Chapter 9

- Critical Binding
Chapter 9
Critical Binding

9.1 INTRODUCTION

One of the distinctive characteristics of quantum mechanics, in contrast to classical mechanics, is the existence of bound states corresponding to discrete energy levels. It is well-known that bound states exist for all attractive potentials, the exact number depending on the specific form of the potential and the dimensionality of the space. In non-relativistic quantum mechanics, several theorems are available on the number of bound states generated by central potentials, the most important being the Bargmann's inequality. Sahu et al.,[1989] have examined various aspects of critical binding in one, two and three dimensions using the attractive square well potential. Cantrell,[1970] has illustrated a simple graphical solution for finding the approximate bound state energies of low-lying states in a deep square well, which also determines the number of bound states for a given potential strength. Coutinho et al.,[1983] have discussed the sufficient condition for existence of at least one bound state in one and two dimensions and have extended the same to N-particle systems using the variational approach [1985]. Recently Nieto [2002] has discussed the energetics of bound states in continuous radial dimensions, extending upto infinity (0 < D < ∞).

While a variety of conditions relating critical binding is known in non-relativistic quantum mechanics, relatively few such conditions are mentioned in relativistic quantum theory. Mention may be made of Coutinho's work [1988] on the general aspects of the bound state solutions of the one-dimensional Dirac equation. The same authors have also obtained sufficient conditions such that the Dirac equation in one dimension supports a bound state [1987] and have later extended the work to two and three space dimensions [1991]. Further Villalba [1989] has considered the Dirac equation with a scalar potential in one dimension. In literature, while authors often deal with the Dirac equation, the Klein-Gordon equa-
tion is generally not addressed. Kagali [2002] has shown that Klein-Gordon equation with certain potentials lead to paradoxical results.

In the present chapter, we address various aspects of binding criteria for well-defined potentials in one, two and three dimensions and check the possible validity and limitations of these conditions in relativistic quantum mechanics.

9.2 Bound State Criteria in Non-Relativistic Quantum Mechanics

The Hamiltonian, $H$, for a non-relativistic particle under the influence of a potential $V(x)$ in one dimension is

$$H = -\frac{d^2}{dx^2} + V(x); -\infty < x < \infty$$

(9.2.1)

If $V(x) < 0$ for all $x$, and vanishes outside some interval, say $|x| > a$, then $V(x)$ satisfies the condition

$$\int V(x) \, dx < 0$$

and has at least one bound state. Simon [1976] has shown that a bound state exists if $V(x)$ satisfies the even weaker condition $\int V(x) \, dx \leq 0$. Brownstein [1999], using a simple trial function, involving a pyramid function, has obtained a criterion for the existence of bound states in one dimension as

$$A\lambda^2 + B\lambda + C < 0$$

(9.2.2)

with

$$A = \int ((V')^2 + V^3) \, dx$$

$$B = 2 \int V^2 \, dx > 0$$

$$C = \int V \, dx$$

and $\lambda$ is any real parameter and $V'$.
This method of Brownstein, using a simple trial function, gives the criterion for the existence of bound states in one dimension, a special case of which gives the Simon's result.

Cameron Reed [1995] has suggested yet another elegant method of generating analytically and numerically ground and excited state wavefunctions and energies of an infinite family of one-dimensional potentials and has carried out explicit calculations for a sixth order polynomial potential.

9.3 Binding Criteria in Relativistic Quantum Mechanics

In this section, we briefly discuss the condition for the existence of bound states of a relativistic particle. In non-relativistic quantum mechanics, as we have seen, a variety of such conditions are known. However, in relativistic quantum mechanics, little seems to be known about this condition.

It is well-known that the one-dimensional relativistic wave equations can be transformed into the Schrödinger like form (Chapter II)

\[
\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E_{\text{eff}} - V_{\text{eff}}) \psi = 0.
\]  

(9.3.1)

As we have seen earlier, in the case of the Klein-Gordon equation, the effective energy, \(E_{\text{eff}}\) and effective potential, \(V_{\text{eff}}\) for a general interaction \(V(x)\) in the vector coupling scheme may be written as

\[
E_{\text{eff}}^V = \frac{E^2 - m^2 c^4}{2mc^2} \quad \text{and} \quad V_{\text{eff}}^V = \frac{2EV(x) - V^2(x)}{2mc^2}
\]  

(9.3.2)

However, when the potential is treated as a Lorentz scalar, \(E_{\text{eff}}\) and \(V_{\text{eff}}\) take the form [Landau, 1996]

\[
E_{\text{eff}}^S = \frac{E^2 - m^2 c^4}{2mc^2} \quad \text{and} \quad V_{\text{eff}}^S = \frac{2mc^2 S(x) + S^2(x)}{2mc^2}
\]  

