Physics 195a
Course Notes
Ideas of Quantum Mechanics – Solutions to Exercises
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1 Exercises

1. Show that L^2 is complete.

2. Complete the proof that the space $L^2(a,b)$ is separable.

3. Show that if $x \in H$, where H is a separable Hilbert space, is orthogonal to every vector in a dense set, then $x = 0$.

   Solution: Let $\{y_\alpha\} \subset H$ be a set of elements dense in H such that

   $$\langle x|y_\alpha\rangle = 0, \qquad \forall\alpha. \tag{1}$$

   Consider an element $y \in H$, in the closure of the set $\{y_\alpha\}$. We wish to show that

   $$\langle x|y\rangle = 0. \tag{2}$$

   If we can show this, then we have demonstrated that x is orthogonal to every element of H (including x), and hence $x = 0$, since H is a metric space.

   Since the closure of the dense set $\{y_\alpha\}$ is obtained by including the limits of all Cauchy sequences of elements of $\{y_\alpha\}$, we may consider such a Cauchy sequence, say, $z_1, z_2, \ldots$, such that

   $$\lim_{n\to\infty} z_n = z. \tag{3}$$

   Thus,

   $$\begin{aligned} |\langle x|z\rangle| &= |\langle x|z\rangle - \langle x|z_n\rangle|, \qquad \text{since } \langle x|z_n\rangle = 0, & (4)\\ &= |\langle x|z - z_n\rangle| & (5)\\ &= |\langle x|\lim_{j\to\infty}(z_j - z_n)\rangle|. & (6) \end{aligned}$$

   But we can pick n to be sufficiently large that the ket vector is as close as we wish to the zero vector. Hence $|\langle x|z\rangle|$ is smaller than any positive number, and must be zero.

4. Complete the proof of the Schwarz inequality.

Solution: Given any two vectors $\phi, \psi \in H$, consider the quantity:

$$\langle \phi + re^{i\theta}\psi | \phi + re^{i\theta}\psi \rangle \geq 0, \tag{7}$$

where r and θ are real numbers. The value 0 is attained if and only if $\phi + re^{i\theta}\psi = 0$. Expand to obtain:

$$r^2\langle \psi|\psi\rangle + 2r\Re\left(e^{i\theta}\langle\phi|\psi\rangle\right) + \langle\phi|\phi\rangle \geq 0. \tag{8}$$

Equality holds if and only if ϕ and ψ are linearly dependent. Suppose they are not; then the relation is a strict inequality, and there is no real solution for r for the equality. Hence, the discriminant must be negative:

$$\left[\Re\left(e^{i\theta}\langle\phi|\psi\rangle\right)\right]^2 - \langle\psi|\psi\rangle\langle\phi|\phi\rangle < 0, \tag{9}$$

or, since this must hold for all phases θ,

$$|\langle\phi|\psi\rangle| < \sqrt{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}. \tag{10}$$

The case where ϕ and ψ are linearly related is readily verified.

5. Complete the derivation of Eqns. 80, 81, and 82.

Solution: For equation 80, first note that:

$$\begin{aligned}
[x_j p_k, x_m p_n] &= x_j p_k x_m p_n - x_m p_n x_j p_k \\
&= x_j x_m p_k p_n + x_j[p_k, x_m]p_n - x_m x_j p_n p_k - x_m[p_n, x_j]p_k \\
&= -i x_j p_n \delta_{mk} + i x_m p_k \delta_{nj}.
\end{aligned}$$

Then,

$$\begin{aligned}
[L_\alpha, L_\beta] &= \epsilon_{\alpha jk}\epsilon_{\beta mn}[x_j p_k, x_m p_n] \\
&= i\epsilon_{\alpha jk}\epsilon_{\beta mn}(-x_j p_n \delta_{mk} + x_m p_k \delta_{nj}) \\
&= i(-\epsilon_{\alpha jm}\epsilon_{\beta mn} x_j p_n + \epsilon_{\alpha jk}\epsilon_{\beta mj} x_m p_k) \\
&= i(-\epsilon_{\alpha mj}\epsilon_{\beta jn} x_m p_n + \epsilon_{\alpha jn}\epsilon_{\beta mj} x_m p_n) \\
&= i(\epsilon_{\alpha jm}\epsilon_{\beta jn} - \epsilon_{\alpha jn}\epsilon_{\beta jm}) x_m p_n.
\end{aligned}$$

For equation 81, start with the definition:

$$E_{\alpha\beta,mn} \equiv \epsilon_{\alpha jm}\epsilon_{\beta jn} - \epsilon_{\alpha jn}\epsilon_{\beta jm}. \tag{11}$$

Note first that $E_{\alpha\beta,mn} = 0$ if $\alpha = \beta$ or if $m = n$, because then the two terms will cancel. Now assume that $\alpha \neq \beta$ and $m \neq n$. If $\alpha \neq m$ and $\alpha \neq n$, then we again get zero, since if $j \neq \alpha$ and $j \neq m$, then $j = n$, which means the first term is zero; similarly for the second term. Likewise, we have zero if $\beta \neq m$ and $\beta \neq n$. Thus, consider $\alpha = m$; in this case:

$$\begin{aligned} E_{m\beta,mn} &= -\epsilon_{mjn}\epsilon_{\beta jm} \\ &= \epsilon_{mjn}\epsilon_{mj\beta} = 1 \quad nb.\ \beta \neq m. \end{aligned} \tag{12}$$

