Bloated square well: Symmetric Fermi-type potential

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Abstract

We utilize the amenability of the Fermi-type potential profile in Schrödinger equation to construct a symmetric well as \( V(x) = -U_n/[1+\exp([-x]/b)] \), \( U_n=V_n[1+\exp[-a/b]] \). For \( b = 0 \), the potential is square (rectangular) well, when \( b \) increases the potential is bloated to acquire round edges or to become thinner around the origin and thicker at the base. We define \( \alpha = a/b \), \( \beta_n = b\sqrt{2\mu U_n}/\hbar \), we find \( \beta_n \) values for which critically the well has \( n \)-node half bound state at \( E=0 \). Consequently, this fixed well has \( n \) number of bound states. Also we derive a semi-classical expression \( G(\alpha, \beta) \) such that the Fermi well has either \( [G] \) or \( [G]+1 \) number of bound states. Here \([.]\) indicates the integer part.

Historically, many phenomena of the microscopic world have been comprehended by hypothesizing that the smallest system is trapped in a potential \( V(x) \). Quantized energies of bound states are obtained by solving the Schrödinger equation

\[
\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi(x) = 0, \quad (1)
\]

for \( V(x) \). Textbooks in quantum mechanics demonstrate this by using a square (rectangular) well of depth \( V_0 \) and width \( 2a \). It is found \([1]\) that the effective radius parameter \( G' = 2\pi^{-1}\sqrt{\frac{2mV_0a^2}{\hbar^2}} \) of the square well determines the number of bound states as \( [G'] + 1 \), where \([.]\) denotes integer part.

Inspired by the low energy scattering of neutron and proton, the concept of scattering-length and the formation of deuteron \([2,3]\), one can define a \( n \)-node Half Bound State (HBS) \([4]\) \( \psi_* \) at \( E = 0 \), for a symmetric well as \( \psi_*(\pm\infty,W_n) = A \) (constant) such that

\[
\psi_*(x = 0,W_n) = 0 \text{ or } \psi'_*(x = 0,W_n) = 0, \quad W_n = \sqrt{2\mu V_0a^2/\hbar} \quad (2)
\]

according to whether \( n(\geq 1) \) is odd or even, respectively. Also odd (even) \( n \) defines an odd (even) parity HBS. It turns out that when in an square well \( W_n = n\pi/2, n = 1,2,3,.. \) \([4]\), \( n \)-node HBS exists at \( E = 0 \) and the potential well has \( n \) number of bound
states. When $W_n$ is slightly increased from these critical values, the well starts possessing one more bound state at an energy a little below $E = 0$. A well has at most one HBS $\psi_*$ and its existence is critical.

Flügge’s book [5] introduces a Fermi-type potential well as an interesting solvable central potential for $s$-wave. We propose to use it as a symmetric one dimensional potential

$$V(x) = -V_0 \frac{1 + e^{-a/b}}{1 + e^{(|x|-a)/b}}, \quad V_0, a, b > 0. \quad (3)$$

$V(0) = -V_0$, $V(\pm \infty) = 0$ and in the limit when $b \rightarrow 0$, $V(x)$ is a rectangular well. In Fig. 1, three instances ($b = 0.1, 0.5, 1$) of $V(x)$ are plotted for $V_0 = 5$ and $a = 3$ to show that it becomes rectangular well with rounded edge, it then spills out of the rectangle to become bell-shaped, further it becomes well which is sharp around the origin and wide on the base.

In this article, we utilize the available exact analytic solutions [5] of the Schrödinger equation (1) for the Fermi well potential (3) to study its bound states and HBS. We find an expression for the effective parameter $G(V_0, a, b)$ from semi-classical consideration for the bloated square well (3). In this well, we fix the values of $V_0$ and $a$ and vary $b$ to find that the bloated well has equal or more number of bound states than that of the rectangular well. Students will find it interesting that any combination of $V_0, a, b$ leading to $G$ will have the number of bound states as $\lfloor G \rfloor$, or $\lfloor G \rfloor + 1$. Further, we fix $\alpha = a/b$ and find values of $\beta$, so that the well (3) has $n$-node HBS at $E = 0$ and hence $n$ number of bound states. We calculate the corresponding value of $G$ and see that either $G$ or $\lfloor G \rfloor + 1$ equals $n$. An analytic formula for semi-classical eigenvalues will also derived.

