Two Particles in a Trap

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Abstract

The Busch-formula relates the energy-spectrum of two point-like particles interacting in a 3-D isotropic Harmonic Oscillator trap to the free scattering phase-shifts of the particles. This formula is used to find an expression for the shift in the spectrum from the unperturbed (non-interacting) spectrum rather than the spectrum itself. This shift is shown to be approximately \( \Delta = -\delta(k)/\pi \times dE \), where \( dE \) is the spacing between unperturbed energy levels. The resulting difference from the Busch-formula is typically \( < \frac{1}{2} \% \) except for the lowest energy-state and small scattering length when it is \( 3\% \). It goes to zero when the scattering length \( \rightarrow \pm \infty \).

The energy shift \( \Delta \) is familiar from a related problem, that of two particles in a spherical infinite square-well trap of radius \( R \) in the limit \( R \rightarrow \infty \). The approximation is however as large as \( 30\% \) for finite values of \( R \), a situation quite different from the Harmonic Oscillator case.

The square-well results for \( R \rightarrow \infty \) led to the use of in-medium (effective) interactions in nuclear matter calculations that were \( \infty \Delta \) and known as the phase shift approximation. Our results indicate that the validity of this approximation depends on the trap itself, a problem already discussed by DeWitt more than 50 years ago for a cubical vs spherical trap.

1 Introduction

In some of his early attempts of developing a many-body theory of nuclei, Brueckner assumed the in-medium (effective) two-body interaction to be \( \propto \tan \delta(k) \), \( \delta(k) \) being the scattering phase-shift as a function of relative momentum \( k \). The initial problem studied was that of an 'infinite' system of nuclear matter for the purpose of calculating binding energy and saturation properties. The \( \tan \delta(k) \) approximation came from the assumption that the Reactance matrix, a part of scattering theory, could be used as an in-medium interaction in the many-body problem. (The diagonal part of this matrix is \( \propto \tan \delta(k) \)). This implies that a principal value Green’s function with an integration over a semi-continuous spectrum would be justified in this case with the box of nuclear matter assumed to be very and even 'infinitely' large. This assumption was substantiated in a paper by Reifman and DeWitt\(^1\). It was however soon realised to be incorrect. Several authors (one of them DeWitt) showed that the correct limit for two particles in a big box would yield an in-medium interaction \( \propto \delta(k) \) rather than \( \tan \delta(k) \).\(^2\)\(^3\)\(^4\)\(^5\) The Reactance matrix is part of scattering theory. The nuclear matter problem assumes a box, although large but still finite with boundary conditions different from that of scattering theory. A particle in this box has a discrete rather than a continuous spectrum and that makes a difference.

The proofs in the referred papers differ but the essential point is that the integration over the continuous spectrum vs the summation over the discrete spectrum differs even though the level-density in a big box goes to zero as the box-size increases. The principal value integration relates to the scattering problem with boundary conditions different from that for a box where the wave-functions are zero at the edge of the box even in the limit of 'infinitely' large.

The exact statement of the results in the referenced papers is that the energy-shift \( \Delta \) due to the interaction of two-particles confined in a spherical box in the limit when the size of the box approaches infinity is given by \( \Delta = S \times dE \) where \( dE \) is the spacing between the levels of the unperturbed spectrum and \( ^6 \)

\[
\Delta = S \times dE
\]

In nuclear matter studies this has been referred to as the ‘phase-shift approximation’ a term adopted here. It was for example used in early calculations on the neutron-gas\(^5\)\(^6\) and used as a first approximation for nuclear matter studies.\(^7\)

The question of the author arose whether the result above might be more general. The problem of two particles trapped in a potential well is of interest for atomic as well as nuclear physics studies. The Busch-formula\(^8\) relates the energy-spectra of the two particles in a Harmonic Oscillator well to the scattering phase-shifts for point-like potentials. This formula is here rewritten in terms of the energy-shifts rather than energy.