(9.3.3)

While the equivalent vector potential is energy dependent, the equivalent scalar potential is energy independent. Nonetheless, the effective energy has the same form in both the coupling schemes.
In Sec.2.41 of Chapter 11, we have shown that the one-dimensional Dirac equation, with an appropriate choice of the Dirac matrices viz., $\beta = \sigma_z$ and $\alpha_x = \sigma_x$, reduces to the Schrödinger form for an interaction included in the vector coupling scheme with effective energy and potential given by

$$E_{\text{eff}} = \frac{E^2 - m^2 c^4}{2mc^2} \quad \text{and} \quad V_{\text{eff}} = \frac{2EV - V^2 - i\hbar c}{2mc^2}$$

(9.3.4)

However, if the potential is treated as a Lorentz scalar, we obtain

$$E_{\text{eff}} = \frac{E^2 - m^2 c^4}{2mc^2} \quad \text{and} \quad V_{\text{eff}} = \frac{2mc^2 S + S^2 - \hbar c}{2mc^2}$$

(9.3.5)

Of course, in this case our choice of the Dirac matrices is $\beta = \sigma_z$ and $\alpha_x = \sigma_y$.

Interestingly, it is seen that the reduction formalism much depends on the choice of the Dirac matrices and is not uniquely defined.

The sufficient condition for a one-dimensional Dirac equation to support a bound state for a pure scalar potential is very similar to the one in non-relativistic case and is given by

$$\int_{-\infty}^{\infty} S(x) \, dx < 0$$

An attractive square well potential obviously satisfies this condition. For well depths greater than $2mc^2$, all the excited states disappear, however the lowest energy state still remains.

An analogous condition for the existence of bound states of a relativistic particle in one dimension is

$$\int_{-\infty}^{\infty} V_{\text{eff}}(x) \, dx \leq 0$$

(9.3.6)

Binding is possible so long as the above inequality is valid.

9.4 RESULTS AND DISCUSSION

In non-relativistic quantum mechanics, while an arbitrarily weak potential can bind particles in one dimension, it is not so in two and three dimensions. Obviously, higher dimensions require stronger binding criteria.
As the well depth is increased, energy levels start appearing in 2D and later in 3D. The occurrence of excited states is seen first in 1D, then in 2D and later in 3D. It may be checked from the table of energies (T 9.2.1) that for a potential of finite depth and specific range, the one dimensional potential allows the maximum number of bound states and the three dimensional one the least. Thus the number of bound states for any potential decreases with the dimensionality of the space but increases with the well-depth or phase space. As is seen from Table T 9.2.1, binding energy is larger in 1D as compared to 2D and 3D. Hence one can conclusively say that the binding criteria is stronger in three dimensional space and weaker in lower dimensions. This may be attributed to the contribution from the orbital angular momentum of the particle, which appears in higher dimensional space.

Interestingly, the situation in relativistic quantum mechanics where spin plays a significant role, is different. While the relativistic wave equations can be transformed to the Schrodinger-like form, with \( E_{\text{eff}} \) and \( V_{\text{eff}} \) in place of \( E \) and \( V \), simple extension of the non-relativistic results to relativistic situations is not always possible. The effective potential being different in different coupling schemes leads to paradoxical results.

In the KG case, it is seen that in vector coupling for any negative potential, \( V_{\text{eff}} \) is always negative and hence bound states are always possible. On the other hand, in scalar coupling, \( V_{\text{eff}} \) may be positive, negative or zero. For small values of \( S(x) \), \( V_{\text{eff}}^S < 0 \), admitting bound states. However for larger \( S(x) \), \( V_{\text{eff}}^S \) can become positive and hence no bound states are possible. As a specific example, it is seen that a square well becomes a barrier beyond a certain \( S(x) \) in scalar interaction and bound states disappear with increasing depth.

Positive potentials exhibit an altogether different behaviour. In vector coupling, for larger \( V(x) \), ie \( V(x) > 2mc^2 \), a barrier leads to a well, admitting bound states. On the contrary, for a scalar interaction, positive potentials can never bind particles.

It is found that the effective potential in the Dirac equation involves an additional \( \left( \frac{dV}{dx} \right) \) term. However, for any symmetric potential, \( \left( \frac{dV}{dx} \right) \) or \( \left( \frac{dS}{dx} \right) \) is antisymmetric and
integration over the symmetric domain vanishes. Thus, on using the integral condition the contribution from the derivative functions at the boundaries cancel out neatly and the same conditions applicable to the KG equation are reflected in the Dirac case. Specifically for a square well potential \( \left( \frac{dV}{dx} \right) \) leads to a \( \delta \)-barrier and \( \delta \)-dip at the boundaries.

