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Analysis of the quasi exact solvable Rydberg dressed atoms interaction model

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Abstract

The exact solvable model of the Rydberg dressed interaction for two particles proposed by Kościk et al. is analyzed in the different dimensions to single out the impact of the dimensionality. First we analyze the effect on the energy spectrum then spatial correlations are studied as the radial density distribution versus the position in the three dimensionalities. The results clarify the effect of the centrifugal forces in the presence of long range interaction.

Keywords: long range interaction, cold atoms, confined atoms, quasi solvable models.

1. Introduction

Experiments involving confined cold few particles are nowadays a matter of routine. In fact number of systems parameters as the confinement potential and the particle-particule interaction features can be controlled on demand [1] [2]. This way, it is possible to verify experimentally the validity of a number of quantum simplified models studied by the past. It is however also true that more efforts are necessary in order to devise new “toy” models aiming at a detailed comprehension of the features of the interaction at different level of approximation as well as different dimensionalities.

Exact solution for the Schrodinger equation established for the case of different and sometimes complicated potentials can be found in the literature (see for example [3]). Most of these solutions are given for the case of single particle systems. The situation becomes quite complicated when considering the case of two particles as a first step on the path towards cold confined mesoscopic systems. The difficulty resides in the consideration of both confinement potential characteristics as well as realistic interaction between particles. The hard core interaction is the most simplified scheme of interaction and in this case it is possible to achieve exact solution for two particles systems by implementing the Bethe ansatz[4]. A theoretical work encompassing the three dimensionalities and a delta like interaction for a system of two particles was elaborated by Bush et al.[5]. A quasi exact solution is hence established where the interaction could be considered to be of contact nature (an s-wave for bosons and p-wave for fermions). This interaction model however ignores the long range nature of interaction for dipolar atoms or Rydberg dressed interaction behaving as $1/r^6$[6]. An analytical solution for this interaction is still to be elaborated. Nevertheless a simplification of this interaction as a step function was proposed by Kościk et al[7]. It was possible in this case to reach a quasi exact solution in one and two dimensions and a study of the different features of the system was elaborated. This kind of quasi solvable models are of extreme importance for advances in cold confined few particles systems. It can be considered as a set of models to be validated experimentally as well as an exact basis to construct the solution for few body systems exploiting different strategies (as variational, ab initio, interacting configurations..) The aim of our present study is to elaborate a comparative analysis of the quasi exact solvable model of Kościk et al. in the three dimensionalities and highlight the most important players for the considered interaction.

2. Theoretical approach

The aim of the different models is to establish an analytical solution for the following Schrodinger equation for a system of two particles having the same mass m:

$$\sum_{i=1}^{2}\frac{-\hbar^2}{2m}\nabla_i^2+\left(V_{ext}+v_{inter}\right)\psi\left(\vec{r}_1,\vec{r}_2\right)=E\psi\left(\vec{r}_1,\vec{r}_2\right) \tag{1}$$

Where V_{ext} is the confining potential, v_{inter} is the interaction potential depending on the particles separation and r_i is the vector position for each particle. The confining potential is considered to be harmonic and the dimensions considered in the harmonic oscillator will define the constraint on the motion of the particles and consequently will define the dimensionality of the problem. The same confining potential is imposed to both particles and the equation becomes:

$$\left(\sum_{i=1}^{2}\left(\frac{-\hbar^2}{2m}\nabla_i^2+\frac{1}{2}m\omega^2 r_i^2\right)+v_{inter}\left(\left|r_1-r_2\right|\right)\right)\psi\left(\vec{r}_1,\vec{r}_2\right)=E\psi\left(\vec{r}_1,\vec{r}_2\right) \tag{2}$$

For this quadratic potential it is possible to single out the center of mass contribution to the motion from the radial one and we can write the equation as:

$$\left(\frac{-\hbar^2}{2M}\nabla_{\vec{R}}^2+\frac{1}{2}M\omega^2R^2+\frac{-\hbar^2}{2\mu}\nabla_{\vec{r}}^2+\frac{1}{2}\mu\omega^2r^2+v(r)-E\right)\psi\left(\vec{R},\vec{r}\right)=0 \quad (3)$$

where $M=2m$, $\mu=m/2$, $\vec{R}=(\vec{r}_1+\vec{r}_2)/2$ and $\vec{r}=\vec{r}_1-\vec{r}_2$