Likewise, when $\alpha = n$ we get -1. Putting all these facts together, we have

$$E_{\alpha\beta,mn} = \epsilon_{\alpha j\beta}\epsilon_{mjn}. \tag{13}$$

For equation 82, we use 80 and 81:

$$\begin{aligned} [L_\alpha, L_\beta] &= iE_{\alpha\beta,mn}x_m p_n \\ &= i\epsilon_{\alpha j\beta}\epsilon_{mjn}x_m p_n \\ &= -i\epsilon_{\alpha j\beta}\epsilon_{jmn}x_m p_n \\ &= -i\epsilon_{\alpha j\beta}L_j \\ &= i\epsilon_{\alpha\beta j}L_j. \end{aligned} \tag{14}$$

6. Time Reversal in Quantum Mechanics:

We wish to define an operation of time reversal, denoted by T, in quantum mechanics. We demand that T be a "physically acceptable" transformation, *i.e.*, that transformed states are also elements of the Hilbert space of acceptable wave functions, and that it be consistent with the commutation relations between observables. We also demand that T have the appropriate classical correspondence with the classical time reversal operation.

Consider a system of structureless ("fundamental") particles and let $\vec{X} = (X_1, X_2, X_3)$ and $\vec{P} = (P_1, P_2, P_3)$ be the position and momentum operators (observables) corresponding to one of the particles in the system. The commutation relations are, of course:

$$[P_m, X_n] = -i\delta_{mn},$$

$$[P_m, P_n] = 0,$$
$$[X_m, X_n] = 0.$$

The time reversal operation $T : t \to t' = -t$, operating on a state vector gives (in Schrödinger picture – you may consider how to make the equivalent statement in the Heisenberg picture):

$$T|\psi(t)\rangle = |\psi'(t')\rangle.$$

The time reversal of any operator, Q, representing an observable is then:

$$Q' = TQT^{-1}$$

(a) By considering the commutation relations above, and the obvious classical correspondence for these operators, show that

$$TiT^{-1} = -i.$$

Thus, we conclude that T must contain the complex conjugation operator K:

$$KzK^{-1} = z^*,$$

for any complex number z, we require that T on any state yields another state in the Hilbert space. We can argue that (for you to think about) we can write: $T = UK$, where U is a unitary transformation. If we operate twice on a state with T, then we should restore the original state, up to a phase:

$$T^2 = \eta 1,$$

where η is a pure phase factor (modulus = 1).

Solution: Consider

$$\begin{aligned} T[P_1, X_1]T^{-1} &= T(-i)T^{-1} & (15)\\ &= T(P_1X_1 - X_1P_1)T^{-1} & (16)\\ &= TP_1T^{-1}TX_1T^{-1} - TX_1T^{-1}TP_1)T^{-1} & (17)\\ &= (-P_1)X_1 - X_1(-P_1) & (18)\\ &= i. & (19) \end{aligned}$$

(b) Prove that $\eta = \pm 1$. Hence, $T^2 = \pm 1$. Which phase applies in any given physical situation depends on the nature of U, and will turn out to have something to do with spin, as we shall examine in the future.

Solution: Consider T^3:

$$\begin{aligned} T^3 &= T^2 T = \eta T \quad (20) \\ &= T T^2 = T\eta = T\eta T^{-1} T = \eta^* T. \quad (21) \end{aligned}$$

Hence $\eta = \eta^*$, and since it is of modulus one, we must have $\eta = \pm 1$.

7. Let us consider the action of Gallilean transformations on a quantum mechanical wave function. We restrict ourselves here to the "proper" Gallilean Transformations: (*i*) translations; (*ii*) velocity boosts; (*iii*) rotations. We shall consider a transformation to be acting on the state (not on the observer). Thus, a translation by $\mathbf{x}_0$ on a state localized at $\mathbf{x}_1$ produces a new state, localized at $\mathbf{x}_1 + \mathbf{x}_0$. In "configuration space", we have a wave function of the form $\psi(\mathbf{x}, t)$. A translation $T(\mathbf{x}_0)$ by $\mathbf{x}_0$ of this state yields a new state (please don't confuse this translation operator with the time reversal operator of the previous problem, also denoted by T, but without an argument):

$$\psi'(\mathbf{x}) = T(\mathbf{x}_0)\psi(\mathbf{x}, t) = \psi(\mathbf{x} - \mathbf{x}_0, t). \quad (22)$$

Note that we might have attempted a definition of this transformation with an additional introduction of some overall phase factor. However, it is our interest to define such operators as simply as possible, consistent with what should give a valid classical correspondence. Whether we have succeeded in preserving the appropriate classical limit must be checked, of course.

Consider a free particle of mass m. The momentum space wave function is

$$\hat{\psi}(\mathbf{p}, t) = \hat{f}(\mathbf{p}) \exp\left(-\frac{itp^2}{2m}\right), \quad (23)$$

where $p = |\mathbf{p}|$. The configuration space wave function is related by the (inverse) Fourier transform:

$$\psi(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{(\infty)} d^3(\mathbf{p}) e^{i\mathbf{x}\cdot\mathbf{p}} \hat{\psi}(\mathbf{p}, t). \quad (24)$$

Obtain simple transformation laws, on both the momentum and configuration space wave functions, for each of the following proper Gallilean transformations:

(a) Translation by $\mathbf{x}_0$: $T(\mathbf{x}_0)$ (note that we have already seen the result in configuration space).

