do not have any cusp. Therefore, taking a finite number of them will not reproduce correctly the shape of the perturbed wave function. The correct shape is restored only in the limit of including an infinite number of states in the expression for $\psi_0^{(1)}$. In practice, this means that the wave function and energy converge rather slowly, see Fig. 4. Exactly the same problem of slow convergence of the wave function and energy is encountered when using perturbation theory for the many-electron problem in atoms, molecules, and solids. In this case the Coulomb interaction gives infinity whenever the distance of two electrons approaches zero. As a result, the exact many-electron wave function also possesses a cusp or cusps, and the energy converges slowly with the number of excited states included in perturbation theory expression. In fact, a cusp appears also when the distance between an electron and nucleus approaches zero. An example is the ground-state wave function of hydrogen atom, proportional to $\exp(-r/a_0)$.

H. The double-well quadratic potential

Consider a particle localized in a one-dimensional linear harmonic oscillator potential. A perturbation $V'(x) = \lambda/(x^2 + a^2)$ is added so that a double minimum potential is formed, see Fig. 5. The magnitude of the perturbation is controlled by a parameter λ. Compute the correction to the lowest energy state within the first order perturbation theory with respect to λ for the cases:

a) $a \ll \sqrt{\frac{\hbar}{m\omega}} \equiv x_0$,

b) $a \gg \sqrt{\frac{\hbar}{m\omega}}$.

Solution:

The ground state wave function for linear harmonic oscillator is of the form

$$\psi_0(x) = \frac{1}{\sqrt{x_0\sqrt{\pi}}} e^{-\frac{x^2}{2x_0^2}} .$$

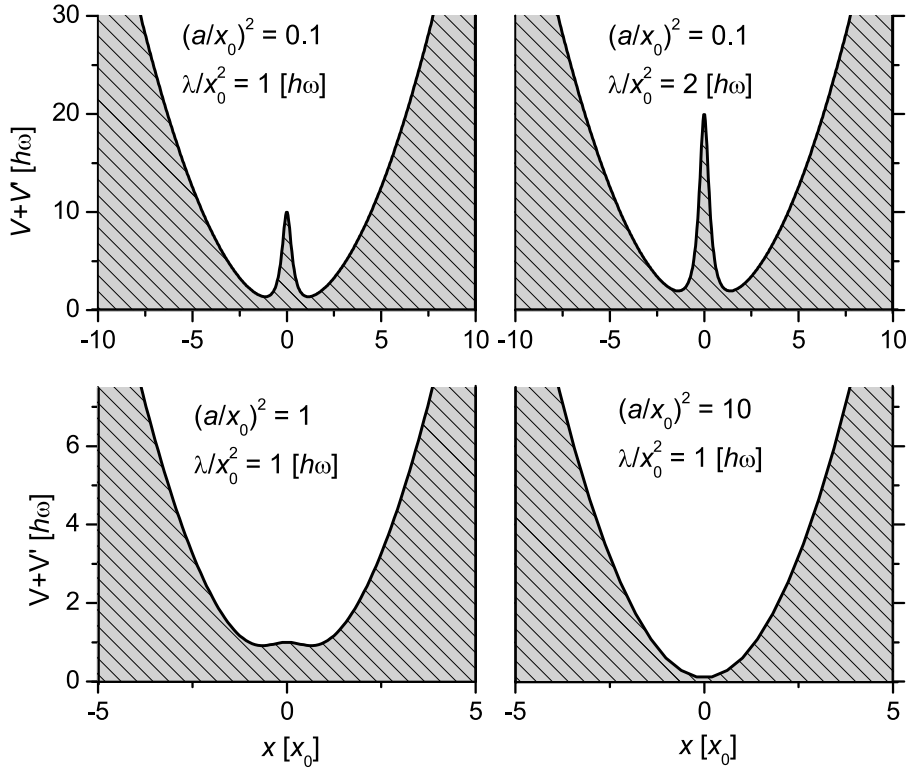

FIG. 5. A quadratic potential perturbed with double minima at the bottom for different sets of parameters a and λ.