The wave function can be written in a separable form as:

$$\psi\left(\vec{R},\vec{r}\right)=\varphi\left(\vec{R}\right)\ \phi(\vec{r}) \quad (4)$$

Consequently we can separate the center of mass and the relative motion equations as:

$$\left(\frac{-\hbar^2}{2M}\nabla_{\vec{R}}^2+\frac{1}{2}M\omega^2R^2-E_c\right)\varphi\left(\vec{R}\right)=0 \quad (5)$$

and

$$\left(\frac{-\hbar^2}{2\mu}\nabla_{\vec{r}}^2+\frac{1}{2}\mu\omega^2r^2+v(r)-E_r\right)\ \phi(\vec{r})=0 \quad (6)$$

with $E=E_c+E_r$. .

The first equation is just an equation for a harmonic oscillator with known solutions and the difficulty resides in finding a solution for the second equation where handling a realistic interaction can be quite challenging.

In one dimension (say for example $x=x_1$-x_2) the relative equation reduces to :

$$\left(\frac{-d^2}{dx^2}+\frac{1}{4}x^2+v(x)-E_r\right)\ \phi(x)=0 \quad (7)$$

Here the equation is written such as the energy and the position are expressed in $\hbar\omega$ and $\sqrt{\frac{\hbar}{m\omega}}$ units respectively.

For two dimensions we convert to polar coordinate $\vec{r}\rightarrow(r,\varphi)$ and with writing the relative wave function as:

$$\phi(r,\varphi)=\frac{1}{\sqrt{r}}\ f(r)e^{\pm i\varphi} \quad (8)$$

The equation for the radial part becomes:

$$\left(\frac{-d^2}{dr^2}+\frac{l^2-1/4}{r^2}+\frac{r^2}{4}+v(r)-E_r\right)f(r)=0 \quad (9)$$

Where l is the angular momentum quantum number and it is expressed in $\sqrt{\hbar m\omega}$ units.

For three dimensions we use spherical coordinates $\vec{r}\rightarrow(r,\theta,\varphi)$ the relative wave function is written as:

$$\phi(r,\theta,\varphi)=\frac{1}{r}f(r)y_l^m(\theta,\varphi) \tag{10}$$

and the equation for the radial part is then given as :

$$\left(\frac{-d^2}{dr^2}+\frac{l(l+1)}{r^2}+\frac{r^2}{4}+v(r)-E_r\right)f(r)=0 \tag{11}$$

Solving these different equations ((7),(9) and(11)) will rely on the form considered for the interaction potential. As matter of fact different forms of the interaction are studied in the literature starting from the hard core potential or impenetrable hard sphere defined as :

$$\begin{cases} v(r)=\infty \quad for \quad 0\le r\le r_0 \\ v(r)=0 \quad \text{elsewhere} \end{cases} \tag{12}$$

r_0 is the radius of the sphere and the Schrodinger equation is solved by considering that the wave function is exactly zero inside the sphere.

The potential is also considered to be of a contact nature and in this case it is given as delta function as:

$$\begin{cases} v(x)=g\delta(x-x_0) \quad for \quad \text{1 dimension} \\ v(r)=g\frac{\partial}{\partial r}r\delta(r-r_0) \ for \quad \text{2 and 3 dimensions} \end{cases} \tag{13}$$

Where g is the strength of the interaction.

We notice that the delta function must be regularized in order to avoid singularity in two and three dimensions[5]. Taking this into account it was possible to solve quasi exactly the problem for the three dimensions.

In order to consider the long range nature of the interaction otherwise the dipolar interaction between two non symmetric neutral charged atoms we should consider a short ranged part of the interaction to which we add a van der waal long ranged interaction. In this case the interaction potential can be given as:

$$v(r)=\frac{g}{1+(r/R_c)^6} \tag{14}$$

Where g gives the strength and R_c is the range of the potential respectively.

