Summary of SI2380 Advanced Quantum Mechanics

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Abstract

This is a summary of SI2380 Advanced Quantum Mechanics.

Contents

1 Useful Mathematics

Hilbert Space and Completeness We will be working with states in some abstract vector space. For finite-dimensional spaces there are no issues and we may always identify a basis. For infinite-dimensional cases one might have convergence issues when trying to construct a state. We therefore impose the condition of completeness on the state space, namely that any infinite series of states in the space such that the infinite series has finite norm also belongs to the space. Such a space is called a Hilbert space.

A Useful Commutation Relation You might happen upon commutation relations of the form $[f(A), B]$ show up. We would like to try to simplify it for the particular case where $[A, B] = C$, where C is some operator commuting with A. To do this, we first study $[A^n, B]$ in a general case. We have

$$[A^n, B] = A\big[A^{n-1}, B\big] + [A, B]A^{n-1},$$

prompting us to find this commutator by induction. For $n = 2$ we have

$$\big[A^2, B\big] = A[A, B] + [A, B]A.$$

For $n = 3$ we obtain

$$\big[A^3, B\big] = A\big[A^2, B\big] + [A, B]A^2 = A(A[A, B] + [A, B]A) + [A, B]A^2 = A^2[A, B] + A[A, B]A + [A, B]A^2.$$

A suitable induction hypothesis looks to be

$$[A^n, B] = \sum_{k=1}^{n} A^{n-k}[A, B]A^{k-1}.$$

Assuming it to be true, we have

$$\begin{aligned}
\big[A^{n+1}, B\big] &= A[A^n, B] + [A, B]A^n \\
&= A\sum_{k=1}^{n} A^{n-k}[A, B]A^{k-1} + [A, B]A^n \\
&= \sum_{k=1}^{n} A^{n+1-k}[A, B]A^{k-1} + [A, B]A^n \\
&= \sum_{k=1}^{n+1} A^{n+1-k}[A, B]A^{k-1},
\end{aligned}$$

proving the hypothesis by induction.

Now we write

$$f(A) = \sum_{n=0}^{\infty} \frac{1}{n!} f_n A^n$$

to obtain

$$\begin{aligned}
[f(A), B] &= \left[\sum_{n=0}^{\infty} \frac{1}{n!} f_n A^n, B\right] \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} f_n [A^n, B] \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} f_n \sum_{k=1}^{n} A^{n-k}[A, B]A^{k-1}.
\end{aligned}$$

Assuming $[A, B]$ to commute with A, we have

$$\begin{aligned}
[f(A), B] &= \sum_{n=0}^{\infty} \frac{1}{n!} f_n A^{n-1} [A, B] \sum_{k=1}^{n} \\
&= [A, B] \sum_{n=1}^{\infty} \frac{1}{(n-1)!} f_n A^{n-1} \\
&= [A, B] \sum_{m=0}^{\infty} \frac{1}{m!} f_{m+1} A^m \\
&= [A, B] \frac{\mathrm{d}f}{\mathrm{d}A}.
\end{aligned}$$

Symmetries on Hilbert Space A symmetry on Hilbert space is a transformation that leaves all inner products unaltered.

Wigner's Theorem Wigner's theorem states that any operator that is a symmetry is either unitary or anti-unitary. An anti-unitary operator is an operator such that $\langle \Phi | U^\dagger U | \Psi \rangle = \langle \Psi | \Phi \rangle$ and $UU^\dagger = 1$. The adjoint of such an operator is defined by $(U |\Phi\rangle, |\Psi\rangle) = (U^\dagger |\Psi\rangle, |\Phi\rangle)$.

Transformation of Operators Consider a symmetry operator u. In order for this to be a symmetry, it must also act on all operators according to $A \to uAu^\dagger$.

Continuous Symmetries Continuous symmetries are found in two forms: One which operates on the coefficients of the state and one which operates on the basis vectors. Denoting some symmetry as $u_{\delta\theta}$, which changes θ to $\delta\theta$, we require symmetries to have the following properties:

- $u_{\delta\theta_1} u_{\delta\theta_2} = u_{\delta\theta_1 + \delta\theta_2}$.
- $u_{\delta\theta}^{-1} = u_{-\delta\theta}$.
- $\lim_{\delta\theta \to 0} u_{\delta\theta} = 1$.