It is seen that for a relativistic particle, a relatively weak potential does not admit a bound state even in one dimension. Stronger potentials alone can bind such particles in two dimensions. These subtle aspects are illustrated in Tables T 9.3.1 and T 9.3.2. In three dimensions, confinement is less, implying weaker binding and the particle behaving more like a free particle.
Table T 9.2.1
Comparative study of the energies of a particle in a square well in one, two and three dimensions

$V_0$ and $E$ in units of $\hbar^2/2ma^2$

<table>
<thead>
<tr>
<th>$V_0$</th>
<th>1D</th>
<th>2D</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0001</td>
<td>-0.0000000998</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>-0.000098687</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>-0.00884214</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>-0.153961</td>
<td>-0.00068846</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>-0.453753</td>
<td>-0.0292019</td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>-1.62256</td>
<td>-0.247163</td>
<td>-0.00026312</td>
</tr>
<tr>
<td>4.0</td>
<td>-2.93937 (-1.53261)</td>
<td>-0.469381</td>
<td>-0.407101</td>
</tr>
<tr>
<td>9.0</td>
<td>-7.63082 (-6.53261)</td>
<td>-7.141600 (-1.107960)</td>
<td>-3.806780</td>
</tr>
<tr>
<td>12.0</td>
<td>-10.52852 (-9.53327) (-0.627512)</td>
<td>-9.02385 (-1.66947)</td>
<td>-6.321370</td>
</tr>
<tr>
<td>16.0</td>
<td>-14.43161 (-13.53261) (-3.07378)</td>
<td>-11.73840 (-3.11842) (-0.0452659)</td>
<td>-9.876470</td>
</tr>
</tbody>
</table>

Note: Value within brackets indicate excited state energies
### Table T 9.3.1

**Binding energy of a particle in a square well potential in One and Two dimensions**

$V_0$ and $E$ in units of $mc^2$

<table>
<thead>
<tr>
<th>$V_0$</th>
<th>$E_{N_R}$</th>
<th>$E_R^{VC}$</th>
<th>$e_b = E_R - 1$</th>
<th>$E_{N_R}$</th>
<th>$E_R^{VC}$</th>
<th>$e_b = E_R - 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0005</td>
<td>-0.000000501</td>
<td>0.999950</td>
<td>-0.000050</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.005</td>
<td>-0.00004934</td>
<td>0.999995</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>-0.00442107</td>
<td>0.995397</td>
<td>-0.004603</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>-0.0158982</td>
<td>0.983002</td>
<td>-0.016998</td>
<td>-5.50234 × 10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>1.00000000</td>
<td>0.00000000</td>
</tr>
<tr>
<td>0.50</td>
<td>-0.226877</td>
<td>0.742494</td>
<td>-0.257506</td>
<td>-0.01460101</td>
<td>0.97215714</td>
<td>-0.02784286</td>
</tr>
<tr>
<td>1.0</td>
<td>-0.603898</td>
<td>0.308959</td>
<td>-0.691041</td>
<td>-0.08443583</td>
<td>0.84964443</td>
<td>-0.15035557</td>
</tr>
<tr>
<td>1.2</td>
<td>-0.769142</td>
<td>0.117729</td>
<td>-0.882271</td>
<td>-0.11576901</td>
<td>0.79081702</td>
<td>-0.20918298</td>
</tr>
<tr>
<td>1.4</td>
<td>-0.939329</td>
<td>-0.0815259</td>
<td>-1.081526</td>
<td>-0.14680811</td>
<td>0.72846513</td>
<td>-0.27153487</td>
</tr>
<tr>
<td>1.6</td>
<td>-1.113310</td>
<td>-0.289766</td>
<td>-1.289766</td>
<td>-0.17708104</td>
<td>0.66242505</td>
<td>-0.33757495</td>
</tr>
<tr>
<td>1.8</td>
<td>-1.290290</td>
<td>-0.511139</td>
<td>-1.511139</td>
<td>-0.20639212</td>
<td>0.59178106</td>
<td>-0.40821894</td>
</tr>
<tr>
<td>2.0</td>
<td>-1.469690</td>
<td>-0.764085</td>
<td>-1.764085</td>
<td>-0.23469003</td>
<td>0.51481900</td>
<td>-0.48518100</td>
</tr>
</tbody>
</table>