Solution: [Should draw a figure...] In configuration space, the result was:

$$\psi'(\mathbf{x}, t) = T(\mathbf{x}_0)\psi(\mathbf{x}, t) = \psi(\mathbf{x} - \mathbf{x}_0, t). \tag{25}$$

Thus, in momentum space, we have:

$$\begin{aligned}
\hat{\psi}'(\mathbf{p}, t) &= T(\mathbf{x}_0)\hat{\psi}(\mathbf{p}, t) && (26)\\
&= \frac{1}{(2\pi)^{3/2}} \int_{(\infty)} e^{-i\mathbf{p}\cdot\mathbf{x}} \psi'(\mathbf{x}, t) d^3(\mathbf{x}) \\
&= \frac{1}{(2\pi)^{3/2}} \int_{(\infty)} e^{-i\mathbf{p}\cdot\mathbf{x}} \psi(\mathbf{x} - \mathbf{x}_0, t) d^3(\mathbf{x}) \\
&= \frac{1}{(2\pi)^{3/2}} \int_{(\infty)} e^{-i\mathbf{p}\cdot(\mathbf{x}+\mathbf{x}_0} \psi(\mathbf{x}, t) d^3(\mathbf{x}) \\
&= e^{-i\mathbf{p}\cdot\mathbf{x}_0} \hat{\psi}(\mathbf{p}, t). && (27)
\end{aligned}$$

(b) Translation by time t_0: $M(t_0)$.

Solution: Let's take the time translation to act on a configuration space wave function in the obvious way:

$$M(t_0)\psi(\mathbf{x}, t) = \psi(\mathbf{x}, t - t_0). \tag{28}$$

Likewise,

$$\begin{aligned}
M(t_0)\hat{\psi}(\mathbf{p}, t) &= \hat{\psi}(\mathbf{p}, t - t_0) && (29)\\
&= \exp\left(\frac{it_0 p^2}{2m}\right) \hat{\psi}(\mathbf{p}, t). && (30)
\end{aligned}$$

(c) Velocity boost by $\mathbf{v}_0$: $V(\mathbf{v}_0)$. (Hint: first find

$$\hat{\psi}'(\mathbf{p}, 0) = \hat{f}'(\mathbf{p}) = V(\mathbf{v}_0)\hat{f}(\mathbf{p}), \tag{31}$$

then

$$\hat{\psi}'(\mathbf{p}, t) = \hat{f}'(\mathbf{p}) e^{-itp^2/2m}, \tag{32}$$

etc.)

Solution: Under a velocity transformation, the space coordinates and momentum transform according to

$$\begin{aligned} \mathbf{x}' &= \mathbf{x} + \mathbf{v}_0 t && (33) \\ \mathbf{p}' &= \mathbf{p} + m\mathbf{v_0}. && (34) \end{aligned}$$

Thus, it appears reasonable to take

$$V(\mathbf{v}_0)\hat{f}(\mathbf{p}) = \hat{f}(\mathbf{p} - m\mathbf{v_0}). \tag{35}$$

Thus,

$$\begin{aligned} \hat{\psi}'(\mathbf{p}, t) &= \hat{f}'(\mathbf{p})e^{-itp^2/2m} && (36) \\ &= \hat{f}(\mathbf{p} - m\mathbf{v_0})e^{-itp^2/2m} \\ &= \hat{\psi}(\mathbf{p} - m\mathbf{v}_0, t) \exp\left[\frac{it(\mathbf{p} - m\mathbf{v}_0)^2}{2m}\right] e^{-itp^2/2m} \\ &= \exp\left[-it\left(\mathbf{p}\cdot\mathbf{v}_0 - \frac{1}{2}m\mathbf{v}_0^2\right)\right]\psi(\mathbf{p} - m\mathbf{v}_0, t). && (37) \end{aligned}$$

In configuration space, this becomes

$$\begin{aligned} \psi'(\mathbf{x}, t) &= \frac{1}{(2\pi)^{3/2}}\int_{(\infty)} d^3(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}}\psi'(\mathbf{p}, t) \\ &= \frac{1}{(2\pi)^{3/2}}\int_{(\infty)} d^3(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} \exp\left[-it\left(\mathbf{p}\cdot\mathbf{v}_0 - \frac{1}{2}m\mathbf{v}_0^2\right)\right]\psi(\mathbf{p} - m\mathbf{v}_0, t) \\ &= \frac{1}{(2\pi)^{3/2}}\int_{(\infty)} d^3(\mathbf{q})e^{i(\mathbf{q}+m\mathbf{v}_0)\cdot\mathbf{x}}e^{\left[-it\left((\mathbf{q}+m\mathbf{v}_0)\cdot\mathbf{v}_0 - \frac{1}{2}m\mathbf{v}_0^2\right)\right]}\psi(\mathbf{q}, t) \\ &= e^{im\mathbf{v}_0\cdot\mathbf{x}}e^{\left[-it\left(mv_0^2 - \frac{1}{2}m\mathbf{v}_0^2\right)\right]}\int_{(\infty)} \frac{d^3}{(2\pi)^{3/2}}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}\exp\left(-it\mathbf{q}\cdot\mathbf{v}_0\right)\psi(\mathbf{q}, t) \\ &= e^{\left[im\mathbf{v}_0\cdot\mathbf{x} - it\left(\frac{1}{2}m\mathbf{v}_0^2\right)\right]}\int_{(\infty)} \frac{d^3}{(2\pi)^{3/2}}(\mathbf{q})\exp\left(i\mathbf{q}\cdot\mathbf{x} - it\mathbf{q}\cdot\mathbf{v}_0\right)\psi(\mathbf{q}, t) \\ &= \exp\left[im\mathbf{v}_0\cdot\mathbf{x} - it\left(\frac{1}{2}m\mathbf{v}_0^2\right)\right]\psi(\mathbf{x} - \mathbf{v}_0 t, t) && (38) \end{aligned}$$

(d) Rotation about the origin given by 3×3 matrix R: $U(R)$.

