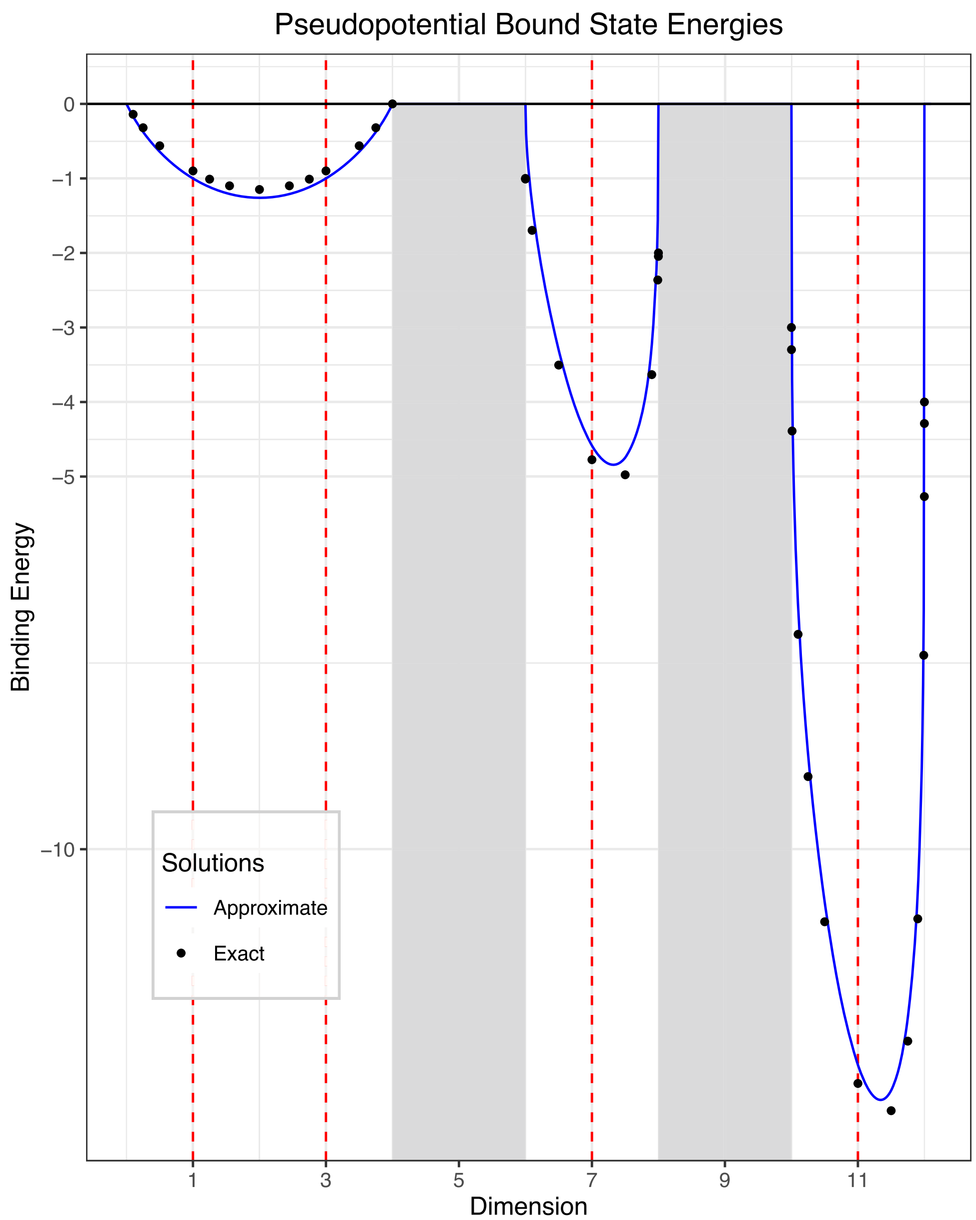

Figure 1. Bound state energies for two cold atoms with pseudopotential interaction and external trap for scattering length $\bar{a}_o = 1$ in oscillator units. Exact numerical solution of equation (6) (black circles) and approximate analytical solution from equation (10) (blue line). For positive scattering length, the exact equation does not have $E < 0$ solutions for dimensions centered on odd $d = 4n + 1$, $n >= 1$ (no bound solutions in the gray intervals $d \in \{(4, 6), (8, 10), (12, 14), \dots\}$). There can be bound state solutions in these intervals if $\bar{a}_o < 0$.