It is not possible yet to find an exact solution to the equations (7) (9) (11) with this realistic interaction but a quasi exact solution was achieved for a potential defined as a step function that mimics the previous expression quite fairly for the short range part and then falls abruptly to zero otherwise and is given as:

$$\begin{cases} v(r) = V_0 & \text{for} \quad 0 \le r \le a \\ v(r) = 0 & \text{elsewhere} \end{cases} \tag{15}$$

Where we can relate V_0 and a to the strength and the range (g and R_C) respectively.
In this case it is possible to establish a quasi exact solution by reducing the radial equation to a Weber form in the case of one dimension and a Kummer form for two and three dimensions and the solution is expressed as function of the confluent hypergeometric function of the first kind *1F1* in the region [0,a] and as function of the Tricomi function *U* elsewhere. In order to guarantee a physical behavior of the whole solution a condition for the continuity of the two functions and their derivative is imposed at $x=a$ and henceforth this gives rise to the quantification of the energy which allows to retrieve the energy spectrum with different combination of strength V_0 and the range a[7]. 0

3. Energy spectrum and impact of the dimensionality

In order to study the effect of the interaction strength and its range, we have elaborated programs in C language for the three dimensionalities. The continuity equation is resolved in order to find the eigen energy for different couple(V_0,a). The wave function is then used to calculate the probability density and other related quantities. We follow the prescription given in[7] to extend the results already known for one and two dimension to three dimensions. Let us now show some of the results we can achieve by exploiting the solutions provided by the previous model bearing in mind that the comparison is made relative to $V_0=0$ where we retrieve the simple equidistant spectrum for a harmonic oscillator. First we can show the effect of the different values of the couple (V_0,a) on the energy spectrum. On figure 1 we are depicting the energy of the fundamental level n=0 with different value of the angular momentum quantum number l=0,1,2,3 and 4. The energy is plotted versus V_0 and the different panels are for different ranges of the interaction. We can see on this figure that levels with increasing value of *l* are affected by the interaction as its range is increased and that the most important impact is observed when the interaction is attractive (V_0 negative). In this case the eigen energy is as negative as the interaction is attractive forcing the system to be in a bound state. When redoing the same figure for n=1 one can see that the energy levels are less affected by the interaction and we have to reach a range as high as 1.25 to obtain a noticeable change for the attractive part of the interaction.
These findings show the effect of the centrifugal force which scales as the square of the angular moment and acts in a way to repel the system at a separation where it does not feel the effect of the interaction. These results are to be contrasted with the case of one dimension in figure 3 where we can see that the absence of an angular momentum makes that

all the curves are more or less equally affected by the attractive interaction depending only on the range of the interaction and the energy level location; and that when the interaction is extremely repulsive the bosons and fermions tend to the same limit. This is related to the Tonk Girardeau limit [8] where the bosons proprieties are similar to the ones for a non interacting fermions (except for the impulsion distribution). It is interesting to notice the decrease of the gap between the first curve l=0 and the curve for l=1 in the extreme repulsion for important ranges in two dimensions, making these two level tending towards being degenerate. This result shows that in this regime the repulsion is able to overcome the amount of the centrifugal potential equivalent to $l=1$ corresponding to the next fermionic level. When comparing the results obtained for two dimensions and three dimensions we can notice the regularity with which the levels react to the interaction whether in the fundamental principal states ($n=0$) fig. 4 or the first principal excited states ($n=1$) fig.5, the three dimension being always higher in energy as the centrifugal potential is naturally higher in this case (l_{2d} corresponds to $l_{3d}+1/2$ for the caluculations). We can notice also the same tendency to "degeneracy" for the three first levels (l=0,1,2). The *m* quantum number (projection of *l*) is not relevant for the case of 3 dimensions since the energy is only dependent on (*n*,*l*).

