Abstract

Regularization scheme dependence of the behavior of wavefunction in the presence of a delta potential is explored in this project by using regularised version of delta function of the form $\delta = v_0 exp(-\lambda\rho^2)$. The project analyzes a non-relativistic system involving two identical particles interacting with a delta potential. The energy eigen function of this system, expressed in spherical coordinates , consists of a radial part $R(r)$ that satisfies a differential equation subject to a delta potential. Numerical simulations for this system were performed using the Numerov method, the main objectives included determining binding energies, verifying the renormalization condition by finding renormalization parameter BE, and analyzing the convergence point (ρ_c), where the numerical solution converges with the $exp(-\gamma * \epsilon_b\rho)$, which is the Analytical solution for $\rho \to \infty$ (universal behavior). This is done initially for regularization parameters $v_0 = 974.443Mev, \lambda = 8fm^{-2}$ and this analysis is extende to various pairs of (v_0, λ). The convergence point ρ_c is identified for each regularization. Results highlight the sensitivity of the wavefunction's behavior to regularization schemes, depicted through graphs, offering insights into the quantum mechanical systems with zero -range potentials.

1 Introduction

Delta potentials and delta functions play an important role in Quantum physics and related areas serving as initial approximations for modeling systems such as quantum wells and nuclear interactions. This project considers a non-relativistic, 3-d system of 2-identical (bosons) interacting with delta potential and explores regularisations of the form $\delta = v_0 exp(-\lambda\rho^2)$.

Regularization of delta functions is a technique used to handle the issue of infinities that arise in the calculation of physical quantities due to the mathematical nature of delta functions. One way of regularization involves modifying the delta function in a way that removes these infinities while preserving the physical properties of the system. This is the approach that is adopted in this project.

Numerov's method is a standard numerical technique that is used to find the solution to a DE and it leverages on numerical integration and the condition of continuity and differentiability of the solution.

2 Defining the system

A non-relativistic, 3-d system of 2-identical particles of mass m_0 interacting with contact potential is considered. Eigenvalue equation for this system in relative coordinates $\bar{r} = \bar{r_1} - \bar{r_2}$ with reduced mass $m = \frac{m_0}{2}$ is given by equation(1).

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\bar{r}) + V(\bar{r})\psi(\bar{r}) = E\psi(\bar{r}) \tag{1}$$

The eigen function when written in spherical coordinates takes the form $\psi(r) = \sum_{l,\mathfrak{m}} R(r)Y^l_{\mathfrak{m}}(\theta,\phi)$ with radial distance r, polar angle θ, and azimuthal angle ϕ and the Azimuthal Quantum Number l and Magnetic Quantum Number $\mathfrak{m}$. The radial part $R(r)$ satisfies .

$$\frac{-\hbar^2}{2m}\left(\frac{1}{r}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r). \tag{2}$$

Substituting $R(r) = \frac{u(r)}{r}$ yeilds :

$$\frac{-\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \left(V(r) + \frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r) = Eu(r). \tag{3}$$

For the convenience we introduce a dimensionless varaiable $\rho = (1/\alpha)r$ and rewrite equation(3) as

$$\frac{-\hbar^2}{2m\alpha^2}\frac{d^2}{dr^2}u(\rho) + \left(V(\rho) + \frac{l(l+1)}{\rho^2}\frac{\hbar^2}{2m\alpha^2}\right)u(r) = Eu(\rho). \tag{4}$$

For a contact potential $V(\rho) = -\delta(\rho)$ and after regularizing the delta potential as $\delta(\rho) = v_0 exp(-\lambda\rho^2)$ the equation(4) further simplifies to

$$\frac{d^2}{d\rho^2}u(\rho) + k(\rho)u(\rho) = 0. \tag{5}$$

where,

$$k(\rho) = \gamma\left(f(\rho) - \frac{l(l+1)}{\gamma\rho^2} - \epsilon\right),$$

$$\gamma = \frac{2m\alpha^2 v_0}{\hbar^2},$$

$$f(\rho) = exp(-\lambda\rho^2), and$$

$$\epsilon = |\frac{E}{v_0}|.$$

The analytical solution does not exist for the equation(5); therefore, we resort to a numerical technique known as Numeov's method that is explained in next section.