For a square well, it is often not realized that this exact quantum mechanical criterion [1] also comes from semi-classical quantization rule that at a discrete energy $E = E_n$

$$\pi^{-1} \int_{x_1}^{x_2} dx \sqrt{\frac{2m}{\hbar^2} [E_n - V(x)]} = n + 1/2, \quad (4)$$

where $x_1$ and $x_2$ are real classical turning points such that $V(x_1) = E_n = V(x_2)$. Here, $n$ gives the quantum number of the discrete energy bound state. The eigenvalues $E_n$ obtained by (4) are only approximate. When a potential well vanishes asymptotically the value of $n$ corresponding to $E = 0$ can give an excellent estimate of the number of bound states in the well. Therefore the integral

$$G = \pi^{-1} \int_{-\infty}^{\infty} dx \sqrt{-\frac{2mV(x)}{\hbar^2}} \quad (5)$$

gives us an effective parameter $G$. We will see that an arbitrary potential well $V(x)$ (other than a square well) which vanishes or saturates to a constant value(s) asymptotically on two sides will have either $G$ or $G + 1$ number of bound states. This dichotomy is due to the approximate nature of the semi-classical quantization (4).

For the square well $G$ equals $G'$. The function $G$ which is actually proportional to the area enclosed by $\sqrt{-V(x)}$ on the $x$-axis for the symmetric Fermi well can be obtained as

$$G(V_0, a, b) = 4\pi^{-1} \beta \sinh^{-1} e^{\beta z}, \quad \beta = \sqrt{\frac{2mU_0 b^2}{\hbar^2}} \quad (6)$$

where $U_0 = V_0[1 + e^{-a/b}]$. For fixed values of $V_0$ and $a$, $G(b)$ can be seen to be an increasing function of $b$ justifying that the square well has the least number of bound states. For large values of $z$, we have $\sinh^{-1} e^z \sim$
FIG. 1: Three modifications of the Fermi well $V(x)$ (3). We fix $V_0 = 5, a = 3$ and vary $b$ as $0.1$ (black, solid), $0.5$ (red, dashed), $1$ (blue, short-dashed).

TABLE I: Bound state calculations using Eq. (13,14)

| $n$ | $V_0$ | $b$ | $a$ | $G$ |
|-----|------|-----|-----|-----|
| 3   | 0.7564 | 2   | 1   | 3   |
| 4   | 0.2565 | 2   | 2   | 3   |
| 6   | 0.5   | 1.1072 | 2   | 3   |
| 6   | 3.4427 | 1   | 6.4 | 3   |
| 7   | 3.5511 | 1   | 6.5 | 3   |
| 7   | 3.6612 | 1   | 6.6 | 3   |
| 8   | 2.9781 | 2   | 8.4 | 4   |
| 9   | 3.0901 | 2   | 8.5 | 4   |
| 9   | 3.2005 | 2   | 8.6 | 4   |

$z + \log 2$. In the limiting case when $b \to 0$, $G(V_0, a, 0) = G'$. In the sequel, we will use symbols $V_{0n}, U_{0n}$, and $\beta_n$ to mean that these parameters are fixed to have just $n$ number of bound states critically. If these are increased slightly the well will have one more bound state slightly below $E = 0$.

