A discrete Schrödinger equation

You may recall the Schrödinger equation in Euclidean space from your physics or chemistry classes. In any case, it is:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(x,t) + V(x,t)\psi(x,t),$$

where $\psi(x,t) \in \mathbb{C}$ is the probability amplitude so we require

$$\int |\psi(x,t)|^2 \,\mathrm{d}x = 1.$$

The Schrödinger equation is, of course, a *partial* differential equation. To turn it into a system of ordinary differential equations we discretize the space in which x takes its values.

And to keep the system low dimensional, we consider a highly symmetric problem, in which $x \in K_N$, the complete graph on N vertices (which implies that the transition amplitude from any vertex to any other vertex is the same), and $V(x,t) = \delta_{xa}$ for some $a \in K_N$. If we further assume that the initial state of the system is an equal superposition $\psi(x,0) = 1/\sqrt{N}$ then $\psi(x,t) = \psi(y,t) =: \beta(t)/\sqrt{N-1}$ for all $x, y \neq a$ and all t. These assumptions produce the two (complex) dimensional system:

$$i\begin{pmatrix}\dot\alpha \\ \dot\beta\end{pmatrix} = -\begin{pmatrix}\gamma+1 & \gamma\sqrt{N-1} \\ \gamma\sqrt{N-1} & \gamma(N-1)\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} =: -\begin{pmatrix}a & b \\ b & d\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix}, \tag{1}$$

where $\alpha(t) := \psi(a,t)$ and γ depends on m. I have omitted the derivation of equation (1), and the motivation for studying it; for both see Childs and Goldstone [1].

The complex-valued functions $\alpha(t)$ and $\beta(t)$ make (1) different from the systems of ODEs you have seen earlier in this course. One way to handle this is to rewrite (1) as a system of real equations by defining $\alpha =: p + iq$ and $\beta =: r + is$, for real-valued functions p, q, r, s. Substituting into (1) and equating the real and imaginary parts of each equation separately gives:

$$\begin{pmatrix}\dot p \\ \dot q \\ \dot r \\ \dot s\end{pmatrix} = \begin{pmatrix}0 & -a & 0 & -b \\ a & 0 & b & 0 \\ 0 & -b & 0 & -d \\ b & 0 & d & 0\end{pmatrix}\begin{pmatrix}p \\ q \\ r \\ s\end{pmatrix}. \tag{2}$$

Now (2) is a linear system for 4 real functions, with a critical point at the origin. Its type depends on the eigenvalues of the coefficient matrix in (2).

Reference

[1] A. M. Childs and J. Goldstone, "Spatial search by quantum walk", *Phys. Rev. A* **70** (2004) 022314/1–11.