QUANTUM MECHANICS
Lecture 13
The Dirac potential well

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D. J. Griffiths: paragraph 2.6

The Dirac potential well

In the previous lecture, we have seen that, for a finite square well of depth $-V_0$ ($V_0 > 0$) and half-width a, the number N of stationary bound states ($E < 0$) is given by

$$N = \frac{R}{\pi/2} + 1$$

where the (adimensional) parameter R is defined as

$$R^2 = \frac{2mV_0}{\hbar^2}\,a^2$$

The Dirac potential well

Clearly, if V_0 grows up (with a constant ...), R increases and also **the number of bound states N increases** as well.

Moreover, when $V = -V_0 \to -\infty$, the solutions for $\xi \equiv a\,k$ become (remember $\xi - \eta$ graphic)

$$\begin{aligned} \xi_n &= n\,\frac{\pi}{2} \quad \Rightarrow \\ \Rightarrow \quad k_n &= \sqrt{\frac{2m(E_n + V_0)}{\hbar^2}} \equiv \frac{\xi_n}{a} = \frac{n\pi}{2a} \end{aligned}$$

and their number tends to become infinite.

The Dirac potential well

1. But is it always true, when V_0 grows up, that also the number N of solutions increases ? **Let us see ...**

2. Let us assume that $V_0 \to +\infty$ with $2aV_0 \equiv S$ constant, which means that, in the above limit, the area S where the energy potential is different from zero remains constant.

3. In this case

$$R^2 = \frac{2m}{\hbar^2} V_0\, a^2 = \frac{2m}{\hbar^2} V_0 \left(\frac{S}{2V_0}\right)^2 = \frac{mS^2}{2\hbar^2 V_0} \to 0$$

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1. But, from what we have seen in the previous lecture, when $R < \pi/2$ there is **one and only one stationary solution** with negative energy.

2. As a consequence, in the above limit, only the first (even) bound state will survive and we will have

$$\psi(x) = \alpha\, e^{-r|x|}$$

where $r = \sqrt{\frac{-2mE}{\hbar^2}} \equiv \frac{\eta}{a}$.

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The Dirac potential well

As a matter of fact, when $R \to 0$, also ξ and η will necessarily tend to zero ($R^2 = \xi^2 + \eta^2 \ldots$); therefore the equation characterizing the only possible (ground) state of the system is such that

$$\eta = \xi \, tg\xi \;\Rightarrow\; ar = ak \; tg(ak) \approx (ak)^2$$
$$\Rightarrow\; r = a\,k^2 = \left(\frac{S}{2V_0}\right) \frac{2m}{\hbar^2} (V_0 + E)$$

The Dirac potential well

1. But
$$r = \left(\frac{S}{2V_0}\right)\frac{2m}{\hbar^2}(V_0+E) = \frac{mS}{V_0\hbar^2}(V_0+E)$$
means
$$\sqrt{\frac{-2mE}{\hbar^2}} = \frac{mS}{\hbar^2}\left(1+\frac{E}{V_0}\right) \Rightarrow \sqrt{-E} = \sqrt{\frac{m}{2}}\frac{S}{\hbar}\left(1+\frac{E}{V_0}\right)$$
2. and squaring, we get
$$-E = \frac{m\,S^2}{2\hbar^2}\left(1+\frac{E}{V_0}\right)^2$$
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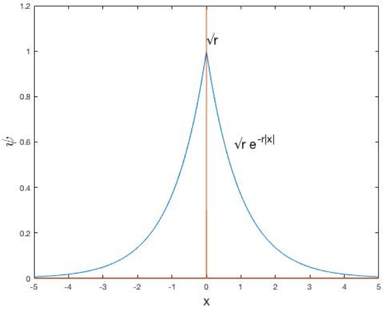

Concerning the w.f., from $E = -\frac{mS^2}{2\hbar^2}$, we obtain

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

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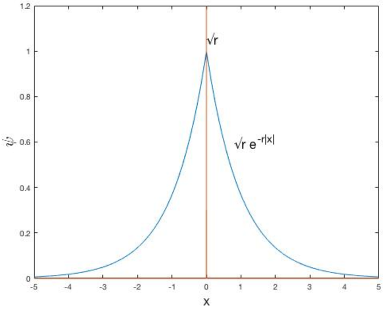
$$\psi(x) = \sqrt{r}\; e^{-r|x|}$$

1. **But, why ψ' has become discontinuous at $x = 0$?**

The Dirac potential well



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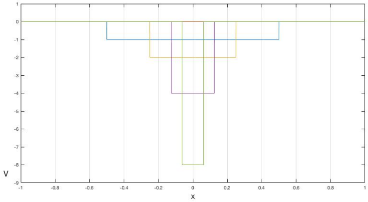

The reason is that, if $V_0 \to \infty; a \to 0$ with $2aV_0 = S\ constant$, we are in presence of a potential energy with a **discontinuity** in $x = 0$ which is **infinite !**

In this case, only ψ remains continuous.

