Tight-Binding Model

Lecture Notes

September 28, 2026

1. Second-Order Ordinary Differential Equations (ODE)

Consider the following second-order linear homogeneous ODE with constant coefficients:

$$a_2 y''(x) + a_1 y'(x) + a_0 y(x) = 0 \tag{1}$$

Assuming a solution of the form $y(x) = \alpha e^{sx}$, we substitute it into the ODE to obtain the characteristic equation:

$$(a_2 s^2 + a_1 s + a_0)\alpha e^{st} = 0 \Rightarrow (a_2 s^2 + a_1 s + a_0) = 0 \tag{2}$$

Let the roots be s_1 and s_2. By comparing the coefficients of the quadratic equation of s, we have

$$\begin{aligned} s_1 + s_2 &= -a_1/a_2, \\ s_1 s_2 &= a_0/a_2. \end{aligned}$$

s_1 and s_2 The most general solution to the ODE in eq. (1) is given by:

$$y(x) = c_1 e^{s_1 x} + c_2 e^{s_2 x}. \tag{3}$$

The two undetermined coefficents c_1 and c_2 are related to the constant of integration, which arises every time we integrate. Since we need to integrate twice to solve the ODE in eq. (1), there will be two unspecified constants of integration. To determine c_1 and c_2, we either need to impose initial condition (I.C.):

$$y(0) = y_0, \quad y'(0) = y_0' \tag{4}$$

or boundary-value condition (B.C.)

$$y(0) = y_0, \quad y(L) = y_1 \tag{5}$$

2. The 1D Wave Equation

2.1 Derivation of the 1D Wave Equation

Consider a vibrating string where the displacement vector at position x and time t is given by:

$$\vec{r}(x,t) = x\hat{x} + y(x,t)\hat{y} \tag{6}$$

The tangent vector along the string is:

$$\vec{t} = \frac{\partial \vec{r}}{\partial x} = \hat{x} + \frac{\partial y}{\partial x}\hat{y} \Rightarrow \hat{t} = \frac{\hat{x} + \frac{\partial y}{\partial x}\hat{y}}{\sqrt{1 + \left(\frac{\partial y}{\partial x}\right)^2}} \tag{7}$$

Assuming small transverse oscillations ($|\frac{\partial y}{\partial x}| \ll 1$), the forces acting at $x = x_0$ and $x = x_0 + \Delta x$ are:

$$\vec{F_1} = -T(x_0)\left(\hat{x} + \frac{\partial y}{\partial x}\hat{y}\right)\Big|_{x=x_0}, \tag{8}$$

$$\vec{F_2} = T(x_0 + \Delta)\left(\hat{x} + \frac{\partial y}{\partial x}\hat{y}\right)\Big|_{x=x_0+\Delta x}. \tag{9}$$

Here $T(x_0)$ and $T(x_0 + \Delta)$ are the tensions acting on the string at $x = x_0$ and $x = x_0 + \Delta$, repectively. Summing up the forces, we have:

$$\vec{F_1} + \vec{F_2} = \left[T(x_0 + \Delta x) - T(x_0)\right]\hat{x} + \left[T(x_0 + \Delta x)\frac{\partial y}{\partial x}(x_0 + \Delta x, t) - T(x_0)\frac{\partial y}{\partial x}(x_0, t)\right]\hat{y}. \tag{10}$$

Since a string wave is purely transversal, the horizontal component of the force vanishes, so $T = T_0$ is a constant independent of x. Applying Newton's second law in the vertical direction:

$$T_0\left\{\frac{\partial y}{\partial x}(x_0 + \Delta x, t) - \frac{\partial y}{\partial x}(x_0, t)\right\} = (\mu_0 \Delta x)\frac{\partial^2 y}{\partial t^2}(x_0, t). \tag{11}$$

Dividing by Δx and taking the limit $\Delta x \to 0$, we have:

$$T_0\frac{\partial^2 y}{\partial x^2}(x_0, t) = \mu_0\frac{\partial^2 y}{\partial t^2}(x_0, t). \tag{12}$$

Define speed $v = \sqrt{\frac{T_0}{\mu_0}}$, and we achieve the standard 1D wave equation:

$$v^2\frac{\partial^2 y}{\partial x^2} - \frac{\partial^2 y}{\partial t^2} = 0. \tag{13}$$