4. Weak interaction analytical approximation for scattering energy (positive energy states) for pseudopotential-perturbed trap in d dimensions

The focus of the current study is bound state energies ($E < 0$). However, for comparison with the analytical bound state energy approximation (equation (10)), we include here the analytical approximation for positive (scattering) energies in the pseudopotential plus trap for all dimensions. These positive energies are harmonic oscillator energies ($2n + d/2$) perturbed by the scattering length from the pseudopotential. In a sense, these are also bound states since the two atoms are confined. In [12], we used a perturbation expansion about $\bar{a}_o$ of equation (6) to obtain a weakly interacting analytical solution for $\bar{E}^{(d)}$ when d is non-even (including non-integer):

$$\bar{E}^{(d\ \text{non-even})}_{\text{trap+pseudo}} \approx 2n + \frac{d}{2} + \frac{2\pi(d-2)}{\sin\left(\frac{d\pi}{2}\right)\Gamma\left(1-\frac{d}{2}\right)\Gamma^3\left(\frac{d}{2}\right)} \frac{\Gamma\left(n+\frac{d}{2}\right)}{\Gamma(n+1)} \bar{a}_o{}^{d-2} \tag{13}$$

Here we resolve the indeterminate form for even d. The denominator of equation (13) contains $\Gamma(1 - d/2)$, which has poles for even d. However, these poles are multiplied by zero limits of $\sin(d\pi/2)$. We can resolve the limit of this product using Euler's reflection formula:

$$\Gamma(z)\Gamma(1 - z) = \frac{\pi}{\sin(\pi z)}. \tag{14}$$

Letting $z = d/2$ gives $\sin\left(\frac{d\pi}{2}\right)\Gamma\left(1 - \frac{d}{2}\right) = \frac{\pi}{\Gamma\left(\frac{d}{2}\right)}$ and then equation (13) can be written as

$$\bar{E}^{(d\neq 2)}_{\text{trap+pseudo}} \approx 2n + \frac{d}{2} + \frac{2(d-2)}{\Gamma^2\left(\frac{d}{2}\right)} \frac{\Gamma\left(n + \frac{d}{2}\right)}{\Gamma(n+1)} \bar{a}_o{}^{d-2} \tag{15}$$

Equation (15) is the preferred approximate formula for positive energy states of the trap plus pseudopotential interaction, but the $d \to 2$ limit is still problematic. Next, we derive a separate analytical approximation for $d \to 2$ similar to our approach in [12] (Appendix H), but here we begin with equation (11) instead of directly from equation (6) and we use $C = \frac{1}{\ln(2/\bar{a}_o^2)}$ as the small perturbation instead of $\bar{a}_o$.

Defining a scaled energy $\epsilon = \frac{1}{2} - \frac{\bar{E}}{2}$, we can rewrite equation (11) as

$$\psi(\epsilon) = 1/C - 2\gamma. \tag{16}$$

To first order in the coupling constant C, we wish to find the perturbation parameters ϵ_o and ϵ_1:

$$\epsilon \approx \epsilon_o + \epsilon_1 C. \tag{17}$$

The zeroth-order perturbation parameter is determined by noting that when $C \to 0$, the solutions of equation (16) are poles of $\psi(\epsilon)$, which are located at negative integers and 0 ($\epsilon = -n$) and, thus, $\epsilon_o = -n$.

We determine the first-order perturbation paraemter by rearranging equation (16) as

$$C = \frac{1}{\psi(\epsilon) + 2\gamma} \tag{18}$$

and then multiplying top and bottom by $\epsilon + n$:

$$C = \frac{1}{(\psi(\epsilon) + 2\gamma)} \frac{(\epsilon + n)}{(\epsilon + n)} \tag{19}$$

From equation (17) and $\epsilon_o = -n$, we can replace the numerator of equation (19) with $\epsilon + n = \epsilon_1 C$:

$$C = \frac{\epsilon_1 C}{(\psi(\epsilon) + 2\gamma)(\epsilon + n)}. \tag{20}$$

Canceling the constants C and rearranging slightly, we have an expression for ϵ_1:

$$\epsilon_1 = [\psi(\epsilon)(\epsilon + n) + 2\gamma(\epsilon + n)]_{\epsilon \to -n}. \tag{21}$$

We are interested in solutions near the unperturbed solution, $\epsilon \to -n$, so the right-most term, $2\gamma(\epsilon + n)$, goes to zero and the term involving ψ can be evaluated by its residual. Since the pole residual of ψ at $-n$ is -1, we have $\lim_{\epsilon \to -n}(\epsilon + n)\psi(\epsilon)$=-1 and equation (21) gives $\epsilon_1 = -1$.

