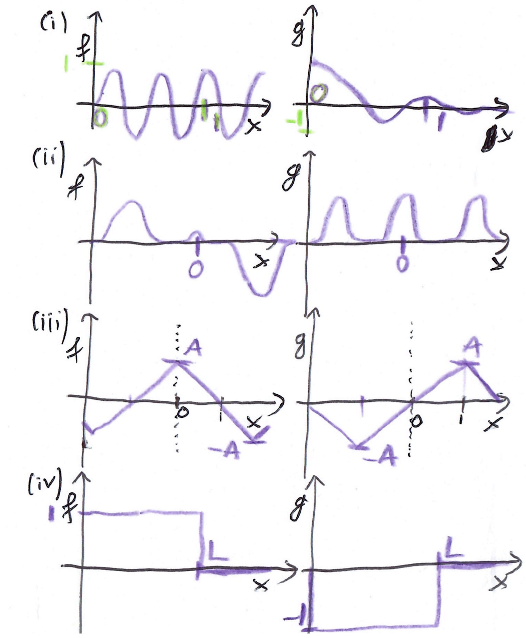
PHY 303, I-Semester 2021/22, Tutorial 2 Solution

Stage 1 *(functions as vectors)*

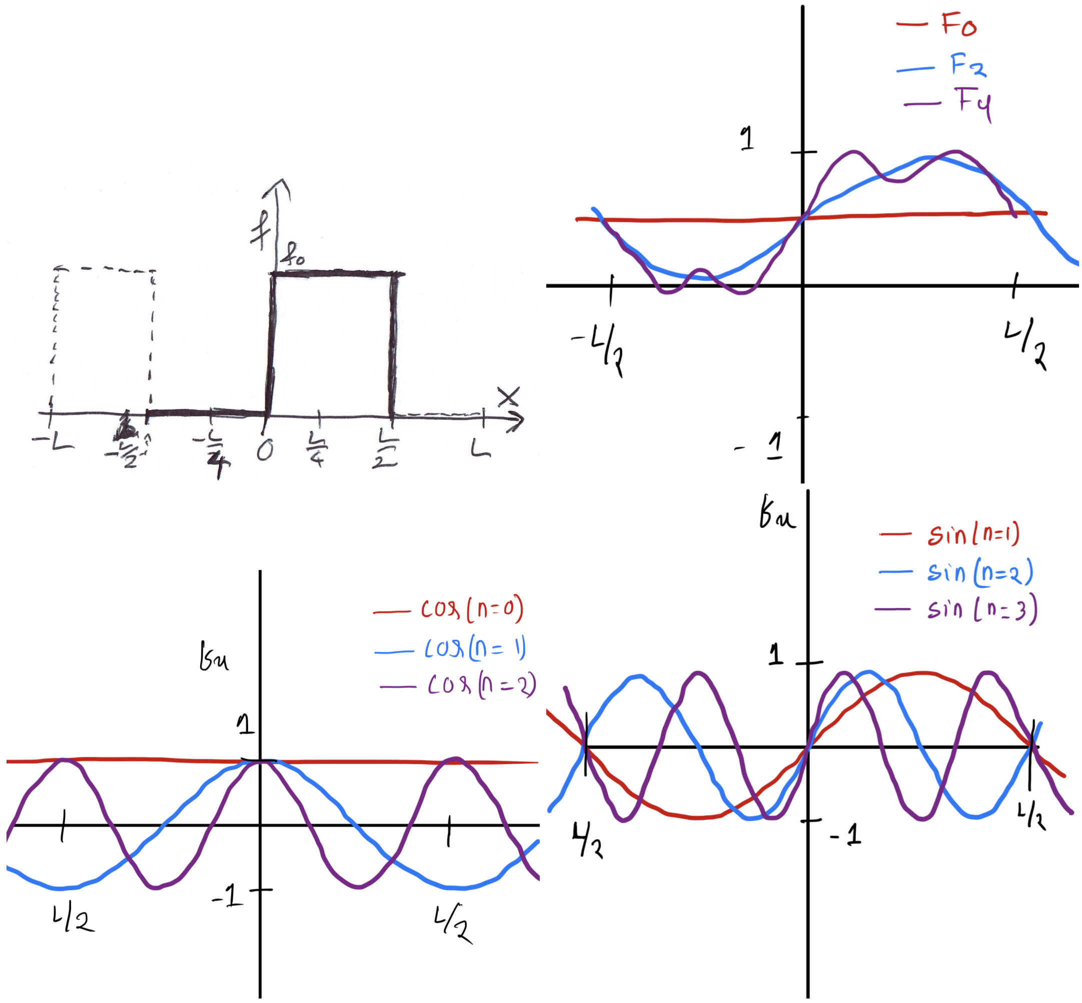
(i) Discuss for the function pairs drawn below how orthogonal they are. Rank/order the pairs (i)-(iv) regarding "how orthogonal" they are.