3 Numerov's method

Numerov's method is a standard numerical technique that is used to find the solution to a DE. In our project it leverages on numerical integration of wavefunction and the condition that wavefunction is both continuous and differentiable at any point ρ_m .

3.1 Methodology

The first step involved discretizing the space with $h$as step size. This converts the DE in equation(5) to a recursion relation that allows us to find the value of the wavefunction at the current location/step based on its values at the previous two steps.

Then a trail reduced energy $\left(\frac{E_t}{v_0}\right)$ is chosen between E_max and E_min. For this trail reduced energy the numerical integration of wavefunction was carried out from $\rho \to 0$ to the point ρ_m. This is carried out by a function named calculate_forward_wavefunction in our implementation and this is referred to as forward integration. The values at ρ_m and ρ_{m-1}were noted (see Appendix A). Similar numerical integration (backward) is carried out from $\rho = b$ to $\rho = \rho_m$ and values of the wavefunction at ρ_m and ρ_{m-1} are noted.

If E_trial is the reduced binding energy $\left(\epsilon_b = \left(\frac{BE}{v_0}\right)\right)$then it must satisfy the condition that the wavefunction for an energy eigenstate should be both continuous and differentiable at any point(ρ_m) implying that logarithmic derivatives from both forward and backward integration at ρ_m should produce the same result. The value of logarithmic derivate at ρ_m for forward wavefunction can be found by using equation(6).

$$\frac{d}{d\rho}\left(log(\psi_f(\rho))\right) = \left(\frac{\frac{d}{d\rho}\left(\psi_f(\rho)\right)}{\psi_f(\rho)}\bigg|_{\rho=\rho_m}\right) \tag{6}$$

Similarly, logarithmic derivative for backward wavefunction at ρ_m can be found by using equation(7).

$$\frac{d}{d\rho}\left(log(\psi_b(\rho))\right) = \left(\frac{\frac{d}{d\rho}\left(\psi_b(\rho)\right)}{\psi_b(\rho)}\bigg|_{\rho=\rho_m}\right) \tag{7}$$

The above condition implies that ϵ_b can be found by determining E_trail for which the equation(8) is satisfied. To achieve this, a standard method for finding roots called the bisection method is implemented in the interval [E_min , E_max] (see Appendix B). The bisection method involves iteratively narrowing down the search interval by bisecting it into two sub-intervals and then selecting the sub-interval where the signs of $logder_f(\rho_c) - logder_b(\rho_c)$ at the endpoints differ, indicating the presence of a root.

$$\frac{d}{d\rho}\left(log(\psi_f(\rho))\right) - \frac{d}{d\rho}\left(log(\psi_b(\rho))\right) \leq \epsilon_1; \epsilon_1 \to 0 \tag{8}$$

Finally, the point where the wavefunction tends to the universal form, termed as convergence point(ρ_c) in our implementation is found by imposing the criteria in equation(9), $\epsilon_2 = 0.005$ is chosen to be as any further refinements are do not produce any significant difference in the anlysis and results.

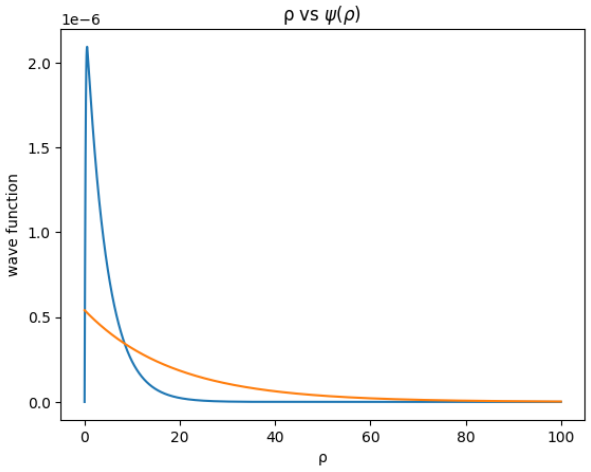
$$|(u(\rho_c)) - (exp(-\gamma * \epsilon_b\rho))| \leq \epsilon_2; \epsilon_2 \to 0 \tag{9}$$

