Consider the problem of an infinite square well (with $V = 0$ for $x \in [0, L]$ and $V = \infty$ otherwise), with a perturbing attractive delta function at the midpoint of the well ($H' = -\alpha\delta(x - L/2)$). The unperturbed problem has eigenfunctions/eigenenergies given by:

$$E_n = \frac{(k\hbar)^2}{2m} = \frac{2\hbar^2}{mL^2}\left(\frac{kL}{2}\right)^2 = \frac{2\hbar^2}{mL^2}\left(\frac{n\pi}{2}\right)^2 \qquad u_n(x) = \sqrt{\frac{2}{L}}\,\sin(kx) \quad \text{where} \quad k = \frac{n\pi}{L}$$

where we have written eigenenegies in terms of the unit $2\hbar^2/mL^2$ to match the results below. Notice a confusing point: if n is odd $(1, 3, 5, \dots)$, the eigenfunction is reflection symmetric ('even'), whereas if n is even $(2, 4, 6, \dots)$, the eigenfunction is reflection antisymmetric ('odd') and hence has a zero at the well midpoint. That is $u_n(L/2) = 0$ — right where H' is non-zero, so the integral:

$$\int_0^L u_m(x)H'u_n(x)\,dx = \langle m|H'|n\rangle = H'_{mn}$$

is zero if either m or n is even. As a result perturbation theory reports that the n=even states are unaffected by H', i.e., $\mathbb{E}(\alpha) = E_n =$ constant.

For the n, m=odd states we use:

$$\langle m|H'|n\rangle = H'_{mn} = -\frac{2}{L}\alpha$$

to conclude:

$$\begin{aligned}\mathbb{E}(\alpha) &= E_n - \frac{2}{L}\alpha + \sum_{k\neq n}^{\text{odd}} \frac{(2\alpha/L)^2}{\frac{(\hbar\pi)^2}{2mL^2}(n^2 - k^2)} + \cdots \\ &= \frac{2\hbar^2}{mL^2}\left\{\left(\frac{n\pi}{2}\right)^2 - 2\frac{mL\alpha}{2\hbar^2} + \frac{16}{\pi^2}\left(\frac{mL\alpha}{2\hbar^2}\right)^2 \sum_{k\neq n}^{\text{odd}} \frac{1}{n^2 - k^2} + \cdots\right\}\end{aligned}$$

From *Mathematica* we learn:

$$\sum_{k\neq n}^{\text{odd}} \frac{1}{n^2 - k^2} = -\frac{1}{4n^2}$$

so using the shorthand $q = mL\alpha/2\hbar^2$ we have:

$$\mathbb{E}(\alpha) = \frac{2\hbar^2}{mL^2}\left\{\left(\frac{n\pi}{2}\right)^2 - 2q - \frac{q^2}{(n\pi/2)^2} + \cdots\right\}$$

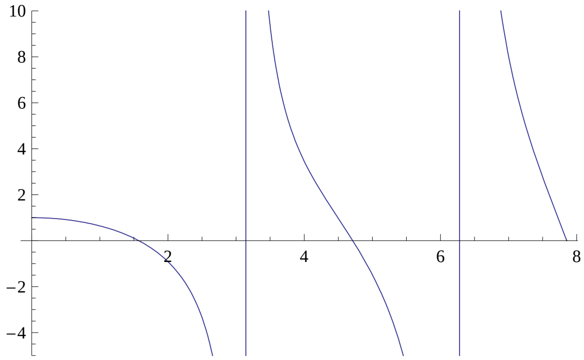
For the exact eigenenergies, we note that except at $x = L/2$, $V = 0$ so $\psi \propto \sin(kx)$. Integrating Schrödinger's across the delta function yields:

$$\frac{-\hbar^2}{2m}\,\Delta\psi'(L/2) = \alpha\psi(L/2)$$

Using the even symmetry of a n =odd state: $\Delta\psi'(L/2) = -2\psi'(L^-/2)$; $\psi \propto \sin(kx)$ produces:

$$\begin{aligned}\frac{-\hbar^2}{2m}\frac{-2k\cos(kL/2)}{\sin(kL/2)} &= \alpha \\ (kL/2)\cot(kL/2) &= \frac{m\alpha L}{2\hbar^2} \\ \theta\cot\theta &= q\end{aligned}$$

Where we have defined the shorthand $\theta = kL/2$. This transcendental equation looks hard to solve. If we graph the lhs as a function of θ, we can see places where the curve would intersect a constant (horizontal) q:



Notice that for small q, such intersections would occur near the zeros of $\cot\theta$, i.e., $\theta =$ odd $\pi/2$ (and so the corresponding energy would equal the unperturbed energy), whereas for large q such intersections would approach (but be a bit above) the asymptotes of $\cot\theta$, i.e., $\theta =$ even $\pi/2$ (and so the corresponding energy would a bit above the unperturbed energy levels for $n =$even). For $q > 1$ there will be no solution in the range $\theta \in [0, \pi/2]$...this is discussed below.

Using *Mathematica* we can find a series expression for θ^2 in terms of q:

```
Series[t Cot[t],{t,(2 k-1) Pi/2,6}]
Simplify[%,Element[k,Integers]]
InverseSeries[%,q]
%^2 /. k->(n+1)/2
```

$$\theta^2 = \left(\frac{n\pi}{2}\right)^2 - 2q - \frac{q^2}{(n\pi/2)^2} + \frac{2\left((n\pi/2)^2 - 3\right)}{3(n\pi/2)^4}\, q^3 + \cdots$$

and

$$\mathbb{E}(\alpha) = \frac{2\hbar^2}{mL^2}\,\theta^2$$

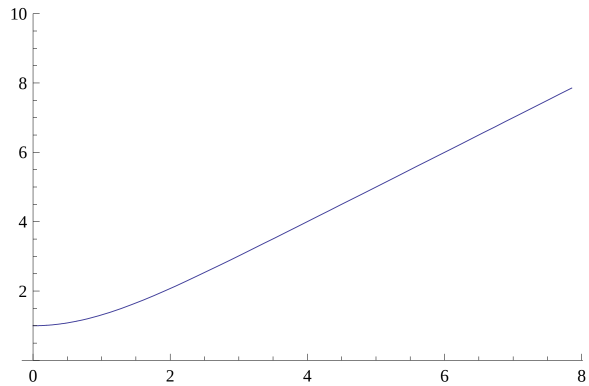
Do remember that the isolated delta function has a single bound state ($E < 0$):

$$E = -\frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right)^2 = -\frac{2\hbar^2}{mL^2}\,q^2$$

so for sufficiently strong delta function we expect the ground state energy to go negative. In fact for $q > 1$, the small θ solution to the equation: $\theta\cot\theta = q$ disappears. To find the ground state energy in this situation we must seek solutions of the form: $\psi \propto \sinh(kx)$ with energy $E = -(\hbar k)^2/2m$, which proceeds exactly as above resulting in

$$\theta\coth\theta = q \qquad \text{where: } E = -\frac{2\hbar^2}{mL^2}\,\theta^2$$

Again graphing the lhs as a function of θ allows you to see solutions:



In this case, notice that as $q \to 1^+$, solution (intersection) $\theta \to 0$, and as $q \to \infty$, $\theta \to q$

Finally, putting together the exact solution with the second order perturbation result we can graph $\mathbb{E}$ as a function of q for the three lowest energy levels. For $n = 3$ the perturbative result lies slightly below the exact result; for $n = 1$ the perturbative result lies slightly above the exact result. Of course, $n = 2$ is unaffected by the perturbation.