Solution: For a rotation on a vector $\mathbf{x}$, rotating it to a new vector $\mathbf{x}'$, $x' = R\mathbf{x}$. Acting on a wave function, the rotated wave function ψ', when evaluated at a rotated point $\mathbf{x}'$, is the same as the unrotated wave function evaluated at the unrotated point $\mathbf{x}$:

$$\psi'(\mathbf{x}', t) = \psi'(R\mathbf{x}, t) = \psi(\mathbf{x}, t). \tag{39}$$

Thus,

$$\psi'(\mathbf{x}, t) = R_{\text{op}}\psi(\mathbf{x}, t) = \psi(R^{-1}\mathbf{x}, t). \tag{40}$$

I have used the notation R_{op} to distinguish the operator on the Hilbert space from the 3×3 matrix R.

In momentum space, we may note that the same argument holds for momenta, or we may Fourier transform the configuration space result. In either event, we obtain

$$R_{\text{op}}\hat{\psi}(\mathbf{p}, t) = \hat{\psi}(R^{-1}\mathbf{p}, t). \tag{41}$$

Make sure your answers make sense to you in terms of classical correspondence.

8. Consider the vector space of real continuous functions with continuous first derivatives in the closed interval $[0, 1]$. Which of the following defines a scalar product?

   (a) $\langle f|g\rangle = \int_0^1 f'(x)g'(x)dx + f(0)g(0)$

   (b) $\langle f|g\rangle = \int_0^1 f'(x)g'(x)dx$

   Solution: A scalar product must satisfy, for any $f, g, h \in V$, the conditions:

   (a) $\langle f|f\rangle \geq 0, \quad$ with $\langle f|f\rangle = 0$ iff $f = 0$.

   (b) $\langle f|g\rangle = \langle g|f\rangle^*$.

   (c) $\langle f|cg\rangle = c\langle f|g\rangle$, where c is any complex number.

   (d) $\langle f|g + h\rangle = \langle f|g\rangle + \langle f|h\rangle$.

   In the present case, we are dealing with real vector spaces, hence the second condition becomes $\langle f|g\rangle = \langle g|f\rangle$ and the constant in the third condition is restricted to be a real number.

   It may be readily checked that the scalar product defined in part (a):

$$\langle f|g\rangle = \int_0^1 f'(x)g'(x)\, dx + f(0)g(0), \tag{42}$$

satisfies all of the properties. However, the product defined in (b):

$$\langle f|g\rangle = \int_0^1 f'(x)g'(x)\,dx, \tag{43}$$

does not. The property that fails is the first – this product will yield zero for $\langle f|f\rangle$ if f is any constant, *i.e.*, not only $f = 0$.

9. Consider the following equation in E_∞ (infinite-dimensional Euclidean space – let the scalar product be $\langle x|y\rangle \equiv \sum_{n=1}^{\infty} x_n^* y_n$):

$$Cx = a,$$

where the operator C is defined by (in some basis):

$$C(x_1, x_2, \ldots) = (0, x_1, x_2, \ldots)$$

Is C:

(a) A bounded operator [*i.e.*, does there exist a non-negative real number α such that, for every $x \in E_\infty$, we have $|Cx| \leq \alpha|x|$ ("$|x|$" denotes the norm: $\sqrt{\langle x|x\rangle}$)]?

(b) A linear operator?

(c) A hermitian operator (*i.e.*, does $\langle x|Cy\rangle = \langle Cx|y\rangle$)?

(d) Does $Cx = 0$ have a non-trivial solution? Does $Cx = a$ always have a solution?

Now answer the same questions for the operator defined by:

$$G(\alpha_1, \alpha_2, \ldots) = (\alpha_1, \alpha_2/2, \alpha_3/3, \ldots). \tag{44}$$

Note that we require a vector to be normalizable if it is to belong to E_∞ – *i.e.*, the scalar product of a vector with itself must exist.

Solution: Both C and G are bounded operators: We note that $|Cx| \leq |x|$ and $|Gx| \leq |x|$. Both C and G are also linear operators:

$$C(ax + by) = aCx + bCy, \tag{45}$$

for any $x, y \in E_\infty$ and any complex numbers a, b. The same holds for operator G. C is not a Hermitian operator:

$$\begin{aligned} \langle x|Cy\rangle &= \sum_{n=2}^{\infty} x_n^* y_{n-1} \\ &\neq \sum_{n=2}^{\infty} x_{n-1}^* y_n. \end{aligned} \tag{46}$$

However, G is Hermitian. Neither the equation $Cx = 0$ nor the equation $Gx = 0$ possess non-trivial solutions.

10. Let $f \in L^2(-\pi, \pi)$ be a summable complex function on the real interval $[-\pi, \pi]$ (with Lebesgue measure).

