Exercise for PCPBT Tool:
Stationary Perturbation Theory

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In quantum mechanics, perturbation theory is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one. The idea is to start with a simple system and gradually turn on an additional "perturbing" Hamiltonian representing a weak disturbance to the system. If the disturbance is not too large, the various physical quantities associated with the perturbed system (e.g. its energy levels and eigenstates) will be continuously generated from those of the simple system. We can therefore study the former based on our knowledge of the latter.

The expressions produced by perturbation theory are not exact, but they can lead to accurate results as long as the expansion parameter, say α, is very small. Typically, the results are expressed in terms of finite power series in α that seem to converge to the exact values when summed to higher order. After a certain order, however, the results become increasingly worse since the series are usually divergent, being asymptotic series). There exist ways to convert them into convergent series, which can be evaluated for large-expansion parameters, most efficiently by Variational method.

There are two categories of perturbation theory: time-independent and time-dependent. In the time-independent perturbation theory, the perturbation Hamiltonian is static (i.e., possesses no time dependence.) Time-independent perturbation theory was presented by Erwin Schrödinger in a 1926 paper [1] shortly after he produced his theories in wave mechanics. In this paper Schrödinger referred to earlier work of Lord Rayleigh [2] who investigated harmonic vibrations of a string perturbed by small inhomogeneities. This is why this perturbation theory is often referred to as Rayleigh-Schrödinger perturbation theory.

The PCPBT tool is used in this exercise to test the validity of the stationary perturbation theory in a quasi-exact way as we are considering double barrier structure formed by the **nine-segment option** with parameters V1=V3=V4=V5=V6=V7=V9=0 eV and V2=V8=1 eV. The lengths of each segment are the same and equal to 4 nm. Calculate the quasi-bound states in this double-well structure and register the lowest four quasi-bound states. In a second experiment add a perturbing potential in the middle of the well by assuming V4=V5=V6 = 50 meV. Register once again the results obtained of the lowest four eigenstates. Can you explain the shift in the energy levels using first and second order stationary perturbation theory? Since the barrier height is 1 eV, you can assume that you are dealing with infinite well potential whose solutions are analytically known for the non-perturbed case.

1. E. Schrödinger, Annalen der Physik, Vierte Folge, Band 80, p. 437 (1926)
2. J. W. S. Rayleigh, *Theory of Sound*, 2nd edition Vol. I, pp 115-118, Macmillan, London (1894)