We may carry out a dimensional analysis to check whether it is correct:

$$[T_0] = MLT^{-2}, \quad [\mu_0] = ML^{-1} \Rightarrow \left[\frac{T_0}{\mu_0}\right] = L^2T^{-2} = [v^2]. \tag{14}$$

2.2 Separation of Variables & Standing Waves

To solve the 1D wave eqution in eq. (13), we assume a product solution:

$$y(x, t) = X(x)T(t). \tag{15}$$

Substituting into the wave equation gives:

$$v^2X''(x)T(t) = X(x)\ddot{T}(t) \Rightarrow \frac{v^2X''(x)}{X(x)} = \frac{\ddot{T}(t)}{T(t)} = -\omega^2. \tag{16}$$

This leads to two decoupled linear ODEs:

$$\ddot{T}(t) + \omega^2T(t) = 0 \Rightarrow T(t) = A_+e^{i\omega t} + A_-e^{-i\omega t}; \tag{17}$$

$$X''(x) + k^2X(x) = 0 \Rightarrow X(x) = B_+e^{ikx} + B_-e^{-ikx}, \tag{18}$$

where $k = \frac{\omega}{v}$.

Fixed-Fixed Boundary Conditions: $X(0) = 0$, $X(L) = 0$

1. $X(0) = 0 \Rightarrow B_+ + B_- = 0$.
2. $X(L) = 0 \Rightarrow B_+ e^{ikL} + B_- e^{-ikL} = 0$. The boundary conditions lead to a coupled homogeneous linear equation of B_+ and B_-. To have a non-trivial solution, the determinant formed by the coefficients of B_+ and B_- must be vanishing, i.e.

$$\begin{vmatrix} 1 & 1 \\ e^{ik_0 L} & e^{-ik_0 L} \end{vmatrix} = 0 \Rightarrow e^{2ikL} = 1. \tag{19}$$

This yields the quantization in the wave number:

$$2kL = 2n\pi \Rightarrow k_n = \frac{n\pi}{L}, \quad n \in \{1, 2, 3, \dots\} \tag{20}$$

If we let $B_+ = B_0$, the the spatial eigenfunctions are given by:

$$X(x) = B_0 \left(e^{ikx} - e^{-ikx} \right) = 2iB_0 \sin\left(\frac{n\pi x}{L}\right) = C_0 \sin\left(\frac{n\pi x}{L}\right). \tag{21}$$

This is the form of a standing wave, which we learn in general physics.

Homework: Consider a Free-Free Boundary Conditions and carry out the analysis by yourself.

3. Linaer Recursive Relation (Difference Equation) with Constant Coefficents

Consider the following second-order linear recursive relation with constant coefficients:

$$a_2 y_{j+2} + a_1 y_{j+1} + a_0 y_j = 0 \tag{22}$$

Similar to the ODE case, we assume a solution of the form $y_j = \alpha s^j$ and substitute it into the above equation to obtain the characteristic equation:

$$(a_2 s^2 + a_1 s + a_0)\alpha s^j = 0 \Rightarrow (a_2 s^2 + a_1 s + a_0) = 0 \tag{23}$$

Let the roots be s_1 and s_2. By comparing the coefficients of the quadratic equation of s, again we have

$$\begin{aligned} s_1 + s_2 &= -a_1/a_2, \\ s_1 s_2 &= a_0/a_2. \end{aligned}$$

The most general solution to the second order recusive relation eq. (22) is given by:

$$y_j = c_1 s_1^j + c_2 s_2^j. \tag{24}$$

To determine c_1 and c_2, we either need to impose initial condition (I.C.):

$$y_1 = z_1, \quad y_2 = z_2 \tag{25}$$

or boundary-value condition (B.C.)

$$y_1 = z_1, \quad y_N = z_N \tag{26}$$

One can see the second order linear ODE and second order linear recursive relation are closely related. Suppose we are interested in solving the ODE in eq. (1) in the range $0 \le x \le L$.