1. The limit condition considered above is very interesting because it allows us to introduce the *generalized function* $\delta(x)$, named **Dirac delta function.**

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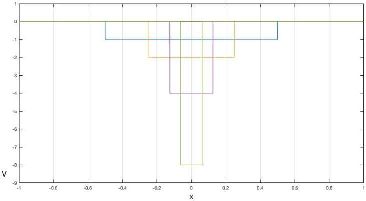

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The Dirac function

The fundamental characteristic of the Dirac-delta function is that

$$\delta(x - x_0) = 0 \ \ for \ \ x \neq x_0$$
$$\int dx \, \delta(x - x_0) = 1$$

and therefore, for any function $f(x)$ continuous in $x = x_0$, we have

$$\int dx \ \delta(x - x_0) \, f(x) = \int dx \ \delta(x - x_0) \, f(x_0) =$$
$$= f(x_0) \int dx \ \delta(x - x_0) = f(x_0)$$

The Dirac function

The limit case studied above corresponds to a potential $V(x) = -S \cdot \delta(x)$
(the potential was centered at $x = 0$, therefore, in this case we have $x_0 = 0 \ldots$).

The Dirac function

1. Strictly speaking, the δ-function is **not** a function in the usual sense, because no function can be different from zero only in one point and have a non-null integral.

2. We arrived to this *generalized* function, considering what happens to a finite square energy potential centered in $x = 0$, when its width $a \to 0$ but the integral

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

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The Dirac function

1. A better way to study the properties of the Dirac function is to consider, for instance, this generalized function as the limit for $\sigma \to 0$ of the following family of gaussians

$$G(x;\sigma) \equiv \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{(x-x_0)^2}{2\sigma^2}}$$

2. For a σ becoming smaller and smaller, these functions become narrower and narrower around $x = x_0$, **remaining normalized**

$$\forall\sigma > 0: \quad \int dx\, G(x;\sigma) = 1$$

so, we can assume that

$$\lim_{\sigma\to 0} \mathbf{G}(\mathbf{x};\sigma) \equiv \delta(\mathbf{x}-\mathbf{x_0})$$

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The Dirac function

1. An important property of the δ-function has to do with the integral of a pure exponential. It turns out, in fact, that

$$\forall \eta \in \Re : \int \mathbf{dx}\, \mathbf{e}^{\mathbf{i}\eta\mathbf{x}} = \mathbf{2}\pi\, \delta(\eta)$$

2. Again, strictly speaking, the above integral does not exist, but ...

3. let us consider the following family of functions

$$F_a(x) \equiv e^{i\eta x}\, e^{-a^2x^2} = e^{[-a^2x^2+i\eta x]}$$

and their integrals

$$I_a(\eta) \equiv \int dx\, F_a(x) = \int dx\, e^{[-a^2x^2+i\eta x]}$$

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The Dirac function

1. Since

$$-a^2x^2 + i\eta\, x = -\left[ax - \frac{i\eta}{2a}\right]^2 - \left(\frac{\eta}{2a}\right)^2$$

2. we have

$$I_a(\eta) \equiv \int dx\, F_a(x) = \int dx\; e^{\left[-a^2x^2 + i\eta x\right]} =$$

$$= e^{-\left(\frac{\eta}{2a}\right)^2} \int \frac{dy}{a}\, e^{-\left[y - \frac{i\eta}{2a}\right]^2} = e^{-\left(\frac{\eta}{2a}\right)^2} \frac{\sqrt{\pi}}{a}$$

where we have used the identity

$$\int dy\, e^{-(y+\alpha)^2} = \int dy\, e^{-y^2} = \sqrt{\pi}$$

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The Dirac function

The functions $I_a(\eta)$ are gaussians centered at zero and normalized to 2π.
In fact

$$\begin{aligned}\int d\eta\, I_a(\eta) &= \frac{\sqrt{\pi}}{a}\int d\eta\, e^{-\left(\frac{\eta}{2a}\right)^2} = \\ &= \frac{\sqrt{\pi}}{a}\, 2a \int d\xi\, e^{-\xi^2} = 2\sqrt{\pi}\sqrt{\pi} = 2\pi\end{aligned}$$

The Dirac function

Clearly, the gaussians $I_a(\eta)$ become narrower and narrower around $\eta = 0$ when $a \to 0$.
In the same limit, $F_a(x) \equiv e^{i\eta\, x} e^{-a^2 x^2} \to e^{i\eta\, x}$;
therefore we can conclude that

$$\lim_{a\to 0} \int dx\, e^{i\eta\, x} e^{-a^2x^2} \equiv \lim_{a\to 0} I_a(\eta) \equiv$$

$$\equiv \lim_{a\to 0} \frac{\sqrt{\pi}}{a}\, e^{-\left(\frac{\eta}{2a}\right)^2} = 2\pi\, \delta(\eta)$$

where the coefficient 2π comes from the integral of the functions $I_a(\eta)$.
In conclusion

$$\lim_{a\to 0} \int dx\, e^{i\eta\, x} e^{-a^2x^2} = \int dx\, e^{i\eta\, x} = 2\pi\, \delta(\eta)$$

Exercise N.5

Exercise

Evaluate the following integrals involving the Dirac delta function

$$a)\quad \int_{-3}^{1} dx\ (x^4 + 4x^2 - 2x + 1) \cdot \delta(x)$$

$$b)\quad \int_{0}^{\infty} dx\ [cos(4x)\ - 2] \cdot \delta(x + \pi)$$

$$c)\quad \int_{-1}^{1} dx\ e^{-x} \cdot \delta(x - 2)$$

$$d)\quad \int_{-\infty}^{+\infty} dx\ e^{-x-3} \cdot \delta(x + 2)$$