Generators of Continuous Symmetries Continuous symmetry operators are smooth maps acting on a manifold - namely, Hilbert space. Hence we can use the language of Lie algebra to study them (if you know nothing about Lie algebra, pretend that I didn't write this and carry on. If you want some reference material, please look at my summary of SI2360). We expand the symmetry operator around the identity as

$$u_{\delta\theta} = 1 - i\,\delta\theta\,T + \ldots$$

for some operator T. We have

$$u_{\delta\theta}^\dagger u_{\delta\theta} = (1 + i\,\delta\theta\,T^\dagger)(1 - i\,\delta\theta\,T) = 1 + i\,\delta\theta \left(T - T^\dagger\right) + \ldots,$$

where we have ignored higher-order terms in $\delta\theta$. The requirement that the symmetry be unitary yields $T^\dagger - T = 0$, and hence the generator T is self-adjoint. By continuous application of this we obtain

$$u_{\delta\theta} = e^{-i\delta\theta T}.$$

This operator satisfies all of the above criteria for a continuous symmetry.

Effect of Symmetries on Wavefunctions Let $u_{\delta\theta}$ act on θ and $\mathbf{x}$ be a vector containing any other parameters describing the basis. We have

$$u_{\delta\theta} |\Psi\rangle = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\theta\, u_{\delta\theta} |\theta, \mathbf{x}\rangle \langle \theta, \mathbf{x} | \Psi \rangle = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\theta\, |\theta + \delta\theta\,, \mathbf{x}\rangle \langle \theta, \mathbf{x} | \Psi \rangle = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\theta\, |\theta, \mathbf{x}\rangle \langle \theta - \delta\theta\,, \mathbf{x} | \Psi \rangle,$$

meaning that the symmetry transforms $\Psi(\theta, \mathbf{x})$ to $\Psi(\theta - \delta\theta\,, \mathbf{x})$.

Suppose instead that θ parametrizes the coefficients - in other words, $|\Psi(\theta)\rangle = \Psi(\theta, \mathbf{x}) |\mathbf{x}\rangle$. In this case, the symmetry transforms the wavefunction to $\Psi(\theta + \delta\theta\,, \mathbf{x})$.

Commutation Relations Between Parameters and Generators For a symmetry of the first kind, we use the transformation rule for operators to obtain commutation relations between parameters and their generators. More specifically, we require

$$(1 - i\,\delta\theta\,T)\theta(1 + i\,\delta\theta\,T) = \theta + \delta\theta$$

to first order. The left-hand side is given by

$$\theta + i\,\delta\theta\,\theta T - i\,\delta\theta\,(T\theta + i\,\delta\theta\,T\theta T) = \theta + i\,\delta\theta\,[\theta, T]$$

to first order, implying

$$i[\theta, T] = 1.$$

Generators in the Operator Basis We have

$$\begin{aligned}(1 - i\,\delta\theta\,T)\,|\Psi\rangle &= \int \mathrm{d}\mathbf{x} \int \mathrm{d}\theta\,|\theta, \mathbf{x}\rangle\,\langle\theta, \mathbf{x}|(1 - i\,\delta\theta\,T)|\Psi\rangle \\ &= \int \mathrm{d}\mathbf{x} \int \mathrm{d}\theta\,|\theta, \mathbf{x}\rangle\,\langle\theta - \delta\theta\,, \mathbf{x}|\Psi\rangle \\ &= \int \mathrm{d}\mathbf{x} \int \mathrm{d}\theta\,|\theta, \mathbf{x}\rangle\,(\langle\theta, \mathbf{x}|\Psi\rangle - \delta\theta\,\partial_\theta\,\langle\theta, \mathbf{x}|\Psi\rangle)\,,\end{aligned}$$

implying

$$\langle\theta, \mathbf{x}|\,T = \frac{1}{i}\partial_\theta.$$

Discrete Symmetries A discrete symmetry is an operator for which the previously described machinery does not hold, namely a symmetry which is not parametrized by a continuous parameter.

Complex Conjugation The complex conjugation operator K is defined as

$$Kc\,|\alpha\rangle = c^\star K\,|\alpha\rangle\,.$$

There is some ambiguity in terms of how this operator acts on the basis. To resolve this, we may choose a representation such that the Hilbert space is spanned by vectors with single ones. These vectors should not be affected by complex conjugation, hence

$$K\,|\alpha\rangle = K \sum_a |a\rangle\,\langle a|\alpha\rangle = \sum_a \langle\alpha|a\rangle\,K\,|a\rangle = \sum_a \langle\alpha|a\rangle\,|a\rangle\,.$$

The trade-off to this solution is that the action of this operator is only clearly specified once a basis has been chosen.

