In curvilinear coordinates $q^1, \ldots, q^n$ the Schrödinger equation has the form (1).[11]

$$H\Psi = \alpha_1 \Psi \quad , \qquad (1)$$

where H is the Hamiltonian operator, $\alpha_1$ the total energy, and $\Psi$ the wave function of the entire system.

$$H = \frac{-\hbar^2}{2} \sum_{s,t=1}^{n} \frac{1}{g^{\frac{1}{2}}} \frac{\partial}{\partial q^s} g^{\frac{1}{2}} g^{st} \frac{\partial}{\partial q^t} + U \qquad (2)$$

The $q^s$ are generalized coordinates, and U is the potential energy; $g^{st}$ is a contravariant tensor[12] conjugate to the metric tensor $g_{st}$ appearing in the line element ds in mass-weighted space; g is the determinant of the $g_{st}$.

$$g^{st} = \sum_{i=1}^{n} \frac{1}{m^i} \frac{\partial q^s}{\partial x^i} \frac{\partial q^t}{\partial x^i} ; \; g_{st} = \sum_{i=1}^{n} m^i \frac{\partial x^i}{\partial q^s} \frac{\partial x^i}{\partial q^t} \qquad (3)$$

$$ds^2 = \sum_{s,t=1}^{n} g_{st}\, dq^s\, dq^t \; ; \; \sum_{r=1}^{n} g_{sr}\, g^{rt} = \delta_s^t \qquad (4)$$

where $x^i$ is a Cartesian coordinate of an atom of mass $m^i$; the coordinates of the k'th atom are given by i = 3k, 3k + 1, 3k + 2 . Both $g_{st}$ and $g^{st}$ are symmetric tensors.