Solution: (iii) fully orthogonal since one is even and one is odd > (ii) Mostly orthogonal, again since the main peaks are even and one and odd in the other. In the middle the tiny bump near $x = 0$ in f will produce a bit of overlapp though. (i) Fair bit of overlap near the origin > (iv) Not at all orthogonal since one is a constant (-1) times the other. For vectors this would imply they are parallel but point in opposite directions.

(ii) Expand the function $f(x) = 1$ for $0 < x < L/2$, $f(x) = 0$ otherwise, in terms of the basis-set $b_n = \{b_n^{(e)}, b_n^{(o)}\} = \{\cos(2\pi nx/L), \sin(2\pi nx/L)\}$ for $n = 0, 1, 2, 3, \cdots$ initially with using drawings. These basis functions are appropriate for periodic functions with period L in between $-L/2$ and $L/2$ [see Eq. (1.20)], so let us assume the function $f(x)$ periodically repeated in this manner as shown by the dashed line. Don't worry about normalisation of the b_n at this point. Draw first the function (as below), then the 5 most slowly varying basis elements, then the first three different terms k in the sequential sum

$$F_k = \sum_{n=0}^{n=k} (f_n^{(e)} b_n^{(e)} + f_n^{(o)} b_n^{(o)}). \quad (1)$$



Solution: See above for (ugly) drawings of the first few basis functions: (bottom left) even, (bottom right) odd. You should make slightly prettier drawings than this, but the really important points in a drawing are usually only: Where are the functions zero? Where are maxima and minima and what values do they take there? Always add axes labels! When drawing these, we see that since the function $f(x)$ is asymmetric, we cannot use the symmetric basis functions. Thus the cumulative sum (top right) only contains the first and 3rd sine function with constant, and consecutively gets closer to the real step function.

(iii) Now, let's check our intuition with a calculation of the basis expansion coefficients f_n, in Eq. (1.18). Discuss how to find these coefficients. Now normalisation will turn out to be important, so first normalize the b_n, carefully distinguishing $n = 0$ and $n > 0$. Then find an equation for the coefficients f_n and compare with your guess from (ii).
Solution: For $n = 0$ the first sine does not exist and the normalisation integral for the first cosine is $\int_{-L/2}^{L/2} dx \cos(0) = L$, hence we write a normalized

basis function $\bar{b}_0(x) = \frac{1}{\sqrt{L}}$*. For higher* n *we need to integrate e.g.*

$$\int_{-L/2}^{L/2} dx\, |b_n(x)|^2 = \int_{-L/2}^{L/2} dx\ \underbrace{\cos(2\pi nx/L)}_{\equiv g(x)}\underbrace{\cos(2\pi nx/L)}_{\equiv h'(x)}$$

$$\overset{I.b.P.}{=} \underbrace{\underbrace{\cos(2\pi nx/L)\left(\frac{L}{2\pi n}\right)\sin(2\pi nx/L)}_{g(x)h(x)}\Big|_{-L/2}^{L/2}}_{=0} - \int_{-L/2}^{L/2} dx\ \underbrace{\underbrace{[-\sin^2(2\pi nx/L)]}_{g'(x)h(x)}}_{=-[1-\cos^2]}.$$

$$\Leftrightarrow 2\int_{-L/2}^{L/2} dx\ \cos^2(2\pi nx/L) = \int_{-L/2}^{L/2} dx\, 1 \Leftrightarrow \int_{-L/2}^{L/2} dx\ \cos^2(2\pi nx/L) = \frac{L}{2}.$$

