Formula Sheet for Wavefunction Animations

Position and momentum eigenstates in 1D

$$\langle x|x'\rangle = \delta(x - x') \tag{1}$$

$$\langle p|p'\rangle = \delta(p - p') \tag{2}$$

$$\langle x|\, p\rangle = \frac{1}{\sqrt{2\pi}} e^{ixp} \tag{3}$$

Gaussian wavepacket in 1D

$$\psi(x,t) \;=\; \sqrt{\frac{\sigma}{\sqrt{\pi}\left(\sigma^2 + \frac{it}{m}\right)}} \quad e^{ip_0 x} \quad e^{-it\,\frac{p_0^2}{2m}} \quad e^{-\frac{\left(x - x_0 - \frac{p_0 t}{m}\right)^2}{2\left(\sigma^2 + \frac{it}{m}\right)}} \tag{4}$$

Relative and center-of-mass coordinates for a 2-particle system

$$\boldsymbol{r} \equiv \boldsymbol{r}_1 - \boldsymbol{r}_2 \qquad\qquad \boldsymbol{r}_1 = \boldsymbol{R} + \frac{m_2}{M}\,\boldsymbol{r}$$

$$\boldsymbol{R} \equiv \frac{m_1 \boldsymbol{r}_1 + m_2 \boldsymbol{r}_2}{M} \qquad\qquad \boldsymbol{r}_2 = \boldsymbol{R} - \frac{m_1}{M}\,\boldsymbol{r}$$

$$\frac{1}{2m_1}\nabla_1^2 + \frac{1}{2m_2}\nabla_2^2 \;=\; \frac{1}{2M}\nabla_R^2 + \frac{1}{2\mu}\nabla_r^2\,, \quad \text{where}$$

$$M \equiv m_1 + m_2 \quad \text{and} \quad \mu \equiv \frac{m_1 m_2}{m_1 + m_2}$$

A 2-particle problem is separable if the potential energy is a function of only the relative coordinate $\boldsymbol{r}$, so that $\Psi_{tot} = \psi_R(\boldsymbol{R}) \cdot \psi_r(\boldsymbol{r})$. However for a scattering problem, we want an initial state of the form $\Psi_{tot} = \psi_{r_1}(\boldsymbol{r}_1) \cdot \psi_{r_2}(\boldsymbol{r}_2)$, representing two widely separated non-interacting particles. Luckily it turns out that, for a particular choice of wavefunctions, we can have it both ways: Let the initial state be a direct product of Gaussian wavepackets for particle 1 and particle 2,

$$\Psi_{tot} \propto \exp\left(-\frac{(\boldsymbol{r}_1 - \overline{\boldsymbol{r}_1})^2}{2\sigma_1^2} + i\boldsymbol{p}_1 \cdot \boldsymbol{r}_1\right) \times \exp\left(-\frac{(\boldsymbol{r}_2 - \overline{\boldsymbol{r}_2})^2}{2\sigma_2^2} + i\boldsymbol{p}_2 \cdot \boldsymbol{r}_2\right),$$

with the Gaussian widths related by $\sigma_2 = \sqrt{\frac{m_1}{m_2}}\,\sigma_1$. With a bit of algebra, you can check that this state is also a direct product in the $\{\boldsymbol{R}, \boldsymbol{r}\}$ coordinates:

$$\Psi_{tot} \propto \exp\left(-\frac{(\boldsymbol{R} - \overline{\boldsymbol{R}})^2}{2\sigma_R^2} + i\boldsymbol{P} \cdot \boldsymbol{R}\right) \times \exp\left(-\frac{(\boldsymbol{r} - \overline{\boldsymbol{r}})^2}{2\sigma_r^2} + i\boldsymbol{p} \cdot \boldsymbol{r}\right).$$

(Here we have introduced the center-of-mass and relative momenta, $\boldsymbol{P} \equiv \boldsymbol{p}_1 + \boldsymbol{p}_2$ and $\boldsymbol{p} \equiv \left(\frac{m_2}{M}\,\boldsymbol{p}_1 + \frac{m_1}{M}\,\boldsymbol{p}_2\right)$, and we have defined $\sigma_R \equiv \sqrt{\frac{m_1}{M}}\,\sigma_1$ and $\sigma_r \equiv \sqrt{\frac{M}{m_2}}\,\sigma_1$.)

Numerical Solution of the Schrodinger Equation

The code makes use of Visscher's technique for numerically propagating wavefunctions forward in time. (Visscher, Comput. Phys. 5, 596 (1991).) The basic idea is to consider the real and imaginary parts of the wavefunction separately, and note that they evolve according to

$$\frac{dR}{dt} = H \cdot I \qquad \text{and} \qquad \frac{dI}{dt} = -H \cdot R\,,$$

where H is the Hamiltonian. The real part R is specified at integer time steps, $0, \Delta t, 2\Delta t, \ldots$, and the imaginary part I at half-odd-integer time steps $\frac{1}{2}\Delta t$, $\frac{3}{2}\Delta t, \ldots$. The discrete-time evolution equations are then

$$R\left(t + \frac{1}{2}\Delta t\right) = R\left(t - \frac{1}{2}\Delta t\right) + \Delta t\, H \cdot I(t)$$

$$I\left(t + \frac{1}{2}\Delta t\right) = I\left(t - \frac{1}{2}\Delta t\right) - \Delta t\, H \cdot R(t)$$

Visscher shows that these equations are second-order accurate in time, and stable for any reasonable choice of parameters.

Finally, note that in most places the code uses the following spatial discretization of the second derivative, which is accurate to fifth order in the spatial step size:

$$f''(x) = \frac{1}{a^2}\left(-\frac{1}{12}f(x-2a) + \frac{4}{3}f(x-a) - \frac{5}{2}f(x) + \frac{4}{3}f(x+a) - \frac{1}{12}f(x+2a)\right) + O(a^6)$$