Antiunitary Operators and Complex Conjucation We claim that any antiunitary operator θ may be written as $\theta = UK$ for some unitary operator U. To show this, we show that this factorization is antiunitary and take UK to be given. We first have

$$\theta(c_1\,|\alpha\rangle + c_2\,|\beta\rangle) = U(c_1^\star K\,|\alpha\rangle + c_2^\star K\,|\beta\rangle) = c_1^\star UK\,|\alpha\rangle + c_2^\star UK\,|\beta\rangle = c_1^\star\theta\,|\alpha\rangle + c_2^\star\theta\,|\beta\rangle\,,$$

hence the given factorization is antilinear. To show antiunitarity, we work in ket space, as the ambiguity with respect to the basis makes it risky to work with bras. We have

$$\begin{aligned}\theta\,|\alpha\rangle &= UK \sum_a |a\rangle\,\langle a|\alpha\rangle\,, \\ &= U \sum_a \langle\alpha|a\rangle\,K\,|a\rangle \\ &= \sum_a \langle\alpha|a\rangle\,U\,|a\rangle\,.\end{aligned}$$

Similarly, the bra corresponding to $\theta\left|\beta\right\rangle$ is

$$\sum_a \langle a|\beta\rangle \langle a| U^\dagger.$$

The inner product between the two is

$$\sum_a \langle a|\beta\rangle \langle a| U^\dagger \sum_b \langle \alpha|b\rangle U |b\rangle = \sum_a \sum_b \langle \alpha|b\rangle \langle a|\beta\rangle \langle a|a\rangle |b\rangle = \sum_a \langle \alpha|a\rangle \langle a|\beta\rangle = \langle \alpha|\beta\rangle ,$$

completing the proof.

Anti-Unitary Operators and Expectation Values Let U be some anti-unitary operator and A some operator. Then

$$\langle \beta|A|\alpha\rangle = \left\langle \tilde{\alpha}\middle|UA^\dagger U^{-1}\middle|\tilde{\beta}\right\rangle ,$$

where the tildes denote vectors acted upon by U.

To prove this, let $|\gamma\rangle = A^\dagger |\beta\rangle$. Then

$$\begin{aligned}
\langle \beta|A|\alpha\rangle &= \langle \gamma|\alpha\rangle \\
&= \langle \tilde{\alpha}|\tilde{\gamma}\rangle \\
&= \langle \tilde{\alpha}|UA^\dagger|\beta\rangle \\
&= \langle \tilde{\alpha}|UA^\dagger U^{-1}U|\beta\rangle \\
&= \left\langle \tilde{\alpha}\middle|UA^\dagger U^{-1}\middle|\tilde{\beta}\right\rangle .
\end{aligned}$$

Tensors A tensor of rank n is a multilinear map from n vectors in some vector space to a scalar.

It is clear that the set of tensors of some rank form a vector space, and so we would like to identify some basis for the space of tensors.

Basis for $n = 1$ We start with rank 1 tensors. The inner product is certainly a rank 1 tensor according to the definition, and so we would like to use that. Now let the set of v_i denote the set of orthonormal basis vectors for the space V. We then choose the basis

$$e_i(v) = \langle v_i|\, v$$

as the basis for the set of rank 1 tensors. This may also be denoted simply as the tensor v_i (the confusion will disappear later).

The Tensor Product To find a basis for tensors of higher order, we first need to introduce the tensor product. We define it for rank 1 tensors as

$$s(v) \otimes t(w) = \langle s|v\rangle \langle t|w\rangle .$$

The tensor product has allowed us to construct a rank 2 tensor from two rank 1 tensors. Repeatedly applying it allows us to construct tensors of any rank. The tensor product is also bilinear, in line with our definition.

The Tensor Product of Operators It follows naturally that

$$(S \otimes T)(v \otimes w) = S(v) \otimes T(w).$$

2 Basic Concepts

Observables An observable is a Hermitian operator whose orthonormal eigenvectors form a basis.

The Postulates of Quantum Mechanics The postulates of quantum mechanics are:

- At any fixed time the state of a physical system is specified by a ket in Hilbert space.
- Every measurable physical quantity corresponds to an observable on Hilbert space. The possible outcomes of a measurement are the eigenvalues of A.
- The probability of measuring the value a of operator A in a normalized state $|\Psi\rangle$ is $P(a) = \langle\Psi|P_a|\Psi\rangle$, where P_a is the projector onto the subspace corresponding to the eigenvalue a given by $P_a = |a\rangle\langle a|$ (possibly with a sum if the eigenspace is degenerate).
- If a measurement of an observable A gives an outcome a, the state of the system immediately after the measurement is the projection of the state onto the subspace with eigenvalue a.
- The time evolution of a state is governed by the Schrödinger equation.
- Physical states in a many-body system are either completely symmetric or completely anti-symmetric with respect to particle exchange (to be discussed later).

Consequences of the Probability Picture The form of writing the projection operator implies $P(a) = |\langle a|\Psi\rangle|^2$, or $P(a)\,\mathrm{d}a = |\langle a|\Psi\rangle|^2\,\mathrm{d}a$ in the continuous case. In order for the probability interpretation to be consistent, i.e. for the sum of all probabilities to amount to 1, it must hold that $\langle\Psi|\Psi\rangle = 1$.