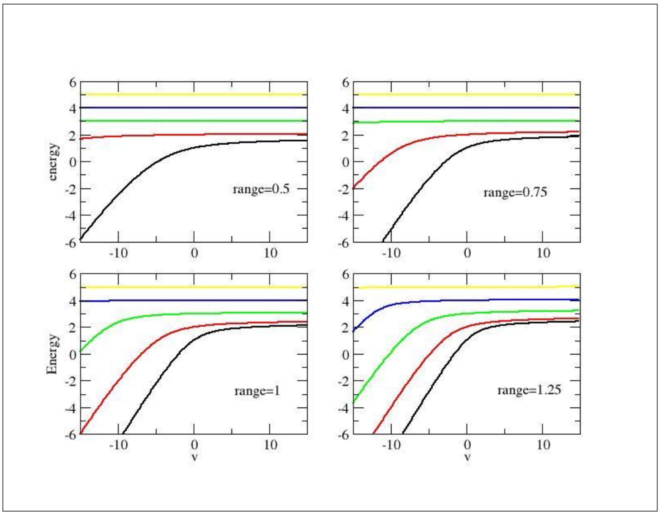

Fig.1. Energy spectrum for the fundamental radial state with increasing value of the angular momentum quantum number (l=0,1,2,3,4 increasingly) in two dimensions. The even value of *l* are for bosons and odd value are for fermions.

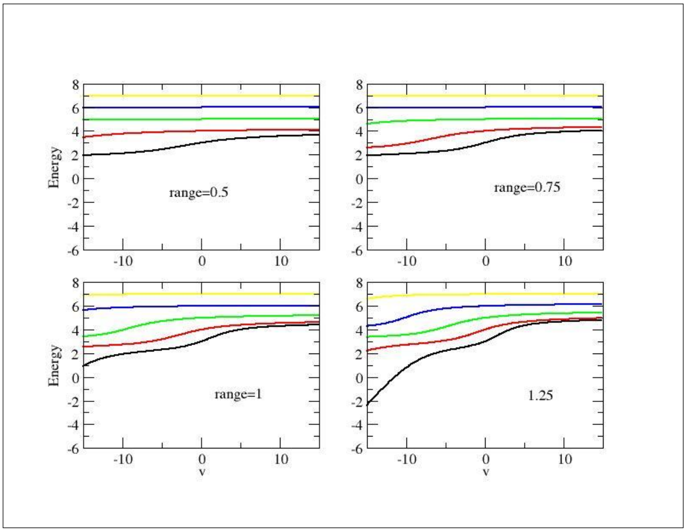

Fig.2. Energy spectrum for the first relative excited state with increasing value of the angular momentum quantum number (l=0,1,2,3,4 increasingly) in two dimensions. The even value of *l* are for bosons and odd value are for fermions.

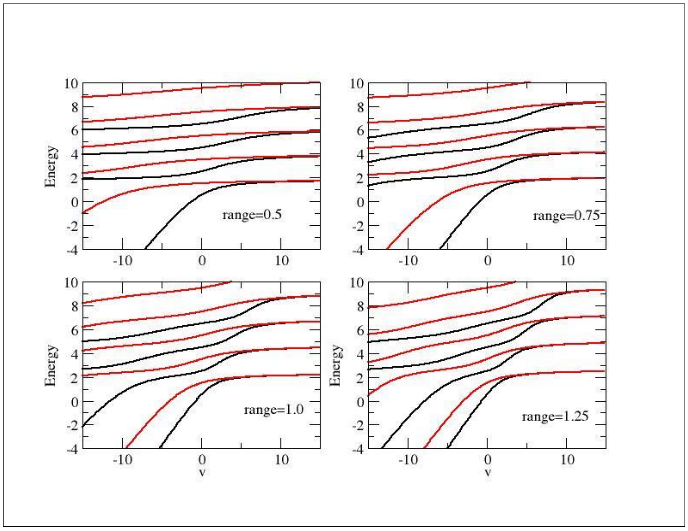

Fig.3. Energy spectrum for the fundamental relative state with increasing value of *n* with even value (black curve) for bosons and odd value(red curve) for fermions in one dimension.

4. Spatial Correlations

Exploiting the wave function derived from the previous calculations it is possible to deduce the probability density distribution as a tool to investigate the possible spatial correlations. In figure 6 we are plotting the radial probability density versus the position *r* for different value of the interaction strength V_0 for a fixed range a=1 and the three figures in one panel are for the three dimensionalities. We want to compare the different dimensionalities for increasing energy states.