The exact same tricks also give you $\int_{-L/2}^{L/2} dx\ \sin^2(2\pi nx/L) = \frac{L}{2}$*, thus all the* $n > 0$ *basis functions are normalized as* $\bar{b}_n = \{\bar{b}_n^{(e)}, \bar{b}_n^{(o)}\} = \{\sqrt{\frac{2}{L}}\cos(2\pi nx/L), \sqrt{\frac{2}{L}}\sin(2\pi nx/L)\}$*.*

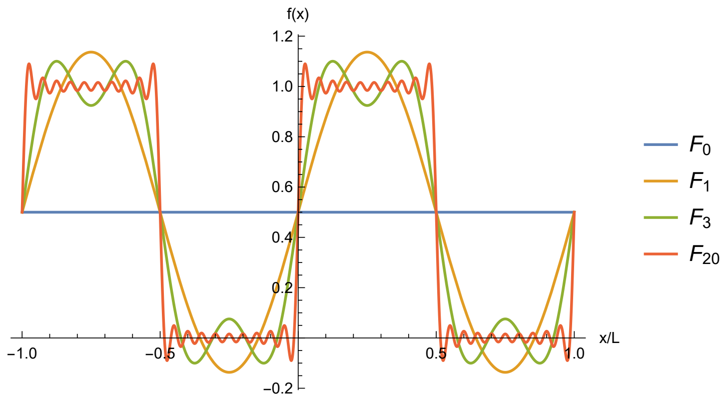
To finally expand the function $f(x)$*, we project* $(\bar{b}_n, f(x))$ *as in the equation below Eq. (1.18), hence* $f(x) = \sum_{n=0}^{\infty}(f_n^{(e)}\bar{b}_n^{(e)} + f_n^{(o)}\bar{b}_n^{(o)})$*, with* $f_n^{(e)} = (\bar{b}_n^{(e)}, f)$*,* $f_n^{(o)} = (\bar{b}_n^{(o)}, f)$*, see Eq. (1.17). Thus*

$$\begin{aligned} f_n^{(o)} &= \int_{-L/2}^{L/2}\sqrt{\frac{2}{L}}\sin(2\pi nx/L)f(x)dx = \int_0^{L/2} dx\ \sin(2\pi nx/L) \times \underbrace{1}_{=f} \\ &= -\sqrt{\frac{2}{L}}\left(\frac{L}{2\pi n}\right)\cos(2\pi nx/L)\Big|_0^{L/2} = \sqrt{\frac{L}{2}}\frac{[1-\cos(n\pi)]}{(n\pi)}. \end{aligned} \tag{2}$$

For n *even* $f_n^{(o)} = 0$ *i.e., only odd order sine functions will be there in the expansion. However for* $n > 0$

$$\begin{aligned} f_n^{(e)} &= \int_{-L/2}^{L/2} dx\ \sqrt{\frac{2}{L}}\cos(2\pi nx/L)f(x) = \int_0^{L/2} dx\ \sqrt{\frac{2}{L}}\cos(2\pi nx/L) \times \underbrace{1}_{=f} \\ &= \sqrt{\frac{2}{L}}\left(\frac{L}{2\pi n}\right)\sin(2\pi nx/L)\Big|_0^{L/2} = \sqrt{\frac{L}{2}}\frac{\sin(n\pi)}{(n\pi)}. \end{aligned} \tag{3}$$