Expectation Values Expectation values are given by

$$\langle A\rangle = \sum aP(a) = \sum a\,\langle\Psi|P_a|\Psi\rangle = \langle\Psi|\sum a\,|a\rangle\,\langle a|\Psi\rangle = \langle\Psi|A|\Psi\rangle\,.$$

Physical States Modifying a state by a phase factor $e^{i\alpha}$ does not change any expectation values.

Pure and Mixed States Pure states are states with a well-defined state vector. Mixed states are states wherein the state vector is not well-defined.

Density Matrices The density matrix is defined as

$$\rho = |\Psi\rangle\langle\Psi|$$

for a pure state and

$$\rho = \sum_j P_j\,|\Psi_j\rangle\langle\Psi_j|$$

for a mixed state, where the P_j are the probability that the state of the system is $|\Psi_j\rangle$. It satisfies:

$$\begin{aligned}
&\mathrm{tr}(\rho) = \sum_n\,\langle n|\rho|n\rangle = \sum_j P_j\,\langle\Psi_j|\sum_n|n\rangle\langle n||\Psi_j\rangle = \sum_j P_j\,\langle\Psi_j|\Psi_j\rangle = 1,\\
&\rho^\dagger = \rho,\\
&\langle A\rangle = \sum_{n,m,j} p_j\,\langle\Psi_j|n\rangle\,\langle n|A|m\rangle\,\langle m|\Psi_j\rangle = \sum_{n,m,j}\,\langle m|\Psi_j\rangle\,\langle\Psi_j|n\rangle\,\langle n|A|m\rangle = \sum_{n,m}\,\langle m|\rho|n\rangle\,\langle n|A|m\rangle = \mathrm{tr}(\rho A).
\end{aligned}$$

For a pure state we also obtain $\rho^2 = \rho$, which is generally not true for a mixed state.

The Time Evolution Operator Consider the operator $u_{t'}(t)$ which evolves $|\Psi(t')\rangle$ to $|\Psi(t)\rangle$. Inserting it into the Schrödinger equation yields

$$\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}u_{t'}(t)\,\big|\Psi(t')\big\rangle &= Hu_{t'}(t)\,\big|\Psi(t')\big\rangle\,,\\
i\hbar\partial_t u_{t'} &= Hu_{t'}(t).
\end{aligned}$$

In the case of a time-independent Hamiltonian, the solution must be of the form $u_{t'}(t) = u(t-t')$, and the equation above can be integrated to yield

$$u_{t'}(t) = e^{-i\frac{t-t'}{\hbar}H}.$$

Hence H generates time translation - at least in time-independent cases.

Time Evolution of the Density Matrix The time evolution of the density matrix is given by

$$\rho(t) = \sum P_i u_{t_0}(t) |\Psi_i\rangle \langle\Psi_i| u_{t_0}(t)^\dagger = u_{t_0}(t)\rho(t_0)u_{t_0}(t)^\dagger.$$

This implies

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\rho = Hu_{t_0}(t)\rho(t_0)u_{t_0}(t)^\dagger - u_{t_0}(t)\rho(t_0)u_{t_0}(t)^\dagger H = H\rho(t) - \rho(t)H = [H, \rho].$$

The Heisenberg Equation Heisenberg's outlook starts from preserving expectation values under time translations in such a way that all (total) time evolution is contained in the operators, arriving at the transformation rule

$$A_{\mathrm{H}} = u_{t_0}^\dagger(t)A_{\mathrm{S}}u_{t_0}(t).$$

A_{H} is the operator according to Heisenberg and A_{S} is the operator according to Schrödinger. We now have

$$\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A_{\mathrm{H}}\rangle &= -u_{t_0}^\dagger(t)HA_{\mathrm{S}}u_{t_0}(t) + u_{t_0}^\dagger(t)(i\hbar\partial_t A_{\mathrm{S}})u_{t_0}(t) + u_{t_0}^\dagger(t)A_{\mathrm{S}}Hu_{t_0}(t) \\
&= -u_{t_0}^\dagger(t)Hu_{t_0}(t)u_{t_0}^\dagger(t)A_{\mathrm{S}}u_{t_0}(t) + u_{t_0}^\dagger(t)(i\hbar\partial_t A_{\mathrm{S}})u_{t_0}(t) + u_{t_0}^\dagger(t)A_{\mathrm{S}}u_{t_0}(t)u_{t_0}^\dagger(t)Hu_{t_0}(t) \\
&= -H_{\mathrm{H}}A_{\mathrm{H}} + u_{t_0}^\dagger(t)(i\hbar\partial_t A_{\mathrm{S}})u_{t_0}(t) + A_{\mathrm{H}}H_{\mathrm{H}} \\
&= -H_{\mathrm{H}}[A_{\mathrm{H}}, +](i\hbar\partial_t A_{\mathrm{S}})_{\mathrm{H}}.
\end{aligned}$$

Symmetries and Conserved Quantities Suppose that there exists some unitary transformation $u = e^{-i\frac{\varepsilon}{\hbar}A}$ such that $u^\dagger Hu = H$. Expanding the symmetry yields

$$\left(1 + i\frac{\varepsilon}{\hbar}A + \dots\right)H\left(1 - i\frac{\varepsilon}{\hbar}A + \dots\right) = H + i\frac{\varepsilon}{\hbar}(-HA + AH) + \dots = H + i\frac{\varepsilon}{\hbar}[A, H] + \dots = H,$$

implying that A and H commute. Assuming A to have no explicit time dependence, Heisenberg's equations yield that $\langle A\rangle$ is conserved. This is essentially a kind of Nöether's theorem in quantum mechanics.