Define $\Delta = L/N$, $x_j = j\Delta$, and $y_j = y(x_j)$, with $0 \leq j \leq N$. To find the solution numerically, we may approximate

$$y'(x_j) \approx \frac{y_{j+1} - y_j}{\Delta};$$
$$y''(x_j) \approx \frac{1}{\Delta}\left\{\frac{y_{j+1} - y_j}{\Delta} - \frac{y_j - y_{j-1}}{\Delta}\right\}. \tag{27}$$

Then we can convert the second order lnear ODE in eq. (1) into a second order linear recursive relation. In the limit that $\Delta \to 0$, we expect the numerical solution would lead to an exact solution to eq. (1). Therefore, it is quiter natural that the ansatz that we used to the linear recursive relation with constant coefficients is very similar to that we used to solve the linear ODE with constant coefficients.

Homework: Verify that in the limit $N \to \infty$ so that $\Delta \to 0$ the solution to the second order linear recursive relation with constant coefficients does give rise to that of a second order linear ODE with constant coefficients.

4. Coupled Harmonic Oscillator System

4.1 Equation of Motion (EOM)

Consider a 1D chain of N particles of mass m connected by springs with spring constant k. Let $X_j(t)$ be the displacement of the j-th particle from its corresponding equilibrium position. After simplification, the EOM for the system are given by:

$$m\ddot{X}_j(t) = k[X_{j+1}(t) + X_{j-1}(t) - 2X_j(t)] \quad \text{for } 2 \leq j \leq N-1. \tag{28}$$

Fixed Boundary Conditions: If the first and N-th particles are both connected by a spring to a wall, the corresponding eqations for them are

$$m\ddot{X}_1(t) = k[X_2(t) - 2X_1(t)];$$
$$m\ddot{X}_N(t) = k[X_{N-1}(t) - 2X_N(t)].$$

Mathemtically, this is equivalent to $X_0(t) = 0$ and $X_{N+1}(t) = 0$.

Assume steady-state solutions $X_j(t) = x_j e^{-i\omega t}$ and define $\omega_0^2 = \frac{k}{m}$. The above eqation simplifies to

$$-\Omega^2 x_j + \{2x_j - x_{j+1} - x_{j-1}\} = 0 \quad \text{for } 2 \leq j \leq N-1. \tag{29}$$

with $x_0 = 0$ and $x_{N+1} = 0$. Here, $\Omega = \omega/\omega_0$.

4.2 Normal Mode Frequencies

To solve the above equation, we assume $a_j = s^j$. As a result, we otain:

$$\Omega^2 = \left\{2 - s - s^{-1}\right\} \Rightarrow s^2 - (2 - \Omega^2)s + 1 = 0. \tag{30}$$

If we factor the equation into $(s - s_1)(s - s_2)$, we see

$$\begin{cases} s_1 + s_2 = 2 - \Omega^2, \\ s_1 \cdot s_2 = 1. \end{cases}$$

Setting $s_1 = s$ and $s_2 = s^{-1}$, the most general solution for a_j is given by:

$$x_j = \alpha_+ s^j + \alpha_- s^{-j} \tag{31}$$

If the system satisfies the fixed BC: $x_0 = 0$, $x_{N+1} = 0$, then, we have

$$\begin{cases} \alpha_+ + \alpha_- = 0, \\ \alpha_+ s^{N+1} + \alpha_- s^{-N-1} = 0. \end{cases} \Rightarrow \begin{vmatrix} 1 & 1 \\ s^{N+1} & s^{-(N+1)} \end{vmatrix} = 0. \tag{32}$$

Therefore, $s = e^{i\theta_k}$ where $\theta_k = \frac{\pi k}{N+1}$, with $k \in 1, 2, \ldots, N$.
The normal frequencies are:

$$\Omega_k^2 = 2 - 2\cos\left(\frac{\pi k}{N+1}\right) = 4\sin^2\left[\frac{\pi k}{2(N+1)}\right]. \tag{33}$$

4.3 The Coupled-Spring System as a Eigenvalue Problem

The coupled-spring system satisfing the fixed-end can be expressed as an eigenvalue problem:

$$\lambda \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_N \end{pmatrix}, \tag{34}$$

where $\lambda = \Omega^2$.

From the result obtained in the previous subsection, we see

$$\lambda_k = 2 - 2\cos\left(\frac{\pi k}{N+1}\right). \tag{35}$$

From the fixed-end BC, $x_0 = 0$, we see that $\alpha_+ + \alpha_- = 0$. Hence,

$$x_j^{(k)} = N_k \sin\left(\frac{\pi k * j}{N+1}\right), \tag{36}$$

Homework: Consider a system of N coupled point masses m connected by springs with spring constant k. Given that the system satisfies the free-end BC:

$$\begin{cases} x_1 = x_0; \\ x_{N+1} = x_N, \end{cases}$$

find all the normal modes $x_j^{(k)}$ and their frequencies $\Omega(k)$.