I. BOUND STATES

The Schrödinger equation (1) for the Fermi potential (3) can be transformed by introducing [5]

$$y = \frac{1}{1 + e^{(\frac{1-x-a}{b})}}$$

and $\psi(x) = y''(1-y)^{\mu} \phi(y)$, (7) to the Gauss hyper geometric equation [6]

$$y(1-y)\phi''(x) + [(2\nu+1) - (2\nu+2\mu+2)y] \phi(x) - (\nu+\mu)(\nu+\mu+1) \phi(x) = 0.$$  

Fig. 2: HBS $\psi_+(x)$ for symmetric Fermi well potential (3) for $4$ and $\beta_1 = 0.3697, \beta_2 = 0.6905, \beta_3 = 0.9947, \beta_4 = 1.2913$

Here, we have $\nu = kb, \mu = ik'b$, with

$$k = \sqrt{-\frac{2mE}{\hbar^2}}$$

and $k' = \sqrt{\frac{2m(E + U_0)}{\hbar^2}}$. (9)

The second order linear differential equation (8) has two linearly independent solutions

$$\phi_1(y) = {}_2F_1[\nu + \mu, \nu + \mu + 1; 2\nu + 1; y(x)],$$

$$\phi_2(y) = \frac{1}{(1-y)^{2\nu}} {}_2F_1[\nu - \mu, \nu - \mu + 1; 1-2\nu; y(x)].$$  

(10)
for (3) can be written as

\[ \psi(x) = x^2 + x^3 \]

Notice that when \( x \to \infty \), \( y \sim e^{-|x|} \) and \( 2F_1 \to 1 \). Therefore, the solution of (1) for (3) can be written as

\[ \psi(x, E) = C' y^\nu (1 - y)^\mu 2F_1[\nu + \mu, \nu + \mu + 1; 2\nu + 1; y], \tag{12} \]

which satisfies Dirichlet condition \( \psi(\pm \infty) = 0 \) representing bound state correctly. On the other hand, the solution due to the other \( 2F_1(x) \) in Eq. (10) is unacceptable as it diverges as \( e^{k|x|} \) when \( x \sim \infty \). The potential (3) being symmetric, the solutions of (1) should be of definite parity. The even parity solutions are given as

\[ \psi'(0, E_{2n}) = 0, \quad \psi_{2n} = \psi(|x|, E_{2n}), \quad n = 0, 1, \ldots, \tag{13} \]

and the odd parity solutions are characterized by

\[ \psi(0, E_{2n+1}) = 0, \quad \psi_{2n+1} = \text{sgn}(x) \psi(|x|, E_{2n+1}). \tag{14} \]

For the Fermi potential the semi-classical eigenvalues can be obtained from Eq. (4) as

\[ F(E) = \frac{2\beta\sqrt{2}}{\pi} \left[ \sqrt{\omega + \tanh(\alpha/2)} + \sqrt{\omega - \tanh(\alpha/2)} \right] = n + 1/2, \]

\[ \omega(E) = (1 + \frac{2E}{U_0}), \quad \alpha = \frac{a}{b}, \quad \beta = b\sqrt{\frac{2mU_0}{\hbar^2}} \tag{15} \]

II. HALF BOUND STATES (HBS)

For HBS, we set \( E = 0 \) or \( \nu = 0 \) \( \mu = i\beta \) in Eq. (12) to get

\[ \psi(x, \beta) = C(1 - y)^{i\beta} 2F_1[i\beta, i\beta + 1, 1; y] = C 2F_1[i\beta, -i\beta; 1; y/(y - 1)] \tag{16} \]

when \( |x| \to \infty, \quad y \to 0 \), then \( \psi_*(\infty) \to C \) which is nothing but the boundary condition on HBS (see above Eq. (2)). Next, the conditions that

\[ \psi_*(0, \beta_n) = 0 \quad \text{and} \quad \psi'_*(0, \beta_n) = 0, \tag{17} \]

for odd and even node solitary HBS of the well (3) at \( E = 0 \). For all the calculations here, we taken \( 2m/\hbar^2 = 1(eV \hat{A}^2)^{-1} \), energies \( (E, V_0, U_0) \) are in \( eV \) and lengths \( (a, b) \) are in \( \hat{A} \). The Table I, is based on exact bound state eigenvalue calculations using Eqs. (13,14). Various combinations of \( (V_0, a, b) \) giving rise to the same value of \( G \) (6) which allow the
TABLE II: For different values of $\alpha$ and $\beta$ studying number of bound states