Density Matrices and Probabilities Consider a Hilbert space spanned by some basis states $|\mathbf{n}\rangle$. If the system is described by the density matrix

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|,$$

the probability that a measurement of $\mathbf{n}$ produces $|m\rangle$ is

$$\begin{aligned}
P(\mathbf{n} = \mathbf{m}) &= \sum_i p_i P(\mathbf{n} = \mathbf{m} \mid \psi_i) \\
&= \sum_i p_i \langle\psi_i|P_{\mathbf{m}}|\psi_i\rangle \\
&= \sum_i p_i \langle\psi_i|P_{\mathbf{m}}|\psi_i\rangle \langle\psi_i|\psi_i\rangle \\
&= \mathrm{tr}(\rho P_{\mathbf{m}}).
\end{aligned}$$

Space and Space Translation We introduce the notion of space as a set of operators x_i on the basis states. These operators are postulated to commute, as are their corresponding translations. The latter implies that their generators k_i commute as well. These are essentially quantum analogues of the canonical Poisson brackets.

The Momentum Operator It turns out that the generators of space translations have a physical interpretation. To understand this, we note that the generating function of a spatial translation in classical mechanics is

$$F(\mathbf{x}, \mathbf{P}) = \mathbf{x}\cdot\mathbf{P} + \mathbf{p}\cdot\mathbf{x},$$

which contains one term generating the identity and one causing the translation. We are therefore prompted to guess that $k_i \propto p_i$. If this were to be true, the constant of proportionality according to de Broglie's hypothesis would be exactly $\hbar$, as expected. We thus arrive at the final analogue to the canonical Poisson brackets, namely

$$[x_i, p_j] = i\hbar\delta_{ij}.$$

One could of course have started with these as postulates instead, prompting a stronger analogy to classical mechanics. But the symmetry approach is nice too.

Spatial Inversion Let Π be the spatial inversion operator, or parity operator, such that $\Pi\mathbf{x}\Pi^{-1} = -\mathbf{x}$. We then have

$$\mathbf{x}\Pi\left|\mathbf{x}'\right\rangle = -\Pi\mathbf{x}\left|\mathbf{x}'\right\rangle = -\mathbf{x}'\Pi\left|\mathbf{x}'\right\rangle,$$

hence $\Pi\left|\mathbf{x}'\right\rangle = \left|-\mathbf{x}'\right\rangle$, as the phase provided by spatial inversion may be chosen freely. Next we have

$$\Pi\Psi = \langle\mathbf{x}|\Pi|\Psi\rangle = \langle-\mathbf{x}|\Psi\rangle = \Psi(-\mathbf{x}).$$

Furthermore, as we chose the operator to provide no phase, we have $\Pi^2 = 1$, hence Π has eigenvalues ± 1 and $\Pi^{-1} = \Pi^\dagger = \Pi$.

The geometry of space implores us to require

$$\Pi e^{-i\frac{1}{\hbar}\delta\mathbf{x}\cdot\mathbf{p}} = e^{i\frac{1}{\hbar}\delta\mathbf{x}\cdot\mathbf{p}}\Pi,$$

namely a spatial translation followed by inversion is equal to inversion followed by an opposite translation. Expanding yields

$$\Pi\left(1 - i\frac{1}{\hbar}\,\delta\mathbf{x}\cdot\mathbf{p}\right)\Pi^\dagger = 1 + i\frac{1}{\hbar}\,\delta\mathbf{x}\cdot\mathbf{p},$$

and we may therefore identify $\Pi\mathbf{p}\Pi^\dagger = -\mathbf{p}$.

Inversion Symmetry and Selection Rules Most observables are either even or odd under inversions, namely $\Pi A\Pi^{-1} = \pi_A A,\ \pi_A = \pm 1$. If we are working with states with definite parity, we have

$$\begin{aligned}\langle\Psi|A|\Phi\rangle &= \pi_A\langle\Psi|\Pi A\Pi|\Phi\rangle \\ &= \pi_A\pi_\Psi\pi_\Phi\langle\Psi|A|\Phi\rangle,\end{aligned}$$

meaning that this matrix element is zero if $\pi_a\pi_\Psi\pi_\Phi = -1$. This is an example of a so-called selection rule.