In figure 6 the comparison is established for $n=0$ and $l=0$ where the value of l is not degenerate in two and three dimensions and consequently the angular distribution is isotropic . For one dimension we are considering the state with n=0. These states are of bosonic nature (the total wave function is symmetric) which explains the possibility of the two particles to be simultaneously in the same position $r=0$ (center of the trap) for one, two and three dimensions where the distributions are quite similar (notice that the 1d results are renormalized to take account of the conversion to polar coordinates). It is interesting to notice that the probability saturates nearly towards the same limit where the repulsion due to the interaction (which is the same in the three cases) is the most dominant player in this regime.

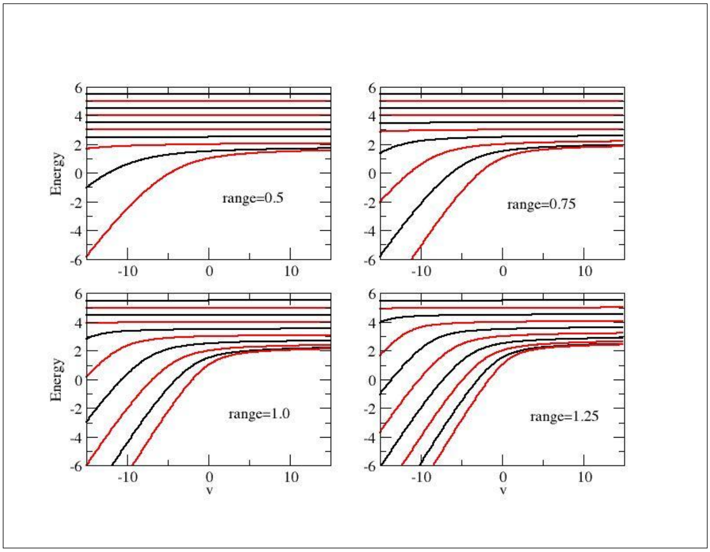

Fig.4. Energy spectrum for the fundamental state (n=0) with increasing value of the angular momentum quantum number (l=0,1,2,3,4) in three (black) and two dimensions (red)

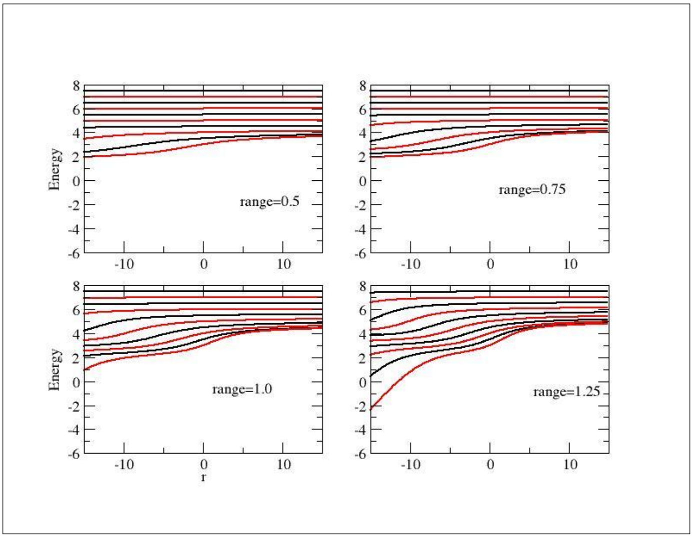

Fig.5. Energy spectrum for the first excited state (n=1) with increasing value of the angular momentum quantum number (l=0,1,2,3,4) in three (black)and two dimensions (red)

We looked also to the radial distribution for higher energy states. We can see on figure 7 the distribution for *n=0* and *l=1* in two and three dimensions and the one for n=1 in one dimension. These distributions are of fermionic nature as the total function is antisymmetric in these cases. It is noticeable on these figures that though the distribution is completely suppressed in the trap center because of the Pauli exclusion principle, the suppression is higher in the case of 3d and 2d because of the centrifugal force. We can also notice that the curves in the attractive part are shifted towards the trap center and that the curve for the repulsive interaction are more repelled from the center as the interaction is acting in the absence of centrifugal potential. The effect of the centrifugal forces increases gradually from two then to three dimensions. For the states n=0 and l=2 in three and two dimensions and n=2 in one dimensions (bosonic states) we have two nodes for the case of one dimension; this makes the comparison less obvious. However it is important to report in this energy regime that at the same time where the distribution is completely suppressed in the center of the trap for three and two dimensions, the two particles are still likely to be found in the center of the trap for one dimension even for the very repulsive interaction (fig.8).