Homework: Consider a system of N coupled point masses m connected by springs with spring constant k. Given that the system satisfies the fixed-end BC on the left-hand side and the free-end BC on the right-hand side:

$$\begin{cases} x_0 = 0; \\ x_{N+1} = x_N, \end{cases}$$

find all the normal modes $x_j^{(k)}$ and their frequencies $\Omega(k)$.

5. One-Dimensional Tight-Binding Model

4.1 Schrodinger Equation of the 1D Tight-Binding Model

Consider a 1D lattice with site positions j. Let v denote the hopping amplitude between nearest-neighbor (n.n) sites:

$$\boldsymbol{H} = \sum_{j=-\infty}^{\infty} \left\{ -v\boldsymbol{a}_{j+1}^\dagger \boldsymbol{a}_j - v\boldsymbol{a}_j^\dagger \boldsymbol{a}_{j+1} \right\} \tag{37}$$

Let $\hbar = 1$, and the Schrödinger equation take the form:

$$i\partial_t \mid \Psi \rangle = \boldsymbol{H} \mid \Psi \rangle . \tag{38}$$

Define $\mid j \rangle = \boldsymbol{a}_j^\dagger \mid 0 \rangle$. It describes the state with an electron at site j, and we will call it the coordinate basis. We may expand the state vector using the coordinate basis:

$$\mid \Psi \rangle = \sum_j A_j(t) \mid j \rangle . \tag{39}$$

Here, $A_j(t)$ is the "wave function" at site j and time t. It is easy to see that $\boldsymbol{a}_{j+1}^\dagger \boldsymbol{a}_j \mid j' \rangle = \delta_{j,j'} \mid j'+1 \rangle$. Hence, we have

$$\boldsymbol{a}_{j+1}^\dagger \boldsymbol{a}_j \mid \Psi \rangle = \sum_j A_j(t) \mid j+1 \rangle = \sum_j A_{j-1}(t) \mid j \rangle . \tag{40}$$

As aresult,

$$\boldsymbol{H} \mid \Psi \rangle = \sum_j \Big\{ -vA_{j-1}(t) - vA_{j+1}(t) \Big\} \mid j \rangle , \tag{41}$$

and the Schrödinger equation becomes:

$$i\partial_t A_j(t) = -vA_{j-1}(t) - vA_{j+1}(t) \tag{42}$$

Let $A_j(t) = e^{-iEt} a_j$. After seperation of variables, we would have the follwing second order recursive relation:

$$Ea_j = -va_{j-1} - va_{j+1}. \tag{43}$$

To solve the above equation, we let $a_j = \alpha s^j$:

$$E = -v(s^{-1} + s) \Rightarrow s^2 + \frac{E}{v} s + 1 = 0. \tag{44}$$

If we factor the equation into $(s - s_1)(s - s_2)$, we see

$$\begin{cases} s_1 + s_2 = -\frac{E}{v}, \\ s_1 \cdot s_2 = 1. \end{cases}$$

Setting $s_1 = s$ and $s_2 = s^{-1}$, the general solution for a_j is:

$$a_j = \alpha_+ s^j + \alpha_- s^{-j} \tag{45}$$

If the system satisfies the periodic BC: $a_N = a_0$, $a_{N+1} = a_1$, then, we have

$$\begin{cases} a_+ s^N + \alpha_- s^{-N} = \alpha_+ + \alpha_-, \\ \alpha_+ s^{N+1} + \alpha_- s^{-N-1} = \alpha_+ s + \alpha_- s^{-1}. \end{cases} \Rightarrow \begin{vmatrix} s^N - 1 & s^{-N} - 1 \\ s(s^N - 1) & s^{-1}(s^{-N} - 1) \end{vmatrix} = 0. \tag{46}$$

After simplification, we have $s^N = 1 \Rightarrow s = e^{ip}$, with $p = 2\pi k/N$ and $k \in \{0, 1, 2, \ldots, N-1\}$ or arbitrary N consecutive integers.