4 Implementation of Numero's method

We have implimented the above Numerov's method for this specific system for regularization parameters $v_0 = 974.443$ and $\lambda = 8$ to validate our implementation.The results are displayed below

4.1 Results A

- The binding energy found : 2.23 MeV.
- The found point of convergence : 98.413
- A graph of wavefunction and $exp(-\gamma * \epsilon_b \rho)$ as a function of ρ is depected below.

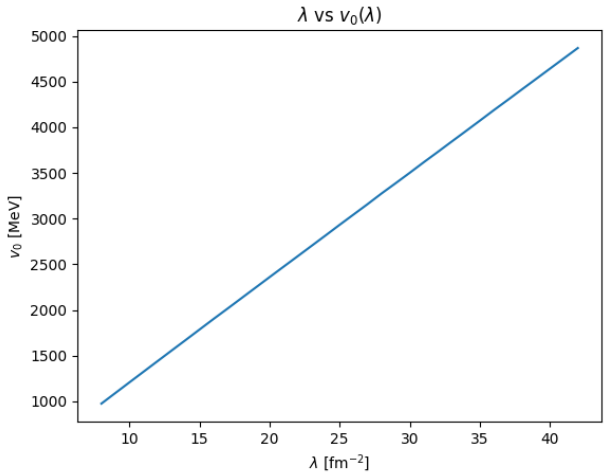


4.2 Finding covergence points

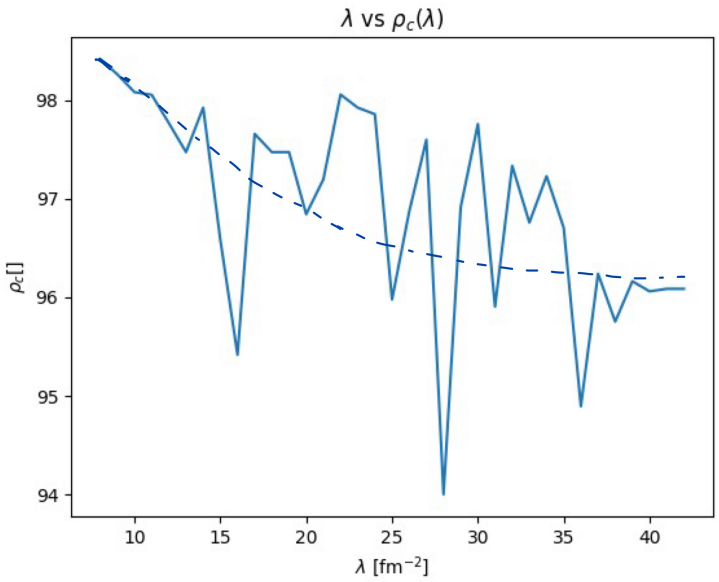
Having gained confidence in our implimentation, the above analysis is Iteratively repeated for various pairs of regularization parameters$(v_0[i], \lambda[i])$ and the point of convergence in each case is found.

- v_0=[974.443, 1090.781, 1206.874,1322.663, 1438.395, 1553.967, 1668.973, 1784.889, 1900.641, 2014.108, 2129.008, 2243.693, 2358.720, 2472.993, 2586.822, 2701.281, 2815.626, 2931.318, 3044.809, 3158.370, 3275.437, 3387.014, 3500.295, 3615.827, 3728.482, 3842.848, 3956.249, 4070.523, 4185.969, 4298.419, 4412.600, 4525.868, 4639.581, 4753.170, 4866.743] MeV
- λ = [8,9,10.....,43] fm^{-2} the relation between the coupling strength and λ is depicted in the graph below

and the results are displayed in next sub-section



4.2.1 Results



The above graph depicts the relationship between convergence point and the regularization parameter λ.The general trend is that the convergence point decreases with the increase in λ with fluctuations we speculate . The following checks and analysis were done to find if there was numerical reason for these fluctuations.