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1 e-mail: kohlers@u.arizona.edu
2 For small \( \delta \) e.g. at low density this might not make any difference but for problems of interest to-day with \( \delta \approx \pi/2 \) it obviously would.
3 It was pointed out by DeWitt\(^3\), after a comment by Brueckner that the result may be different for a box other than spherical.
Results below show that the phase-shift approximation for these shifts is (surprisingly) in practically exact agreement with the Busch-formula. The largest difference is found for the lowest energy-state \((n = 0)\) and small scattering length but it decreases rapidly for \(n > 0\) and larger scattering lengths. For comparison are also shown results for the spherical infinite square well as a function of the radius of the sphere. Although the approximation becomes exact in the limit \(R \to \infty\), it is in general much worse in this case than for the H.O.

## 2 3-D Harmonic Oscillator Well

With the energy in units of \(\hbar \omega\) the total energy for two non-interacting particles with zero angular momentum in a 3-D Harmonic Oscillator well is

\[
E_{\text{tot}} = E + E_{\text{cm}} = 2n + 3
\]

where \(E_{\text{cm}} = \frac{3}{2}\) is the center-of-mass energy. It is convenient to choose

\[
a_{\text{osc}} = \sqrt{\frac{\hbar}{m\omega}}
\]

as the unit of length. With \(\eta = 2E\) the Busch-formula reads\(^9\)

\[
\tan \delta(k) = -\frac{\sqrt{\eta\Gamma[(1 - \eta)/4]}}{2\Gamma[(3 - \eta)/4]} \tag{2}
\]

where \(k = \sqrt{\eta}/a_{\text{osc}}\).

The level-spacing in the uncorrelated system is \(dE = 2\) and following the notation above one finds the level-shift to be \(\Delta = 2S\). In the case of the spherical box above \(S\) is given by eq. \(1\). It is the purpose of the present work to find \(S\) for the 3-D H.O. with the Busch spectrum. One finds

\[
\eta = 4n + 3 + 4S
\]

Using the reflection formula for \(\Gamma\)-functions

\[
\Gamma(1 - x) = \frac{\pi}{\Gamma(x)\sin(\pi x)} \tag{3}
\]

one finds

\[
\tan \delta(k) = -A(z) \tan(S\pi) \tag{4}
\]

where

\[
A(z) = \frac{\sqrt{z - \frac{1}{4}}\Gamma(z)}{\Gamma(z + \frac{1}{2})} \tag{5}
\]

with \(z = n + S + 1\).

The beta-function \(B(x, y)\) is defined by

\[
B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x + y)} \tag{6}
\]

and for \(y\) fixed and \(x\) large one has\(^3\)

\[
B(x, y) \approx \Gamma(y)x^{-y} \tag{7}
\]

so that for \(z\) large one would have

\[
\frac{\Gamma(z + \frac{1}{2})}{\Gamma(z)} \approx \sqrt{z}
\]

but in eq. \(5\) one has the factor

\[
\sqrt{z - \frac{1}{4}}
\]

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\(^4\) I owe my thanks to Dr Jerry Yang for showing me this relation on Wikipedia
Numerical tests show that a better approximation indeed is
\[ \frac{\Gamma(z + \frac{1}{2})}{\Gamma(z)} \approx \sqrt{z - \frac{1}{4}} \]

One finds that the values of \( z \) that is needed in the Busch-formula is \( z \geq \frac{1}{2} \) and Fig. 1 shows the function \( A(z) \) for a useful range of \( z \).

One finds \( A \to 1 \) quite rapidly with \( z \) (and consequently with \( n \)) so that in this limit eq. (4) yields
\[ S \to -\frac{\delta(k)}{\pi} \]
which is the phase-shift approximation given in eq. (1).