In the limit $N \to \infty$, $p \in [0, 2\pi)$ or $(-\pi, \pi]$. p is the lattice momentum, and $[0, 2\pi)$ or $(-\pi, \pi]$ is the Brillouin Zone (BZ). We may expand the annihilation and creation operators in the momentum space:

$$\begin{cases} \boldsymbol{a}_j = \int_0^{2\pi} \frac{dp}{2\pi} \boldsymbol{a}(p) e^{ipj}, \\ \boldsymbol{a}_j^\dagger = \int_0^{2\pi} \frac{dp}{2\pi} \boldsymbol{a}^\dagger(p) e^{-ipj}. \end{cases} \tag{47}$$

In terms of $\boldsymbol{a}(p)$ and $\boldsymbol{a}^\dagger(p)$, the Hamiltonian in eq. (37) may be re-written as

$$\boldsymbol{H} = \int_0^{2\pi} \frac{dp}{2\pi} E(p) \boldsymbol{a}^\dagger(p) \boldsymbol{a}(p). \tag{48}$$

Here, $E(p) = \omega(p) = -2t \cos p$ gives the dispersion relation in the momentum space.

$$\frac{d\omega}{dk} = 2t \sin p, \tag{49}$$

is the group velociy. For $p \approx 0$, $E(p) \approx -2t \left\{1 - \frac{p^2}{2}\right\}$. Consequently, the dispersion relation is equivalent to that of a classical particle with effective mass

$$m_{\text{eff}} = \frac{1}{2t}. \tag{50}$$

The energy eigenstate

$$\mid \psi \rangle = \sum_j \psi_j \boldsymbol{a}_j^\dagger \mid 0 \rangle = \int_0^{2\pi} \frac{dp}{2\pi} \left\{ \tilde{\psi}(p) \mid p \rangle \right\}. \tag{51}$$

Here,

$$\mid p \rangle = \boldsymbol{a}^\dagger(p) \mid 0 \rangle \tag{52}$$

is the momentum eigenstate, and

$$\tilde{\psi}(p) = \sum_j \psi_j e^{-ipj}. \tag{53}$$

is the wave function in the momentum space.

4.2 Finite Lattice

Consider a finite lattice with N sites ($j = 1, 2, \ldots, N$). The interior equations are:

$$v(a_{j-1} + a_{j+1}) = \Omega a_j \quad \text{for } j = 2, \ldots, N-1. \tag{54}$$

Open Boundary Conditions: $a_0 = 0$ and $a_{N+1} = 0$.

$$\begin{cases} a_0 = 0 \Rightarrow \alpha_+ + \alpha_- = 0, \\ a_{N+1} = 0 \Rightarrow \alpha_+ s^{N+1} + \alpha_- s^{-(N+1)} = 0. \end{cases} \tag{55}$$

For non-trivial solutions ($\alpha_+, \alpha_- \neq 0$), the characteristic determinant must vanish, leading to:

$$s^{2(N+1)} = 1 \tag{56}$$

Thus, r lies on the unit circle in the complex plane:

$$s_k = e^{i\theta_k}, \quad \theta_k = \frac{\pi k}{N+1}, \quad k = 1, \ldots, N. \tag{57}$$

Dispersion Relation and Wavefunctions of Energy Eigenstate:
Substituting $s_1 = e^{i\theta_k}$ and $s_2 = e^{-i\theta_k}$ into $s_1 + s_2 = \frac{E}{v}$:

$$E_k = -2v \cos\left(\frac{\pi k}{N+1}\right), \quad k = 1, \ldots, N. \tag{58}$$

With $\alpha_- = -\alpha_+$, the standing-wave spatial eigenfunctions become:

$$a_j^{(k)} = \beta_k \sin\left(\frac{\pi k j}{N+1}\right). \tag{59}$$

Again, this may be viewed as the following eigenvalue problem:

$$\tilde{E}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \\ a_N \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 & \cdots & 0 \\ -1 & 0 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -1 & 0 & -1 \\ 0 & \cdots & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \\ a_N \end{pmatrix}, \tag{60}$$

where $\tilde{E} = E/v$. Note that the above matrix commutes with that in eq. (34). Thus, it is no wonder that the two matrices may be simultaneously diagonalized by the same eigenvectors.

Homework: Choose $N = 30$ and use mathematica or python to find the eigenvalues of the matrix in eq. (60) numerically and compare the result with the analytic one given in eq. (58).