Mirror Symmetries Other discrete spatial symmetries exist. One example is mirror symmetry. This particular example may be written as a composition of an inversion and a rotation.

Time Reversal We will now proceed to define time reversal - or rather, motion reversal, which is what we really mean. To get a sense of what we want it to do, imagine a particle moving in some direction. Applying motion reversal to such a particle just flips its velocity. The fundamental property which defines this operation is therefore the following: For any state, we require that motion reversal followed by a small forward time step is equivalent to a small backward time step followed by time reversal (think of the particle, and see if this makes sense). In the language of quantum mechanics:

$$\left(1 - \frac{it}{\hbar}H\right)T\left|\Psi\right\rangle = T\left(1 + \frac{it}{\hbar}H\right)\left|\Psi\right\rangle,$$

where T is the time reversal operator. This is only true if $-iHT = TiH$.

Why do I leave the i? It is because T cannot be linear. Otherwise, we would have $TH = -HT$. Considering a particular eigenstate, we would then have

$$HT\left|n\right\rangle = -TH\left|n\right\rangle = -E_nT\left|n\right\rangle,$$

namely, $T\left|n\right\rangle$ is an eigenstate with eigenvalue $-E_n$. This does not work in many cases, however - a free particle is a typical example of a system where the energy spectrum is non-negative. It can, however, be anti-linear, and if it is to represent a symmetry for certain systems, it must be anti-unitary. If this is true, then we have

$$HT = TH.$$

Observables Under Time Reversal For an observable, time reversal changes the corresponding operator according to $A \to TAT^{-1}$, as A must be Hermitian. We define evenness and oddness under time reversal the same as we did for parity, and from this a selection rule follows, this time as

$$\langle\beta|A|\alpha\rangle = \pm\left\langle\tilde{\beta}\middle|A\middle|\tilde{\alpha}\right\rangle^{\star},$$

where the tildes denote time-reversed states.

Our intution tells us that position should be even and momentum odd under time reversal. We can show this by enforcing a stricter criterion, namely that time reversal preserve the canonical commutation relations. This requirement is reasonable because we expect that time reversed motion should also adhere to the laws of physics, which ought to happen if the canonical commutation relations are preserved. We have

$$T[x_i, p_j]T^{-1} = -i\hbar\delta ij.$$

For this to be satisfied, either position or momentum must be odd under time reversal.

So which one is it? We can make a choice by requiring that translations and time reversal commute. This will lead to

$$\left(1 - \frac{i}{\hbar}\mathbf{a}\cdot\mathbf{p}\right)T = T\left(1 - \frac{i}{\hbar}\mathbf{a}\cdot\mathbf{p}\right).$$

The anti-linearity of T yields

$$-i\mathbf{a}\cdot\mathbf{p}T = iT\mathbf{a}\cdot\mathbf{p},$$

or equivalently

$$T\mathbf{p}T^{-1} = -\mathbf{p}.$$

Note that no other answer could really immerge from this calculation - baked into the requirement that we started with was an implicit idea of position being invariant under time reversal.

Propagators The probability amplitude at some point x at time t is given by

$$\Psi(x,t) = \langle x|\Psi(t)\rangle = \langle x|u_0(t)|\Psi(0)\rangle = \int \mathrm{d}x' \, \left\langle x\middle|u_0(t)\middle|x'\right\rangle\left\langle x'\middle|\Psi(0)\right\rangle.$$

Defining the propagator $G_{x',t'}(x,t) = \langle x|u_{t'}(t)|x'\rangle$, we arrive at

$$\Psi(x,t) = \int \mathrm{d}x' \, G_{x',0}(x,t)\left\langle x'\middle|\Psi(0)\right\rangle = \int \mathrm{d}x' \, G_{x',0}(x,t)\Psi(x',0).$$

Hence the propagator acts as a Green's function with respect to time, in some sense.

Arriving at Path Integrals The general propagator of some state is given by

$$G_{x',t'}(x,t) = \sum_{\gamma} G_{\gamma;x',t'}(x,t),$$

where the summation is performed over all possible paths γ between the two points.