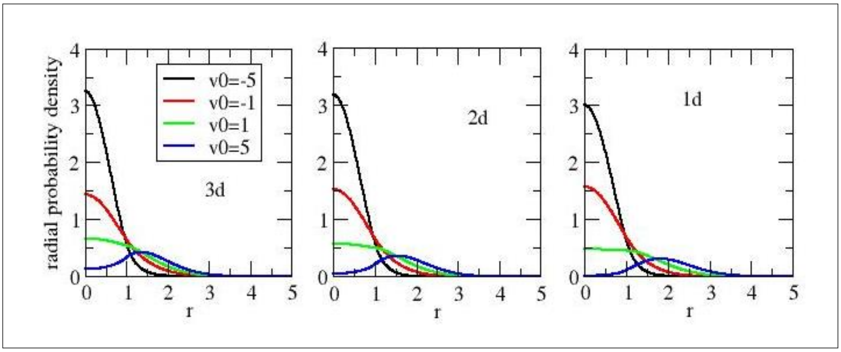

Fig.6. comparison of the ground state normalized radial distribution for (l=0, n=0) in three dimensions, two dimensions and (n=0) for one dimension

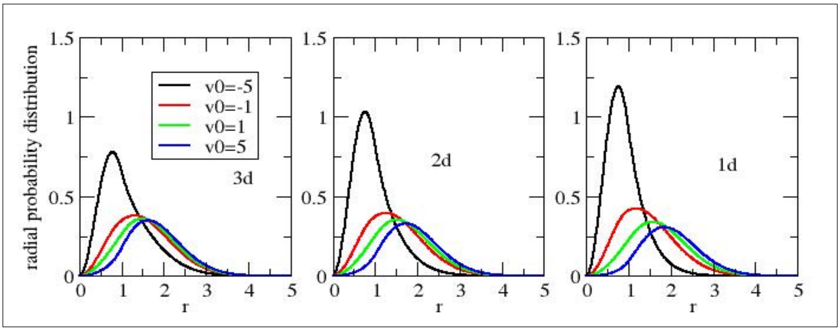

Fig.7. comparison of the normalized radial probability distribution for the states (l=1, n=0) in the three dimensions, two dimensions and (n=1) for one dimension

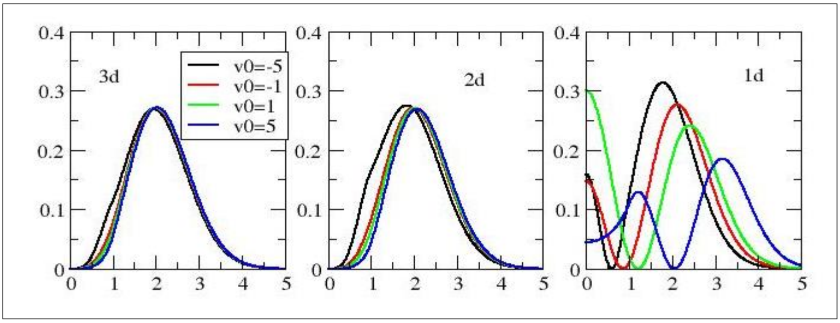

Fig.8. comparison of the normalized radial probability distribution for the states (l=2, n=0) in the three dimensions, two dimensions and (n=2) for one dimension.

5. Conclusion

It was possible by extending the results already established for a simplified step like potential to three dimensions to elaborate a comparative study for the three dimensionalities. This study aimed at singling out the effect of the different dimensionalities in the presence a long ranged interaction for

two particles confined in a harmonic potential. The study shows clearly that the effect is globally related to the centrifugal forces which are in turn dependent on the angular momentum. The effect is more pronounced in three dimensions because of the natural momentum excess from one end and is totally absent in one dimension in the other end. This contribution is a try to comprehend the details of the correlation for bosonic and fermionic systems and shed light on the major players for different energies and interaction regimes. This paper for preliminary results was written in a very compact form, more details and results are to be worked out in a coming publication.

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