A correction \( dS \) to \( S \) due to \( A(z) \neq 1 \) is obtained from
\[ dS \approx -\frac{1}{\pi}(1 - A^{-1}(z)) \frac{\tan \delta(k)}{1 + \tan^2 \delta(k)} \]  
(9)

This shows a dampening of the correction with increasing value of \( \tan^2 \delta \). In the limit when \( \delta = \frac{\pi}{2} \) the correction goes to zero. The energy-shift is then exactly given by \( \frac{1}{\pi^2} = \frac{1}{4} \), a well-known result. Fig. 2 shows the difference between the energy shifts calculated by the Busch-formula and the phase-shift-approximation for quantum levels \( n = 0, 1 \) and 2 as a function of scattering length. It is seen to decrease rapidly with \( n \) and also with \( \pm a \). The peaks are a result of the competition between the \( A(z) \) and \( \tan \delta \) corrections respectively shown in eq. (9). Fig. 3 shows the same differences but in % of the Busch result for \( n = 1, 2, 3 \) again showing the rapid decrease with increasing values of \( n \) and with \( \pm a \).

### 3 Spherical Square Well

The problem of two particles in a spherical box was treated by several authors referred to in the Introduction. In these several works the emphasis was on the energy-shift in the limit of the radius of the sphere going to 'infinity' with the result given by eq. (1), the phase-shift approximation. For comparison with the 3-D H.O. it
Figure 2: The difference between the energy-shifts calculated with the Busch-formula and that obtained in the phase-shift approximation for $n = 0, 1, 2$. The largest difference is as expected for $n = 0$ (red on-line), while it is appreciably smaller for $n = 1$ (green on-line) and $n = 2$ (blue on-line). The smallest value of $z$ in the function $A(z)$ is $\frac{1}{2}$ (see Fig. 1), which occurs for $n = 0$ and $\delta = -\frac{\pi}{2}$. The largest difference shown is consequently for this value of $n$ and for $a < 0$ where the shift is negative.

Figure 3: Similar to Fig. 2 but the difference is here shown as the percentage of the energy-shift. The maximum difference is $\approx -3\%$ (for $n = 0$, red on-line) but a rapid decrease with increasing $n$ is seen and is less than $\frac{1}{2}\%$ for $n = 1$ (green on-line) and even smaller for $n = 2$ (blue on-line).
is of interest to also display the shift as a function of the ratio of scattering length to radius and as a function of quantum-numbers $n$ of the spherical box.

The simplest solution [2, 10] of the problem at hand is to explicitly consider the wave-functions of the two particles in this box. Considering only $s$-states the radial wavefunctions of free non-interacting particles are

$$
\Psi(r) \propto \frac{1}{r} \sin(k^{(0)}r) \tag{10}
$$

With two-body interaction the wave-function outside the range of the two-body interaction is

$$
\Psi(r) \propto \frac{1}{r} \sin(kr + \delta(k)) \tag{11}
$$

The boundary condition implies that the wave-functions vanish at the boundary of the sphere assumed to have a radius $R$. (One immediately sees the simplicity of the formalism relative to that of the 3-D H.O. or a cubical box.) Thus, for the non-interacting case

$$
k^{(0)}_n R = n\pi \tag{12}
$$

and for the interacting case

$$
k_n R + \delta(k_n) = n\pi \tag{13}
$$

The spacing between unperturbed levels is

$$
dE = k^{(0)}_{n+1}^2 - k^{(0)}_n^2 = (k^{(0)}_{n+1} + k^{(0)}_n) \left( \frac{\pi}{R} \right) \tag{14}
$$

The energy shift

$$
\Delta = k^2 - k^{(0)}_n^2 = -(k_n + k^{(0)}_n) \left( \frac{\delta(k_n)}{R} \right) \tag{15}
$$

divided by the unperturbed energyspacing, i.e. $S$, is then

$$
S = \frac{k_n + k^{(0)}_n}{k^{(0)}_{n+1} + k^{(0)}_n} \left( \frac{\delta(k_n)}{\pi} \right) \tag{16}
$$

The energy-shifts and -spacings decrease with $R$ and $n \to \infty$ and then

$$
S \to -\frac{\delta(k_n)}{\pi} \tag{17}
$$

as before.