Suppose now that the time evolution is divided into steps such that

$$u_{t'}(t) = \prod_{k=1}^{n} u_{t_{k-1}}(t_k), \; t_0 = t', \; t_n = t, \; t_k - t_{k-1} = \delta t.$$

Then

$$G_{x',t'}(x,t) = \left\langle x\middle|\prod_{k=1}^{n} u_{t_{k-1}}(t_k)\middle|x'\right\rangle.$$

For every k we now introduce an identity according to

$$
\begin{aligned}
G_{x',t'}(x,t) &= \left\langle x \middle| \prod_{k=1}^{n} u_{t_{k-1}}(t_k) \int \mathrm{d}x_k \, |x_{k-1}\rangle\langle x_{k-1}| \middle| x' \right\rangle \\
&= \left\langle x \middle| \prod_{k=1}^{n} \int \mathrm{d}x_k \, u_{t_{k-1}}(t_k) \, |x_{k-1}\rangle\langle x_{k-1}| \middle| x' \right\rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, \langle x_k | u_{t_{k-1}}(t_k) | x_{k-1} \rangle \, .
\end{aligned}
$$

The time translation operator has the form $u_{t_{k-1}}(t_k) = e^{-i\frac{\Delta t}{\hbar}H}$. For a Hamiltonian of the form $H = \frac{p^2}{2m} + V(\mathbf{x})$, the terms do not necessarily commute. However, to second order we have

$$
\begin{aligned}
e^{\alpha A} e^{\alpha B} &= \left(1 + \alpha A + \frac{1}{2}\alpha^2 A^2 + \dots\right)\left(1 + \alpha B + \frac{1}{2}\alpha^2 B^2 + \dots\right), \\
e^{\alpha(A+B)} &= 1 + \alpha A + \alpha B + \frac{1}{2}\alpha^2 (A^2 + B^2 + AB + BA) + \dots, \\
&= e^A e^B \left(1 - \frac{1}{2}\alpha^2 AB + \frac{1}{2}\alpha^2 BA + \dots\right) \\
&= e^{\alpha A} e^{\alpha B} e^{\frac{1}{2}\alpha^2 [A,B]}.
\end{aligned}
$$

Ignoring the second-order term yields

$$
\begin{aligned}
G_{x',t'}(x,t) &= \int \prod_{k=1}^{n} \mathrm{d}x_k \, \langle x_k | e^{-i\frac{\Delta t}{\hbar}(T+V)} | x_{k-1} \rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \, \langle x_k | e^{-i\frac{\Delta t}{\hbar}T} | x_{k-1} \rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \left\langle x_k \middle| e^{-i\frac{\Delta t}{\hbar}T} \int \mathrm{d}p_k \, |p_k\rangle\langle p_k| \middle| x_{k-1} \right\rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \left\langle x_k \middle| \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{\hbar}T} \, |p_k\rangle\langle p_k| \middle| x_{k-1} \right\rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{2m\hbar}p_k^2} \, \langle x_k | p_k \rangle \, \langle p_k | x_{k-1} \rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{2m\hbar}p_k^2} \frac{1}{2\pi\hbar} e^{i\frac{p_k(x_k - x_{k-1})}{\hbar}} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} e^{i\frac{m}{2\hbar\Delta t}(x_k - x_{k-1})^2} \frac{1}{2\pi\hbar} \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{2m\hbar}\left(p_k - \frac{m}{\Delta t}(x_k - x_{k-1})\right)^2} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} e^{i\frac{m}{2\hbar\Delta t}(x_k - x_{k-1})^2} \sqrt{\frac{m}{2\pi^2\hbar\Delta t i}} \int \mathrm{d}v_k \, e^{-v_k^2} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} e^{i\frac{m}{2\hbar\Delta t}(x_k - x_{k-1})^2} \sqrt{\frac{m}{2\pi\hbar\Delta t i}} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \sqrt{\frac{m}{2\pi\hbar\Delta t i}} e^{i\frac{1}{\hbar}\sum_{k=1}^{n}\left(\frac{1}{2}m\left(\frac{x_k - x_{k-1}}{\Delta t}\right)^2 - V(x_{k-1})\right)\Delta t} .
\end{aligned}
$$

In the continuous limit the exponent becomes

$$
i\frac{1}{\hbar}\int \mathrm{d}t \, \frac{1}{2}m\dot{x}^2 - V(x) = i\frac{S}{\hbar}
$$

where S is the action. The remaining factor, termed the measure, is

$$D(x(t)) = \lim_{\Delta t \to 0} \prod_{k=1}^{n} \mathrm{d}x_k \sqrt{\frac{m}{2\pi\hbar\Delta t i}}.$$

Finally the propagator is given by

$$G_{x',t'}(x,t) = \int D(x(t)) e^{-i\frac{S}{\hbar}}.$$

This is termed the path integral.

As a side note, if the action is large compared to $\hbar$, the action varies strongly, causing destructive interference from all paths except for the one such that

$$\frac{\delta S}{\delta x} = 0.$$

This is Hamilton's principle, the fundamental postulate of classical mechanics.