| $\alpha$ | $n$ | $\beta_n$ | $G$ | $\alpha$ | $n$ | $\beta_n$ | $G$ |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 0.8774 | 1.4238 | 1 | 0.6226 | 1.3679 |
| 2 | 1.4975 | 2.4302 | 2 | 1.0000 | 2.4166 |
| 3 | 2.1402 | 3.4731 | 3 | 1.5723 | 3.4541 |
| 4 | 2.7494 | 4.4617 | 4 | 2.0281 | 4.4555 |
| 5 | 3.3789 | 5.4833 | 5 | 2.4907 | 5.4716 |
| 6 | 3.9892 | 6.4735 | 6 | 2.9449 | 6.4694 |
| 7 | 4.6142 | 7.4787 | 7 | 3.4046 | 7.4794 |
| 8 | 5.2255 | 8.4798 | 8 | 3.8586 | 8.4767 |

$\alpha$ and $\beta$ to possess $[G]$ or $[G]+1$ number of bound states. Most often it turns out that if the fractional part of $G$ namely $\{G\}$ is $<1/2$, $n = [G]$, otherwise $n = [G]+1$.

The Table II, is based on calculations for the solitary $n$-node HBS at $E = 0$ of the Fermi wells using Eq. (17). The critical $\beta_n$ values for four values of $\alpha$ have been calculated and the corresponding value of the effective parameter $G$ are given. In Fig. 2, for $\alpha = 4$, four $n$-node HBS for the critical values of $\beta_n (n = 1, 2, 3, 4)$ are presented. These four potentials are characterized with $\beta_1 = 0.30697, \beta_2 = 0.6905, \beta_3 = 0.9947$, and $\beta_4 = 1.2913$ (see Table II), The corresponding number of nodes are 1,2,3 and 4, and so are the corresponding number of bound states $[G]$. An inaccurate value of $\beta$ may lead to the non-vanishing of $\psi_n(x)$ or its derivative at $x = 0$, this would disturb the definite parity of the HBS. If $\beta$ is slightly increased from $\beta_n$, the well will have $n+1$ bound states, the last one will be at an energy little below $E = 0$.

Fig. 3, three bound states and one HBS with three nodes are presented when $\alpha=2$ and $\beta=1.5723(1.572333)$. The plot of HBS is very sensitive to accurate value of $\beta$ which is root of Eq. (17). Notice that 3-node HBS means three bound states in the potential well. In Fig. 3, the eigenfunctions of 3 bound states ($E_0 = -1.6202, E_1 = -0.7786, E_2 = -0.2244$) and the solitary 3-node HBS at $E = 0$ are presented. The corresponding semi-classical bound state eigenvalues obtained from Eq. (15) are $-1.5827, -0.7612, -0.2023$, which are approximate but in a good agreement with the exact ones given above.

**CONCLUSION**

One dimensional symmetric Fermi potential has been presented here as a bloated square well potential to study its bound states and the critical $n$-node half bound states. To the best of our knowledge, this as a one-dimensional potential well has been left out in the literature so far. Moreover, our discussion of the number of bound states in this well semi-classically and in terms of $n$-node half bound state is instructive.

**REFERENCES**
[1] Merzbacher E, *Quantum Mechanics* (John Wiley and Sons, Inc.: New York, 1970), 2nd edition.

[2] Blatt J M and Weisskopf V F, *Theoretical Nuclear Physics* 1st edn (London: Wiley, 1952) p 68.

[3] Ahmed Z, ‘Studying the scattering length by varying the depth of the potential well’ Am. J. Phys. 78 418 (2010).

[4] Ahmed Z, Sharma V, Sharma M, Singhal A, Kaiwart R, and Priyadarshani P, ‘The paradoxical zero reflection at zero energy’ Eur. J. Phys. 38 (2017) 025401 (2017).

[5] Flugge S, 1994 *Practical Quantum Mechanics* (Springer Verlag, Berlin Heidelberg) Prob. 64.

[6] Abramowitz and I. A. Stegum, *Hand book of Mathematical Functions* (Dover, 1965) pp. 256-259.