   (a) Define the scalar product by:

$$\langle f|g\rangle = \int_{-\pi}^{\pi} f^*(x) g(x) dx, \tag{47}$$

   for $f, g \in L^2(-\pi, \pi)$. Starting with the intuitive, but non-trivial, assumption that there is no vector in $L^2(-\pi, \pi)$ other than the trivial vector ($f \sim 0$) which is orthogonal to all of the functions $\sin(nx)$, $\cos(nx), n = 0, 1, 2, \ldots$, show that any vector f may be expanded as:

$$f(x) = \sum_{n=0}^{\infty} \left(a_n \cos nx + b_n \sin nx \right), \tag{48}$$

   where

$$a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) dx \tag{49}$$

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx dx \qquad (n > 0) \tag{50}$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx dx. \tag{51}$$

   [You may consult a text such as Fano's *Mathematical Methods of Quantum Mechanics* for a full proof of the completeness of such functions.]

Solution: Let us start a bit more generally. We argued in the solutions to problems 2 and 3 that: If we have an orthonormal set of vectors $\{e_\alpha\}$ in a Hilbert space H, then this set is complete if and only if there is no vector in H, other than the zero vector, which is orthogonal to all elements of $\{e_\alpha\}$. Recall also that $\{e_\alpha\}$ is complete if and only if the closure of the subspace formed by $\{e_\alpha\}$ is H.

Let us show that, if $\{e_\alpha\}$ is a complete set of vectors, then we also have that we may expand any vector $f \in H$ as:

$$f = \sum_\alpha \langle e_\alpha | f \rangle e_\alpha, \tag{52}$$

where at most a denumerable number of terms are non-zero.

Consider a finite dimensional subspace, S, formed by a subset of the $\{e_\alpha\}$, giving them labels $\{e_1, e_2, \ldots, e_n\}$. We can make a projection of $f \in H$ onto this subspace according to:

$$f_S = \sum_{i=1}^{n} \langle e_i | f \rangle e_i. \tag{53}$$

Take the scalar product of both sides with e_j ($j \in 1, 2, \ldots, n$):

$$\langle e_j | f_S \rangle = \langle e_j | f \rangle. \tag{54}$$

Then $\langle e_j | f - f_S \rangle = 0$, or $f - f_S$ is orthogonal to S. In this case, the Pythagorean theorem applies, and

$$|f|^2 = |f_S|^2 + |f - f_S|^2. \tag{55}$$

Thus, we have proven the following form of **Bessel's inequality**:

$$|f|^2 \geq \sum_{i=1}^{n} |\langle e_i | f \rangle|^2, \tag{56}$$

where the vector norm appears on the left, and absolute value signs on the right.

We may now see that at most a countable set of coefficients $\langle e_i | f \rangle$ can be non-vanishing: If the set is uncountable, then there must be a limit point in the set of coefficients other than zero, and hence the right hand side of Bessel's inequality can be made arbitrarily large. Hence, we consider the expansion in a countable set:

$$f' = \sum_{i=1}^{\infty} \langle e_i|f\rangle e_i. \tag{57}$$

Similarly with the above, we take the scalar product of both sides with e_j and learn that $f - f'$ is orthogonal the the subspace generated by $\{e_i\}$; Bessel's inequality generalizes to

$$|f|^2 \geq \sum_{i=1}^{\infty} |\langle e_i|f\rangle|^2, \tag{58}$$

Consider now the scalar product of $f - f'$ with any element e_α of $\{e_\alpha\}$, where $\alpha \neq 1, 2, \ldots$ This scalar product must be zero. Hence, $f - f'$ is orthognonal to the subspace generated by $\{e_\alpha\}$. Since this is a complete set, $f - f' = 0$, which is the desired result.

The remainder of the exercise, deriving the expansion coefficients, and showing that the functions are orthonormal, is straightforward.

(b) Consider the function:

$$f(x) = \begin{cases} -1 & x < 0, \\ 0 & x = 0, \\ +1 & x > 0. \end{cases} \tag{59}$$

Determine the coefficients $a_n, b_n, n = 0, 1, 2, \ldots$ for this function for the expansion of part (a).

Solution: Since f is an odd function, all of the a_i coefficients are zero. The remaining coefficients are:

$$\begin{aligned} b_n &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin nx\, dx \\ &= \frac{2}{\pi}\int_{0}^{\pi} \sin nx\, dx \\ &= \begin{cases} 0 & n \text{ even} \\ \frac{4}{n\pi} & n \text{ odd}. \end{cases} \end{aligned} \tag{60}$$

In Fig. 1 we show the first 52 partial series expansions, $f_N(x)$.