The phase-shift approximation was tested for convergence as a function of box radius $R$ and quantum number $n$. For this purpose the expression for $S$ was rewritten as follows

$$
S = \frac{1}{\pi} \left( \frac{\delta(k_n) - 2n\pi}{2n} \right) \frac{\delta(k_n)}{\pi} \tag{18}
$$

The radius $R$ only appears implicitly through the relation

$$
k_n = (n\pi - \delta(k_n))/R \tag{19}
$$

to be solved selfconsistently.

In the (unphysical) case that $\delta$ would be independent of $k$ one would have the situation where $S$ is independent of $R$, but only of $n$ and of course of $\delta$.

Fig. 4 shows the difference between the ‘exact’ shift and the phase-shift approximation $-\frac{\delta}{\pi}$ of eq. (11), while Fig. 5 shows the difference in % of the exact shift.

Compared with the analogous result for the H.O. there are notable differences. While the largest deviation from the phase-shift approximation is 3% (and typically much smaller) in the H.O. case, it can for the sphere be even as large as 30%. But even though the deviation from the phase-shift approximation in the H.O. is small it has its maximum for large values of $a_{osc}$ (or small scattering lengths) while going to zero for small values (or large scattering lengths), which is opposite to the situation encountered for the spherical well. Both Figs. 4 and 5 illustrate however the known result that $S \to -\frac{\delta(k)}{\pi}$ as $R \to \infty$ as shown in previous works already referred to above [2, 3, 4].
Figure 4: The difference between the exact and phase-shift approximation for two-particles in the spherical trap for three values of the quantum-number $n = 1$, (red on-line), $n = 2$ (green on-line) and $n = 3$ (blue on-line). Notice the difference with the similar plot in Fig. 2 for the H.O. trap.

Figure 5: Similar to Fig. 4 but the difference is shown as percentage of the energy-shift.
The phase-shift approximation $-\frac{1}{2}\delta(k)dE$ for the energy-shift due to the interaction of two particles in a trap, where $\delta(k)$ is the free particle scattering phase-shift and $dE$ the energy-level spacing of the unperturbed spectrum, has been investigated.

The traps considered were a 3-D Harmonic Oscillator and a spherical infinite square well. The square-well case was treated a long time ago as referenced above, with the main emphasis on the large size limit of the trap with the result expressed by eq. (1). Somewhat of a surprise was the finding of the present investigation that a not only somewhat similar situation exists for the H.O. trap but that the approximation is so much more accurate for this trap.

The differences between the results for the two respective traps are seen by comparing Figs. 2 and 3 for the H.O. trap with the Figs. 4 and 5 for the square-well trap. While in the square well case, the differences (errors) by using the phase-shift approximation are as large as 30%, the differences are much smaller and even practically zero in the H.O. case. With $a \to \pm \infty$ the phase-shift approximation becomes exact in the H.O. case while in the spherical case the error increases. While Figs 4 and 5 show that the approximation becomes perfect when $a/R$ goes to zero (or the radius of the square well goes to $\infty$) that is when (unexpectedly) the largest correction, although still small, is found in the H.O. case.

In all the work above like in the Busch-formula, it is assumed that the range of the potential is small compared to the size of the trap. Considerations of range corrections are beyond the scope of this investigation. It has been the subject of a recent publication.[11]

The question arises of course whether the phase-shift approximation has a more general validity e.g. for the shifts in a cubical box, as derived by Lüscher.[12] It is however already seen that the situation is rather different in the 3-D H.O. case compared to the case of a spherical well. The conceptual differences between scatterings and interactions in the spherical vs cubical box was already pointed out by DeWitt in a detailed discussion of this matter.[3] [5]

References

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*Quote: Only the spherical box (with spherical waves) is suitable for establishing a connection between single scattering processes and discrete spectrum theory....*