which show good local (short-time) accuracy but when applied to Hamiltonian systems will lead to a regularly increasing deviation in energy.

To be specific, the simple first-order symplectic algorithm

$$\mathbf{p}_{n+1} = \mathbf{p}_n + \mathbf{F}(\mathbf{q}_n)\Delta t\,, \quad \mathbf{q}_{n+1} = \mathbf{q}_n + \mathbf{P}(\mathbf{p}_{n+1})\Delta t \tag{4.153}$$

exactly conserves a Hamiltonian $\tilde{H}$ that is associated to the given Hamiltonian H by

$$\tilde{H} \equiv H + H_1\Delta t + H_2(\Delta t)^2 + H_3(\Delta t)^3 + \ldots \tag{4.154}$$

where

$$H_1 = \frac{1}{2}H_pH_q\,, \quad H_2 = \frac{1}{12}(H_{pp}H_q^2 + H_{qq}H_p^2)\,, \quad H_3 = \frac{1}{12}H_{pp}H_{qq}H_pH_q \;\ldots \tag{4.155}$$

(H_q being shorthand for $\nabla_q H$ etc.) In particular, for the harmonic oscillator the perturbed Hamiltonian

$$\tilde{H} = H_{ho} + \frac{\omega^2\Delta t}{2}pq \tag{4.156}$$

is conserved exactly.

Incidentally, the one-step algorithm 4.153 is also known as the *Euler-Cromer method.* When applied to oscillator-like equations of motion it is a definite improvement over the (unstable) Euler-Cauchy method of equ. 4.7.

EXERCISE: Apply the (non-symplectic) RK method and the (symplectic) Størmer-Verlet algorithm (or the Candy procedure) to the one-body Kepler problem with elliptic orbit. Perform long runs to assess the long-time performance of the integrators. (For RK the orbit should eventually spiral down towards the central mass, while the symplectic procedures should only give rise to a gradual precession of the perihelion.)

4.2.6 Numerov's Method

This technique is usually discussed in the context of *boundary value problems* (BVP), although it is really an algorithm designed for use with a specific *initial value problem* (IVP). The reason is that in the framework of the so-called *shooting method* the solution to a certain kind of BVP is found by taking a detour over a related IVP (see Sec. 4.3.1). An important class of BVP has the general form

$$\frac{d^2y}{dx^2} = -g(x)y + s(x) \tag{4.157}$$

with given boundary values $y(x_1)$ and $y(x_2)$. A familiar example is the one-dimensional Poisson equation for the potential $\phi(x)$ in the presence of a charge density $\rho(x)$,

$$\frac{d^2\phi}{dx^2} = -\rho(x) \tag{4.158}$$