1. Varying the numerical parameters grid size b, and equating it to b=100,b=120,b=150 but the nature of the graph doesn't change.
2. Varying the precision parameter ϵ_2 and result only finds convergence points more precisely, but the nature of the graph doesn't change.
3. suspecting that Numerov's method produced pathological results for specific rgularization parameters, the graphs for parameters where fuclution is observed were visually analysed and after the analysis it was conclude that were no irregularities in the wavefunction produced.

5 Conclusion

The analysis of regularization scheme dependence on the behavior of the wavefunction is done, and the results convey that the wavefunction for this regularization form tends to its universal form at a very large value of ρ, counterintuitive to the assumption that for a zero-range potential, the wavefunction tends to the universal form close to the end of range of the potential. The convergance point for each regularization is found. Although the source of fluctuations was not found, a general that the convergence point decreases with the increase in λ is establisheds.

6 Appendix

6.1 Appendix A

```
def calculate_wavefunction_forward(u_0, E_trail, ro_m, h, x, wavefunction_forward, lamda, gamma):

    r_0 = 0
    wavefunction_current_1 = u_0
    wavefunction_current_2 = h * (l + 1) * (r_0**l) + wavefunction_current_1
    wavefunction_forward[0] = u_0
    wavefunction_forward[1] = wavefunction_current_2
    i = 2 * h     # error handling due to appending
    if len(wavefunction_forward) != 2 and len(x) != 2:
```

```
        wavefunction_forward = [u_0, wavefunction_current_2]
        x = [0, h]
    while i <= ro_m:
        v = calculate_reducedPotential(i, lamda)
        k = np.float128(gamma * (v - E_trail))
        wavefunction_current_3 = np.float128((-k * (h**2) + 2) * wavefunction_current_2
        - wavefunction_current_1)
        wavefunction_current_1 = wavefunction_current_2
        wavefunction_current_2 = (wavefunction_current_3)
        x.append(i)
        wavefunction_forward.append(wavefunction_current_2)
        if wavefunction_current_2 - wavefunction_current_1 < 0:
        i = i + h
return (x, wavefunction_forward, ro_m)
```

6.2 Appendix B

```
def log_difference(E_trail,u_inf,b,h,y,wavefunction_backward,u_0,ro_m,
    x,wavefunction_forward,lamda,gamma):
    forward = calculate_wavefunction_forward(u_0, E_trail, ro_m, h, x,
        wavefunction_forward, lamda, gamma)
    ro_mid = forward[2]
    backward = claculate_wavefunction_backward(u_inf, E_trail, ro_mid, b, h, y,
        wavefunction_backward, lamda, gamma)
    der_wavefunction_forward = (forward[1][-1] - forward[1][-2]) / h
    log_der_wavefunction_forward = der_wavefunction_forward / forward[1][-1]
    der_wavefunction_backward = (backward[1][-2] - backward[1][-1]) / h
    log_der_wavfunction_backward = der_wavefunction_backward / backward[1][-2]
return log_der_wavfunction_backward - log_der_wavefunction_forward
```

6.3 Appendix C

```
 E_bound = bisect(log_difference,E_min,E_max,
       args=(u_inf,b,h,y,wavefunction_backward,
       u_0, ro_m,x,wavefunction_forward,lamda,gamma,),xtol=tolerance,)
```

7 Acknowledgements

I would like to express my sincere appreciation to my supervisor Dr.Johannes Kirscher whose support and expertise were invaluable to the success of this project

8 References

1. A hint of renormalization Bertrand Delamottea.Laboratoire de Physique The´orique et Hautes Energies, Universite´s Paris VI, Pierre et Marie Curie, Paris VII, Denis Diderot, 2 Place Jussieu, 75251 Paris Cedex 05, France ˜Received 28 January 2003; accepted 15 September 2003
2. Regularization, Renormalization, and Dimensional Analysis: Dimensional R egularization meets ,Freshman E&M