Problem 1 – Hartree product

Do exercise 2.2 on page 48 in Szabo and Ostlund.

Problem 2 – linear operators

(a) Prove that the time derivative $\frac{\partial}{\partial t}$ is a linear operator. Use the definition of a derivative and the definition of a linear operator.

(b) Prove that $V(x)$ is a linear operator.

(c) Prove that the sum of two linear operators is linear.

Problem 3 – vector spaces

The motivation for this question is to help you understand the linear vector space structure of quantum mechanics.

For finite-dimensional vector spaces, the concept of a basis, and of an orthonormal basis, is straightforward. In the Euclidean space $\mathbb{R}^n$, two vectors $u, v$ are orthogonal if $u \cdot v = 0$. The length of a vector $u$ is $\|u\| = \sqrt{u \cdot u}$. The projection of $u$ on $v$ is given by $\frac{u \cdot v}{v \cdot v}v$. The only operator we used in all of this is the scalar product $(\cdot)$ defined on the vector space, which in this case is the dot product.

A basis is a set of vectors $\{e_1, e_2, \ldots\}$ for which any vector $x$ can be written as a linear combination of the basis vectors, namely $x = c_1e_1 + c_2e_2 + \cdots$, where $\{c_1, c_2, \ldots\}$ are real numbers. The basis is normalized if all the basis vectors have unit length, $\|e_1\| = 1$, $\|e_2\| = 1$, $\cdots$. The basis is orthogonal if $e_i \cdot e_j = 0$ for $i \neq j$. The basis is called orthonormal if it is both normalized and orthogonal.

In $\mathbb{R}^2$, the orthonormal basis $\{e_1 = (1, 0), e_2 = (0, 1)\}$ is very easy to work with, because any vector $x = (a, b)$ can simply be written $x = ae_1 + be_2$. See Fig. 1 for a geometrical picture.

In general, to resolve a vector into a linear combination of basis vectors, we need to solve the linear equation $x = c_1e_1 + c_2e_2$. For the example we are discussing here, things work out nicely because if we take the scalar product with $e_1$ on both sides we get

$$x \cdot e_1 = c_1e_1 \cdot e_1 + c_2e_2 \cdot e_1$$

which simplifies to $x \cdot e_1 = c_1$ because of the orthonormality of the basis, and we easily find $c_1$ because we can calculate $x \cdot e_1 = (a, b) \cdot (1, 0) = a$. 1
FIG. 1: For the basis \( \{e_1 = (1, 0), e_2 = (0, 1)\} \), we have \( x = (a, b) \) as \( x = ae_1 + be_2 \).

(a) In \( \mathbb{R}^2 \), consider the basis \( \{e_1 = (1, 0), e_2 = \frac{1}{\sqrt{2}}(-1, 1)\} \). Is this basis normalized? Is it orthogonal? For the general vector \( x = (a, b) \), write \( x \) as a linear combination of the basis vectors. For the specific vector \( x = (2, 1) \), write \( x \) as a linear combination of the basis vectors and draw a picture for this case similar to Fig. 1.

(b) In \( \mathbb{R}^2 \), consider the basis \( \{e_1 = \frac{1}{\sqrt{2}}(1, 1), e_2 = \frac{1}{\sqrt{2}}(1, -1)\} \). Is this basis normalized? Is it orthogonal? For the general vector \( x = (a, b) \), write \( x \) as a linear combination of the basis vectors. For the specific vector \( x = (2, 1) \), write \( x \) as a linear combination of the basis vectors and draw a picture for this case similar to Fig. 1.

(c) For the infinite dimensional vector space of quantum mechanics, the dot product is replaced with integration, and we have

\[
f \cdot g = \int f(x)g(x)dx
\]
for functions $f(x)$, $g(x)$ of one variable. Otherwise things are pretty much the same as for the finite dimensional cases discussed above. Consider the square well potential, defined by the potential

$$V(x) = \begin{cases} \infty & (x < 0) \\ 0 & (0 < x < L) \\ \infty & (x > L) \end{cases}$$

Write down the Hamiltonian operator for this problem, and write down the eigenfunctions (eigenvectors) for the time-independent Schrödinger equation. You do not have to show any work. Normalize the eigenfunctions if they are not already normalized. The (normalized) eigenfunctions resulting from solving the time-independent Schrödinger equation form an orthonormal basis. This is a deep mathematical result (Sturm-Liouville theory). This means that for any function $f(x)$, we should be able to express $f(x)$ as a linear combination of the basis functions. Consider the function

$$f(x) = \begin{cases} 0 & (x < 0) \\ x & (0 < x < L/2) \\ -x + L & (L/2 < x < L) \\ 0 & (x > L) \end{cases}$$

Write this function as a linear combination of the basis functions (by explicitly finding the expansion coefficients). We plotted this series in class.

Hints:

- integration by parts is useful for this problem
- for any integral, $\int_a^b g(x)dx = \int_a^c g(x)dx + \int_c^b g(x)dx$ for any $a,b,c$ real numbers.

(d) Is the function $f(x)$ a solution to the time-independent Schrödinger equation (for the square well problem we are considering here)?

**Problem 4 – operators**

Explain why

$$A = |\psi\rangle\langle\phi|$$

is an operator.

**Problem 5 – bra/ket**

What bra should you associate with the ket $\lambda_1|\phi_1\rangle + \lambda_2|\phi_2\rangle$?
Let $\phi(r)$ and $\psi(r)$ be two wave functions which can be expanded in the $u$ basis as follows:

$$\phi(r) = \sum_i b_i u_i(r)$$  \hspace{1cm} (4)

$$\psi(r) = \sum_j c_j u_j(r)$$  \hspace{1cm} (5)

Derive an expression for the scalar product $(\phi, \psi)$ in terms of the $b$ and $c$ expansion coefficients.