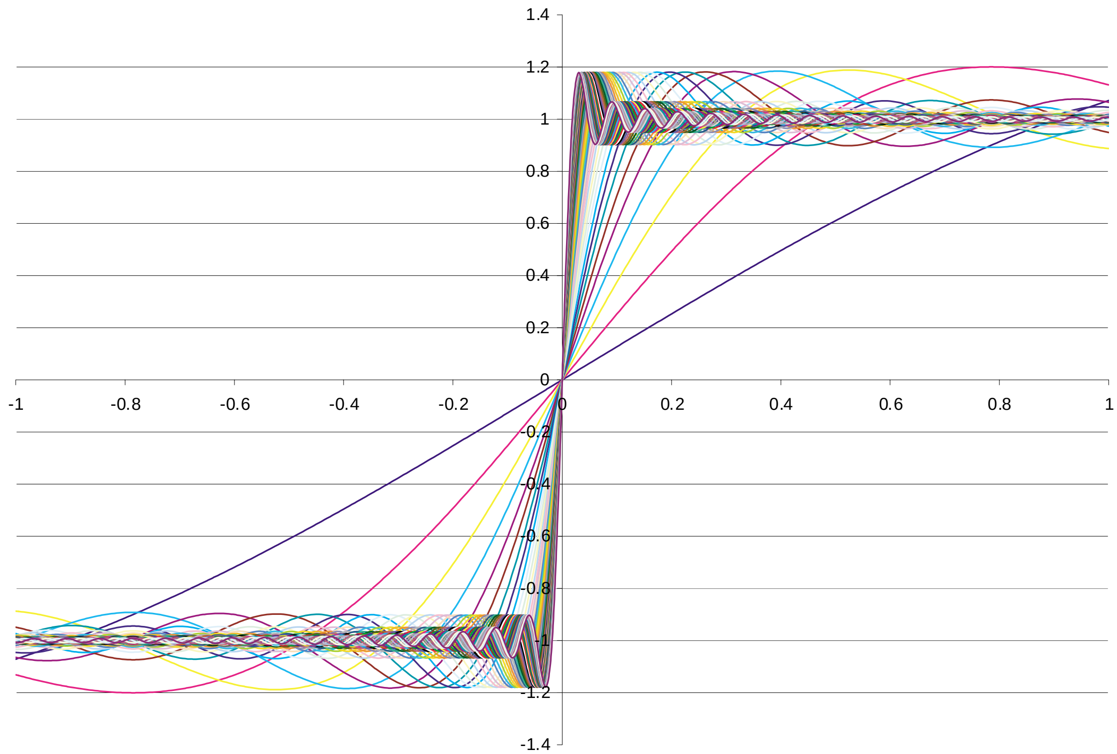

Figure 1: The first 52 functions $f_N(x)$.

(c) We wish to investigate the partial sums in this expansion:

$$f_N(x) = \sum_{n=0}^{N} (a_n \cos nx + b_n \sin nx) \,. \tag{61}$$

Find the position, x_N of the first maximum of f_N (for $x > 0$). Evaluate the limit of $f_N(x_N)$ as $N \to \infty$. Give a numerical answer. In so doing, you are finding the maximum value of the series expansion in the limit of an infinite number of terms. [You may find the following identity useful:

$$\sum_{n=1}^{N} \cos(2n-1)x = \frac{1}{2}\frac{\sin 2Nx}{\sin x}.] \tag{62}$$

Solution: Only odd terms in the sum will contribute, so substitute index n with $2k-1$

$$
\begin{aligned}
f_N(x) &= \frac{4}{\pi}\sum_{n=1,\text{odd}}^{N}\frac{\sin nx}{n} \\
&= \frac{4}{\pi}\sum_{k=1}^{[(N+1)/2]}\frac{\sin(2k-1)x}{2k-1}. \qquad (63)
\end{aligned}
$$

Take the derivative and set equal to zero to find the extrema:

$$
\begin{aligned}
0 &= f'_N(x) = \frac{4}{\pi}\sum_{k=1}^{[(N+1)/2]}\cos(2k-1)x \\
&= \frac{2}{\pi}\frac{\sin 2[(N+1)/2]x}{\sin x}. \qquad (64)
\end{aligned}
$$

If N is even, the first maximum is at $Nx_N = \pi$, and if N is odd, it is at $(N+1)x_N = \pi$. We want the limit:

$$
\begin{aligned}
\lim_{N\to\infty} f_N(x_N) &= \lim_{N\to\infty}\int_0^{x_N} f'_N(x)\,dx \\
&= \frac{2}{\pi}\lim_{N\to\infty}\int_0^{x_N}\frac{\sin 2[(N+1)/2]x}{\sin x}\,dx \\
&= \frac{2}{\pi}\lim_{N\to\infty}\int_0^{\pi}\frac{\sin y}{\sin\{y/2[(N+1)/2]\}}\frac{dy}{2[(N+1)/2]} \\
&= \frac{2}{\pi}\int_0^{\pi}\frac{\sin y}{y}\,dy \qquad (65) \\
&= \frac{2}{\pi}\mathrm{Si}(\pi) = 1.179, \qquad (66)
\end{aligned}
$$

using the *Handbook of Mathematical Functions* to determine $\mathrm{Si}(\pi) \approx 1.85193$.

(d) Obviously, the maximum value of $f(x)$, defined in part (b), is 1. If the value you found for the series expansion is different from 1, comment on the possible reconciliation of this difference with the theorem you demonstrated in part (a).

Solution: Two (related) points may be noted here: First, there is no contradiction with the assertion that $f(x)$ may be arbitrarily closely approximated, at any x, by taking the expansion to sufficiently high numbers of terms. Second, in the limit $N \to \infty$, the expansion differs from $f(x)$ at a set of measure zero, and hence is not considered to be a distinct function in our Hilbert space.