The sought correction term is given by

$$E_0^{(1)} = \langle\psi_0|\,\hat{\mathrm{V}}'\,|\psi_0\rangle = \frac{\lambda}{x_0\sqrt{\pi}}\int_{\mathbb{R}}\frac{1}{x^2+a^2}e^{-\frac{x^2}{x_0^2}}\mathrm{d}x = \frac{\lambda}{x_0\sqrt{\pi}}\int_{\mathbb{R}}\frac{1}{a(1+y^2)}e^{-\frac{a^2y^2}{x_0^2}}\,\mathrm{d}y\,,$$

where we used an integral substitution $x = ay$.

In the case a) the exponential will be close to one, and thus the Lorentzian function $1/(1+y^2)$ will dictate the behavior of the integrand, see the bottom right panel of Fig. 6. This results in

$$E_0^{(1)} \approx \frac{\lambda}{ax_0\sqrt{\pi}}\int_{\mathbb{R}}\frac{1}{1+y^2}\mathrm{d}y = \frac{\lambda}{ax_0\sqrt{\pi}}\Big[\arctan y\Big]_0^{\infty} = \frac{\lambda\sqrt{\pi}}{ax_0}\,.$$

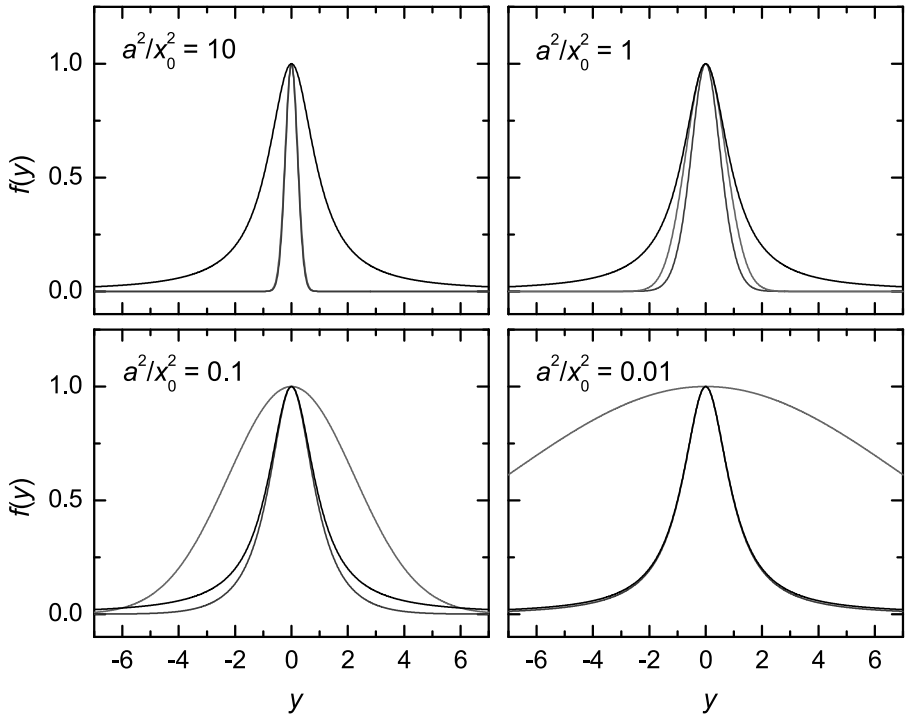

FIG. 6. Dependence of the shape of the (blue) curve $f(y) = \exp\left(-a^2y^2/x_0^2\right)/(1+y^2)$ on the size of parameter a/x_0. Black curve is $1/(1+y^2)$ and the red one is $\exp\left(-a^2y^2/x_0^2\right)$.

In the case b), in the comparison of exponential with a fast decay versus power law in the denominator, the exponential dominates, and therefore y^2 can be neglected with respect to one, see the top left panel of Fig. 6. We have

$$E_0^{(1)} \approx \frac{\lambda}{ax_0\sqrt{\pi}} \int_{\mathbb{R}} e^{-\frac{a^2y^2}{x_0^2}}\,\mathrm{d}y = \frac{\lambda}{ax_0\sqrt{\pi}}\sqrt{\frac{\pi}{a^2}x_0^2} = \frac{\lambda}{a^2}\,.$$

I. A ramp-like infinite square well

A quantum particle is trapped in a one-dimensional infinitely deep square well potential of the length a with perturbation $\hat{\mathsf{H}}' = \frac{V_0}{a}x$, $x \in [0, a]$, see Fig. 7. Find the energy corrections within the first order of perturbation theory for the three