Using our values for the perturbation parameters, equation (17) becomes

$$\epsilon \approx -n - C. \tag{22}$$

Finally, expressing the scaling definition, $\epsilon = \frac{1}{2} - \frac{\bar{E}}{2}$, in terms of the original energy ($\bar{E}$) and using the definition of the coupling constant C and equation (22), the approximate energy for $d = 2$ is

$$\bar{E}^{(d=2)}_{\text{trap+pseudo}} \approx 2n + 1 + \frac{2}{\ln(2/\bar{a}_o^2)}. \tag{23}$$

In summary, equations (15) and (23) provide approximate formulas for positive energy states of the ultra-cold trap perturbed by the pseudopotential interaction for all dimensions.

5. Conclusions

We examined the effect of the spatial dimension d on the existence of bound state energies for two cold atoms in a trap with a pseudopotential interaction parameterized by d. In three dimensions, it is known the pseudopotential supports a bound state for positive scattering length, and we find this also to be the case for $d = 1, 2$ and certain higher odd dimensions, $d = 4n + 3$ ($n = 0, 1, 2, \ldots$). However, for $d = 5$ and higher odd dimensions $d = 4n + 1$ ($n = 1, 2, \ldots$), we find bound state solutions do not exist for positive scattering length, but negative scattering lengths do support bound states. These oscillations of bound state solutions between positive and negative scattering lengths with d is due to a $\sin(d\pi/2)$ term in the energy functional (Equation (6)).

The sine term arises in the derivation (Appendix G of [12]) from an identity for the confluent hypergeometric function U in terms of Kummer's function, M (13.1.2 and 13.1.3 from [15]).

We derived an analytical approximation of equation (6) for the bound state energies of the trapped pseudopotential system (equations (10) and (12), which is in very good agreement with numerical solutions (figure 1). Pseudopotential bound state energies exist for $d = 2$, but for even-$d > 2$, the bound state energy is zero due to the sin term in equation (6). However, there are positive energy perturbed trap solutions of equation (6) for all d, and in the positive-energy analytical approximations (equations (15) and (23)), we show how the sin term cancels with a pole to give a non-zero limit for the energy. Further study is needed to determine whether there are wavevector ($k > 0$) correction terms for even-$d > 2$. The wavevector-dependent scattering phase coefficient (Equation (3)) in the pseudopotential goes to zero for even d because of the poles in $\Gamma(2 - d/2)$. However, there is a wavevector-dependent logarithmic term in the even-d pseudopotential that may contribute to the pseudopotential binding energy [16].

Forbidden quantum bound states or stable classical orbits for $d > 3$ have been used to explain the observed dimensionality of space or to place constraints on the dimensionality of hypothetical universes. Such explanations assume an anthropic principle and that the laws of d-dimensional physics have similar characteristics to $d = 3$. Our analysis is based on a generalization of the Fermi pseudopotential, and we find oscillations from positive to negative scattering lengths that permit bound states as d varies. These oscillations may influence the type of complex chemical systems that can emerge. However, the pseudopotential is a contact potential, and shape dependent effects may be important when extrapolating to complex systems.

One of the oscillations from positive scattering length bound states (e.g., $d = 3$) to negative scattering lengths occurs at $d = 9$, which is a dimension of importance in string theory. To understand the discrepancy between the nine dimensions at the Planck scale and the three dimensions of our experience, there may be mechanisms whereby three of the nine compactified dimensions at the Planck scale expanded in the early universe [17]. The ability to form bound states and complex systems at the microscopic scale at $d = 3$ but not $d = 9$ could contribute to our understanding of these expansion mechanisms. The oscillations that we observe in the bound state energies do not necessarily preclude the evolution of complex systems at other dimensions, but such systems may have different characteristics.

Data availability statement

No new data were created or analysed in this study.

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