11. Show that, with a suitable measure, any summation over discrete indices may be written as a Lebesgue integral:

$$\sum_{n=1}^{\infty} f(x_n) = \int_{\{x\}} f(x)\mu(dx). \tag{67}$$

Solution:

12. Resonances II: Quantum mechanical resonances – Earlier we investigated some features of a classical oscillator with a "resonant" behavior under a driving force. Let us begin now to develop a quantum mechanical analogue, of relevance also to scattering and particle decays. For concreteness, consider an atom with two energy levels, $E_0 < E_1$, where the transition $E_0 \to E_1$ may be effected by photon absorption, and the decay $E_1 \to E_0$ via photon emission. Because the level E_1 has a finite lifetime – we denote the mean lifetime of the E_1 state by τ – it does not have a precisely defined energy. In other words, it has a finite width, which (assuming that E_0 is the ground state) can be measured by measuring precisely the distribution of photon energies in the $E_1 \to E_0$ decay. Call the mean of this distribution ω_0.

    (a) Assume that the amplitude for the atom to be in state E_1 is given by the damped oscillatory form:

    $$\psi(t) = \psi_0 \; e^{-i\omega_0 t - \frac{t}{2\tau}}$$

    Show that the mean lifetime is given by τ, as desired.

    Solution: The probability to be in the state ψ depends on time according to:

    $$P(t) = |\psi(t)|^2 = \frac{1}{\tau} e^{-t/\tau}, \tag{68}$$

    where I have assumed the normalization $|\psi_0|^2 = 1/\tau$. Note that with this normalization, we have a properly normalized probability. The mean lifetime is thus:

    $$\langle t \rangle = \int_0^{\infty} \frac{t}{\tau} e^{-t/\tau}\, dt = \tau. \tag{69}$$

(b) Note that our amplitude above satisfies a "Schrödinger equation":

$$i\frac{d\psi(t)}{dt} = (\omega_0 - \frac{i}{2\tau})\ \psi(t)$$

Suppose we add a sinusoidal "driving force" $Fe^{-i\omega t}$ on the right hand side, to describe the situation where we illuminate the atom with monochromatic light of frequency ω. Solve the resulting inhomogeneous equation for its steady state solution.

Solution: The new Scrödinger equation is

$$i\frac{d\psi(t)}{dt} = (\omega_0 - \frac{i}{2\tau})\ \psi(t) + Fe^{-i\omega t}. \tag{70}$$

The steady state solution is

$$\psi(t) = \frac{F}{\omega - \omega_0 + \frac{i}{2\tau}} e^{-i\omega t}. \tag{71}$$

(c) Convince yourself (*e.g.*, by "conservation of probability") that the intensity of the radiation emitted by the atom in this steady-state situation is just $|\ \psi(t)\ |^2$. Thus, the incident radiation is "scattered" by our atom, with the amount of scattering proportional to the emitted radiation intensity in the steady state. Give an expression for the amount of radiation scattered (per unit time, per unit amplitude of the incident radiation), as a function of ω. For convenience, normalize your expression to the amount of scattering at $\omega = \omega_0$. Determine the full-width at half maximum (FWHM) of this function of ω, and relate to the lifetime τ.

Solution: Population of state ψ in steady state must be achieved by absorbing photons from the light source. In steady state, the same rate of radiation by de-exciting atoms must prevail to keep a balance. The population probability is just $|\psi|^2$, hence this gives the intensity of the emitted radiation. The amount of radiation scattered per unit time per unit incident amplitude normalized to the intensity at ω_0 is:

$$\begin{aligned} \frac{1/(4\tau^2)}{F^2}|\psi|^2 &= \left|\frac{1/(4\tau^2)}{\omega - \omega_0 + \frac{i}{2\tau}}\right|^2 \\ &= \frac{1}{(\omega - \omega_0)^2 + 1/(4\tau^2)}. \end{aligned} \tag{72}$$

The maximum of this distribution occurs at $\omega = \omega_0$, with peak value $4\tau^2$. Half maximum is at $\omega - \omega_0 = \pm 1/(2\tau)$. Thus, the FWHM is $\Gamma = 1/\tau$.

Note that the "Breit-Wigner" function is just the Cauchy distribution in probability.

13. Time Reversal in Quantum Mechanics, Part II

We earlier showed that the time reversal operator, T, could be written in the form:

$$T = UK,$$

where K is the complex conjugation operator and U is a unitary operator. We also found that

$$T^2 = \pm 1.$$

Consider a spinless, structureless particle. All kinematic operators for such a particle may be written in terms of the $\vec{X}$ and $\vec{P}$ operators, where

$$\begin{aligned}
[P_j, X_k] &= -i\delta_{jk} \\
T\vec{X}T^{-1} &= \vec{X} \\
T\vec{P}T^{-1} &= -\vec{P}
\end{aligned}$$

(where the latter two equations follow simply from classical correspondence).

If we work in a basis consisting of the eigenvectors of $\vec{X}$, the eigenvalues are simply the real position vectors, and hence:

$$U\vec{X}U^{-1} = \vec{X}.$$

In this basis, the matrix elements of $\vec{P}$ may be evaluated:

$$\vec{P} = -i\vec{\nabla} :$$

$$\begin{aligned}
\langle \vec{x}_1 \mid \vec{P} \mid \vec{x}_2 \rangle &= \int_{(\infty)} \delta^{(3)}(\vec{x} - \vec{x}_1)(-i\vec{\nabla}_x)\delta^{(3)}(\vec{x} - \vec{x}_2) d^{(3)}\vec{x} \\
&= -i\vec{\nabla}_{x_1}\delta^{(3)}(\vec{x}_1 - \vec{x}_2).
\end{aligned}$$

Thus, these matrix elements are pure imaginary, and

$$K\vec{P}K^{-1} = -\vec{P},$$

which implies finally

$$U\vec{P}U^{-1} = \vec{P}.$$

We conclude that for our spinless, structureless particle:

$$U = 1e^{i\theta},$$

where the phase θ may be chosen to be zero if we wish. In any event, we have:

$$T = e^{i\theta}K,$$

and

$$T^2 = e^{i\theta}Ke^{i\theta}K = 1.$$

(a) Show that, for a spin 1/2 particle, we may in the Pauli representation (that is, an angular momentum basis for our spin-1/2 system such that the angular momentum operators are given by one-half the Pauli matrices) write:

$$T = \sigma_2 K,$$

and hence show that:

$$T^2 = -1.$$

Note that the point here is to consider the classical correspondence for the action of time reversal on angular momentum.

