Here I present some summary tables for various discrete variable representation (DVR) bases using the following notations and terminology (mostly following [1] with the exception that we use $w_n \equiv 1/K_n$ for the integration weights).

$$k_c : \qquad \text{(momentum cutoff (UV))}$$

$$x_n : \quad z_n \equiv k_c x_n \qquad \text{(abscissa and dimensionless abscissa)}$$

$$P : \quad P = P^\dagger = P^2 = \sum_{|k|<k_c} |k\rangle\langle k| \qquad \text{(projector)}$$

$$|x_n\rangle : \quad \langle x|x_n\rangle = \delta(x - x_n) \qquad \text{(delta-function)}$$

$$|\Delta_n\rangle : \quad |\Delta_n\rangle = P|x_n\rangle \qquad \text{(projected delta-functions)}$$

$$w_n : \quad w_n = 1/\langle\Delta_n|\Delta_n\rangle = 1/\Delta_n(x_n) \qquad \text{(quadrature weights)}$$

$$|L_n\rangle : \quad |f\rangle = \sum_n f(x_n)|L_n\rangle, \quad \langle L_m|\Delta_n\rangle = \delta_{mn} \qquad \text{(interpolating functions)}$$

$$|F_n\rangle : \quad \langle F_m|F_n\rangle = \delta_{mn} \qquad \text{(orthonormal basis functions)}$$

The conventional DVR bases satisfy $|L_n\rangle = \sqrt{w_n}\,|F_n\rangle = w_n|\Delta_n\rangle$: i.e. the projected delta-functions form an orthogonal basis:

$$\langle\Delta_m|\Delta_n\rangle = \Delta_m(x_n) = w_n^{-1}\delta_{mn}. \tag{1}$$

In other words, the basis functions $F_n(x)$ have nodes at all abscissa $x = x_{m\neq n}$. This is a non-trivial requirement and generally requires these bases to be built from orthogonal polynomials. The key to the utility of these DVR bases is that they are quasi-local: to express a function $f(x)$ in the basis, one simply evaluates it at the abscissa. Likewise, the potential energy matrix can be approximated by a diagonal matrix. Coupled with the kinetic operator, this can yield exponential accuracy for the eigenvalues and eigenfunctions (for appropriate potentials and boundary conditions)

$$|f\rangle = \sum_n f_n|F_n\rangle, \quad f_n = f(x_n)\sqrt{w_n} \qquad \text{(quasi-locality)}$$

$$K_{mn} = \langle F_n|\widehat{\mathbf{K}}|F_m\rangle \qquad \text{(kinetic energy)}$$

$$V_{mn} = \langle F_n|\widehat{\mathbf{V}}|F_m\rangle \approx \delta_{mn}V(x_n) \qquad \text{(potential energy)}$$

Selected References

[1] R. G. Littlejohn, M. Cargo, T. Carrington, Jr., K. A. Mitchell, and B. Poirier, J. Chem. Phys. **116**, 8691 (2002).

[2] D. Baye, J. Phys. B **28**, 4399 (1995).

[3] D. Baye, physica status solidi (b) **243**, 1095 (2006).

[4] R. G. Littlejohn and M. Cargo, J. Chem. Phys. **117**, 27 (2002).

[5] D. Baye and P.-H. Heenen, J. Phys. A **19**, 2041 (1986).

[6] D. Baye, M. Hesse, and M. Vincke, Phys. Rev. E **65**, 026701 (2002).

[7] H. Karabulut and E. L. Sibert III, J. Phys. B **30**, L513 (1997).

[8] R. G. Littlejohn and M. Cargo, J. Chem. Phys. **116**, 7350 (2002).

Fourier Basis The simple Fourier basis over an interval of length $L = Na$ is just a quasi-local rearrangement of the usual Fourier basis e^{ik_nx} with wave-vectors $k_n = 2\pi n/L$ in terms of the "periodic sinc functions" $\text{psinc}(z)$ (see [2]):

$$\text{psinc}(z) = \frac{\sin z}{N \sin \frac{z}{N}} = \frac{1}{N} \sum_{m=-(N-1)/2}^{(N-1)/2} e^{imz}, \tag{2a}$$

$$x_n = x_0 + an\Big|_{n=-(N-1)/2}^{(N-1)/2}, \quad k_c = \pi/a, \quad w_n = \pi/k_c = a, \tag{2b}$$

$$L_n(x) = \text{psinc}\Big(k_c(x - x_n)\Big), \tag{2c}$$

$$K_{m\neq n} = \frac{2\pi^2(-1)^{m-n}}{L^2} \frac{\cos \frac{k_c(x_m-x_n)}{N}}{\sin^2 \frac{k_c(x_m-x_n)}{N}}, \quad K_{nn} = \frac{\pi^2}{3a^2}\left(1 - \frac{1}{N^2}\right). \tag{2d}$$

Sinc Function Basis For N abscissa, one can represent functions over an interval of length aN (non-periodic) with $\text{sinc}(x) \equiv \sin(x)/x$ functions. This follows from the Fourier basis in the limit $N \to \infty$ (see [2]):

$$x_n = x_0 + an, \quad k_c = \pi/a, \quad w_n = \pi/k_c = a, \tag{3a}$$

$$L_n(x) = \text{sinc}\Big(k_c(x - x_n)\Big), \tag{3b}$$

$$K_{m\neq n} = \frac{2(-1)^{m-n}}{(x_m - x_n)^2}, \quad K_{nn} = \frac{\pi^2}{3a^2}. \tag{3c}$$

Bessel Function Basis For central problems one expands the radial wavefunction $u(r) = r^{(d-1)/2}\psi(r)$ for each angular momentum $\nu = l + d/2 - 1$. In practice, one can often use just a few basis: in $d = 3$ for example, one can use the $l = 0$ basis for all even l and the $l = 1$ basis for all odd l. The abscissa and basis functions are defined in terms of the Bessel functions $J_\nu(z)$ (see [4]):

$$\frac{d^2u(r)}{dr^{2\,2}} - \frac{\nu^2 - 1/4}{r^2}u(r) + \frac{2m}{\hbar^2}[E - V(r)]u(r) = 0 \tag{4a}$$

$$J_\nu(z_{\nu n}) = 0, \quad w_n = \frac{2}{k_c z_{\nu n} J'_\nu(z_{\nu n})^2}, \tag{4b}$$

$$F_n(r) = (-1)^{n+1} \frac{k_c z_{\nu n}\sqrt{2r}}{k_c^2 r^2 - z_{\nu n}^2} J_\nu(k_c r), \tag{4c}$$

$$K_{m\neq n} = \frac{8k_c^2(-1)^{m-n} z_{\nu n} z_{\nu m}}{(z_{\nu n}^2 - z_{\nu m}^2)^2}, \quad K_{nn} = \frac{k_c^2}{3}\left[1 + \frac{2(\nu^2 - 1)}{z_{\nu n}^2}\right] \tag{4d}$$