The function $\sin(x)/x$ *is called "sinc function" (google). For* $n = 0$ *we separately find* $f_0^{(e)} = \int_0^{L/2} dx\ 1/\sqrt{L} = \sqrt{L}/2$*. While for* $n \neq 0$ *we have* $f_n^{(e)} = 0$*. This corroborates our view in point (ii) not to use any cosines expect of order* $n = 0$ *which is* 1*. With these exact coefficients, we can now plot the requested cumulative terms* F_k *from Eq. (1) one by one and find e.g. the graph below.*



(iv) Discuss similarities and differences between the above and how you expand a geometrical vector $\mathbf{x}$ in terms of a basis.
Solution: The procedure is almost the same, also for writing $\mathbf{v} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3$, *we find the coefficients by projecting the vector onto each basis vector* $v_k = \mathbf{b}_k \cdot \mathbf{v}$. *The key difference is, that we now have an infinite number of basis functions, and the scalar-product takes a slightly different form.*

Stage 2 *(Discretized operators)* Discuss the operator discretisation that we did in example 10 of the lecture for two new operators: (i) the second derivative $\hat{O} = \frac{d^2}{dx^2}$ and the Hamiltonian $\hat{H}$ including some potential $V(x)$. Discuss which matrix you expect. Hint: Either use a finite version of the limit for the second derivative, or matrix multiplication.
Solution: From math courses, we know that

$$\frac{d^2}{dx^2}f(x) = \lim_{\Delta x \to 0} \frac{-f(x-\Delta x) + 2f(x) - f(x+\Delta x)}{(\Delta x)^2} \tag{4}$$

If we again skip the limit $\Delta x \to 0$, *we can write this in a similar form as example 10, so we get:*

$$\underline{\underline{O}}^{(2)} = \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & \\ 1 & -2 & 1 & 0 & 0 & 0 & \\ 0 & 1 & -2 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & -2 & 1 & 0 & \\ 0 & 0 & 0 & 1 & -2 & 1 & \\ 0 & 0 & 0 & 0 & 1 & -2 & \\ & & & \vdots & & & \end{bmatrix}, \tag{5}$$

We could also use $\frac{d^2}{dx^2}\cdots = \frac{d}{dx}\frac{d}{dx}\cdots$ *and thus take* $\underline{\underline{O}} \cdot \underline{\underline{O}}$, *where* $\underline{\underline{O}}$ *is the matrix* *from example 10. This will give us*

$$\underline{\underline{O}}^{(2)} = \frac{1}{2(\Delta x)^2}\begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 & \\ 0 & -2 & 0 & 1 & 0 & 0 & \\ 1 & 0 & -2 & 0 & 1 & 0 & \cdots \\ 0 & 1 & 0 & -2 & 0 & 1 & \\ 0 & 0 & 1 & 0 & -2 & 0 & \\ 0 & 0 & 0 & 1 & 0 & -2 & \\ & & & \vdots & & & \end{bmatrix}, \tag{6}$$

which looks very similar and does in fact almost the same job (why are the residual differences ok?). Since the Hamiltonian contains a second derivative and the potential $V(x)$, we can plug the corresponding matrix together as:

$$\underline{\underline{H}} = -\frac{\hbar^2}{2m}\underline{\underline{O}}^{(2)} + \underline{\underline{V}}, \tag{7}$$

where

$$\underline{\underline{V}} = \begin{bmatrix} V(x_1) & 0 & 0 & 0 & \\ 0 & V(x_2) & 0 & 0 & \\ 0 & 0 & V(x_3) & 0 & \cdots \\ 0 & 0 & 0 & V(x_4) & \end{bmatrix}, \tag{8}$$

(see also assignment 2 Q4).