By considering a direct product space made up of many spin-0 and spin 1/2 states (or by other equivalent arguments), this result may be generalized: If the total spin is 1/2-integral, then $T^2 = -1$; otherwise $T^2 = +1$.

Solution: The Pauli matrices are:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{73}$$

We assume that spin angular momentum behaves similarly with orbital angular momentum under time reversal. Since $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, we have that angular momentum reverses sign under time reversal. Hence, we must have:

$$-\sigma_i = T\sigma_i T^{-1} = UK\sigma_i K^{-1}U^{-1} = U\sigma_i^* U^{-1}. \tag{74}$$

Thus,

$$U\sigma_1 U^{-1} = -\sigma_1; \quad U\sigma_2 U^{-1} = \sigma_2; \quad U\sigma_3 U^{-1} = -\sigma_3. \tag{75}$$

That is, U commutes with σ_2 and anticommutes with σ_1 and σ_3. Since any 2×2 matrix can be written as a complex linear combination of the identity and the three Pauli matrices, we see that U must be of the form $U = e^{i\theta}\sigma_2$, where we may pick the phase *theta* to be zero. Hence, we can write $T = \sigma_2 K$. Then,

$$T^2 = \sigma_2 K \sigma_2 K = -\sigma_2^2 = -1. \tag{76}$$

(b) Show the following useful general property of an antiunitary operator such as T:

Let

$$|\psi'\rangle = T|\psi\rangle$$
$$|\phi'\rangle = T|\phi\rangle.$$

Then

$$\langle\psi'|\phi'\rangle = \langle\phi|\psi\rangle.$$

This, of course, should agree nicely with your intuition about what time reversal should do to this kind of scalar product.

Solution: We have:

$$\begin{aligned} |\psi'\rangle &= T|\psi\rangle = UK|\psi\rangle = U(|\psi\rangle)^* \\ |\phi'\rangle &= T|\phi\rangle = UK|\phi\rangle = U(|\phi\rangle)^*. \end{aligned} \tag{77}$$

Hence,

$$\begin{aligned} \langle\psi'|\phi'\rangle &= (\langle\psi|)^* U^\dagger U(|\phi\rangle)^* \\ &= \langle\psi|\phi\rangle^* \\ &= \langle\phi|\psi\rangle. \end{aligned} \tag{78}$$

(c) Show that, if $|\psi\rangle$ is a state vector in an "odd" system ($T^2 = -1$), then $T|\psi\rangle$ is orthogonal to $|\psi\rangle$.

Solution: Let $|\phi\rangle = T|\psi\rangle$. From part (b), we have the final step in the sequence:

$$\langle\phi|\psi\rangle = -\langle\phi|T^2|\psi\rangle = -\langle\phi|T|\phi\rangle = -\langle\phi|\psi\rangle. \tag{79}$$

This can only be true if $\langle\phi|\psi\rangle = 0$, that is, $T|\psi\rangle$ is orthogonal to $|\psi\rangle$.

14. Suppose we have a particle of mass m in a one-dimensional potential $V = \frac{1}{2}kx^2$ (and the motion is in one dimension). What is the minimum energy that this system can have, consistent with the uncertainty principle? [The uncertainty relation is a handy tool for making estimates of such things as ground state energies.]

Solution: The Hamiltonian is:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2.$$

We consider expectation values in the ground state. The average momentum and position are zero (by symmetry):

$$\langle p\rangle = 0; \qquad \langle x\rangle = 0.$$

Thus:

$$\begin{aligned}(\Delta p)^2 &= \langle p^2\rangle - \langle p\rangle^2 \\ &= \langle p^2\rangle, \\ (\Delta x)^2 &= \langle x^2\rangle.\end{aligned}$$

Let E be the ground state energy:

$$E = \langle H\rangle = \frac{(\Delta p)^2}{2m} + \frac{1}{2}k(\Delta x)^2.$$

The uncertainty relation for x and p is:

$$(\Delta p)^2(\Delta x)^2 \geq \frac{1}{4}\left|[x,p]\right|^2 = \frac{1}{4}.$$

Thus,

$$E \geq \frac{1}{8m(\Delta x)^2} + \frac{k}{2}(\Delta x)^2.$$

This has a minimum at:

$$0 = \frac{dE}{d(\Delta x)^2} = -\frac{1}{8m(\Delta x)^4} + \frac{k}{2},$$

or,

$$(\Delta x)^2 = \frac{1}{2\sqrt{mk}}.$$

Therefore,

$$E \geq \frac{1}{2}\omega,$$

Where $\omega = \sqrt{k/m}$ is the classical oscillator frequency. We note that the minimum is actually achieved in this case: the ground state energy of the simple harmonic oscillator is $\omega/2$, in quantum mechanics.