Stage 3 *(Normalisation)* Find out which of the following wavefunctions can be normalized and normalise those as suggested in section 1.6.1. You may do any integrations with `mathematica` or Wolfram Alpha . *In either the relevant command is, e.g.* ***`Integrate[sin[x],x,0,∞]`*** *for e.g.* $\int_0^\infty dx\ \sin(x)$*, followed by shift-ENTER. You enter ∞ as* ***`ESC inf ESC`*** *or* ***`inf`*** *respectively.*

$$\begin{aligned} \Psi(r) &= \frac{\cos(r)}{r}, \quad \text{on } 0 \le r \le \infty, \\ \Psi(x) &= \theta(D - |x|), \text{ with } D > 0 \text{ on } -\infty \le x \le \infty, \\ \Psi(x) &= e^{-|x|} \quad \text{on } -\infty \le x \le \infty. \end{aligned} \tag{9}$$

Above $\theta(x)$ is the Heaviside step function.

Solution: We find $\int_0^\infty dr \left|\frac{\cos(r)}{r}\right|^2 \to \infty$*, is not convergent on* $[0, \infty)$*. To have an idea which function we expect to be normalisable and which not, have a look at*

$$\int_\epsilon^R dr \frac{1}{r^\alpha} = -\frac{1}{(\alpha-1)R^{\alpha-1}} + \frac{1}{(\alpha-1)\epsilon^{\alpha-1}}, \qquad \textit{for } \alpha \neq 1, \tag{10}$$

$$\int_\epsilon^R dr \frac{1}{r^\alpha} = \log\left(\frac{R}{\epsilon}\right) \qquad \textit{for } \alpha = 1. \tag{11}$$

where we later want to make R arbitrarily large, and ϵ arbitrarily small. Now we see, that if $\alpha > 1$, the limit $\epsilon \to 0$ gives infinity, while the limit $R \to \infty$ is finite. For $\alpha = 1$ both give infinity, and for $\alpha < 1$ the limit $\epsilon \to 0$ remains finite, but the limit $R \to \infty$ is infinite. Now, whenever we know that in one of these limits a function approximately behaves like on of these power laws, we can know integral convergence without doing the calculation. In this case, since $\frac{\cos(r)}{r} \approx 1/r$ at small r, its integral will be logarithmically divergent at $r \to 0$.

$\int_{-\infty}^{\infty} dx\ |\theta(D - |x|)|^2 = \int_{-D}^{D} dx 1 = 2D$, hence this function is normalisable.

$\int_{-\infty}^{\infty} dx\ e^{-2|x|} = 2\int_0^{\infty} dx\ e^{-2x} = -e^{-2x}\Big|_0^{\infty} = 1$ hence this function is already normalized.

Stage 4 Suppose a quantum wavefunction is $\phi(x) \sim f(x)$, where $f(x)$ is the function from Stage 1 (ii), without the periodic repeats at $|x| > L$. Normalise that wavefunction, and then find the expectation value of position and uncertainty of position.

Solution: We have $\int_{-\infty}^{\infty} dx\,|\phi(x)|^2 = \int_{-\infty}^{\infty} dx\, f(x)^2 = \int_0^{L/2} dx\, 1 = L/2$. Using the procedure below Eq. (1.27), we know that $\bar{\phi}(x) = f(x)\sqrt{2/L}$ will be normalized correctly. Then:

$$\langle \hat{x} \rangle \overset{Eq.\ (1.28)}{=} \int_{-\infty}^{\infty} dx\, x|\bar{\phi}(x)|^2 = \frac{2}{L}\int_0^{L/2} dx x = \frac{L}{4}. \tag{12}$$

$$\begin{aligned}\langle \hat{x}^2 \rangle &= \int_{-\infty}^{\infty} dx\, x^2|\bar{\phi}(x)|^2 = \frac{2}{L}\int_0^{L/2} dx x^2 \\ &= \frac{2}{L}\left(\frac{x^3}{3}\Big|_0^{L/2}\right) = 2 \times \frac{L^2}{3 \times 2^3} = \frac{L^2}{12}.\end{aligned} \tag{13}$$

Assembling both into the uncertainty σ_x from Eq. (1.35) gives

$$\sigma_x = \sqrt{\frac{L^2}{12} - \frac{L^2}{16}} = \frac{L}{4\sqrt{3}}, \tag{14}$$

which seems reasonable considering the drawing.