The Interaction Picture

3 Angular Momentum

Rotations Consider an axis $\mathbf{n}$. The rotation symmetry operator about this axis is termed $u(\theta\mathbf{n})$. In three dimensions we have

$$u_{-\delta\theta_y \mathbf{e}_y} u_{-\delta\theta_x \mathbf{e}_x} u_{\delta\theta_y \mathbf{e}_y} u_{\delta\theta_x \mathbf{e}_x} = u_{-\delta\theta_x \delta\theta_y \mathbf{e}_z},$$

with similar relations obtained by cyclic permutations. In quantum mechanics there must be three generators of rotations in three dimensions, and if we want the corresponding transformations to correspond to the classical notion of rotations, they must satisfy this same property. Expanding to second order in generators yields

$$\begin{aligned}&\left(1 + i\,\delta\theta_y\,T_y - \frac{1}{2}\,\delta\theta_y{}^2\,T_y^2\right)\left(1 + i\,\delta\theta_x\,T_x - \frac{1}{2}\,\delta\theta_x{}^2\,T_x^2\right)\left(1 - i\,\delta\theta_y\,T_y - \frac{1}{2}\,\delta\theta_y{}^2\,T_y^2\right)\left(1 - i\,\delta\theta_x\,T_x - \frac{1}{2}\,\delta\theta_x{}^2\,T_x^2\right)\\ =&1 + i\,\delta\theta_x\,\delta\theta_y\,T_z.\end{aligned}$$

Expanding the parentheses we obtain

$$1 + \delta\theta_x\,\delta\theta_y\,(-T_yT_x + T_xT_y) = 1 + i\,\delta\theta_x\,\delta\theta_y\,T_z,$$

implying the commutation relation

$$[T_x, T_y] = iT_z.$$

Cyclic permutation as well as the antisymmetry of the commutator finally yields

$$[T_i, T_j] = i\varepsilon_{ijk}T_k,$$

with summation.

As we will show later, these generators are related to angular momentum according to

$$J_i = \hbar T_i.$$

This produces the commutation relation

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k.$$

We will be working with these for the rest of the discussion.

The total angular momentum is given by $J^2 = J_iJ_i$, and thus commutes with all of its component. Hence we can find a basis for Hilbert space composed of joint eigenvectors of J^2 and any one component of $\mathbf{J}$ (usually J_z).

Properties of Angular Momentum To study the properties of angular momentum, we will use the method of raising and lowering operators. Working in the basis of eigenvectors of J^2 and J_z, the raising and lowering operators are

$$J_+ = J_x + iJ_y,\ \ J_- = J_x - iJ_y.$$

We have

$$[J_z, J_\pm] = [J_z, J_x \pm iJ_y] = i\hbar(J_y \mp iJ_x) = \hbar(iJ_y \pm J_x) = \pm\hbar(J_x \pm iJ_y) = \pm\hbar J_\pm.$$

Now introduce the eigenstates $|j, m\rangle$ such that $J^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle$ and $J_z |j, m\rangle = \hbar m |j, m\rangle$. We have

$$J_z J_\pm |j, m\rangle = (J_\pm J_z \pm \hbar J_\pm) |j, m\rangle = (m \pm \hbar) J_\pm |j, m\rangle .$$

Hence the raising and lowering operators do indeed raise and lower the angular momentum. Next we have

$$J^2 J_\pm |j, m\rangle = J_\pm J^2 |j, m\rangle = \hbar^2 j(j+1) J_\pm |j, m\rangle .$$

Hence the raising and lowering operators do not change the value of the total angular momentum. This imposes a constraint on the possible set of angular momenta - namely, all components of the angular momentum are Hermitian, meaning that J_z^2 may not have eigenvalues larger than j^2. Hence states exists such that

$$J_- |j, m\rangle = 0,\ \ J_+ |j, m\rangle = 0.$$

To identify these, consider the operators

$$\begin{aligned} J_- J_+ &= J_x^2 + J_y^2 + i[J_x, J_y] = J_x^2 + J_y^2 - \hbar J_z = J^2 - J_z^2 - \hbar J_z, \\ J_+ J_- &= J_x^2 + J_y^2 - i[J_x, J_y] = J_x^2 + J_y^2 + \hbar J_z = J^2 - J_z^2 + \hbar J_z \end{aligned}$$

Suppose now that we are working on the first eigenstate such that $J_+ |j, m\rangle = 0$. Then

$$J_- J_+ |j, m\rangle = (J^2 - J_z^2 - \hbar J_z) |j, m\rangle = \hbar^2 (j(j+1) - m(m+1)) |j, m\rangle = 0.$$

Hence this m satisfies $m = j$. Similarly, for the state such that $J_- |j, m\rangle = 0$, we have

$$J_- J_+ |j, m\rangle = (J^2 - J_z^2 + \hbar J_z) |j, m\rangle = \hbar^2 (j(j+1) - m^2 + m) |j, m\rangle = \hbar^2 (j(j+1) - m(m-1)) |j, m\rangle = 0.$$

Hence this m satisfies $m = -j$. Now, as we know that m changes in integer steps between real numbers from $-j$ to $+j$, we must have that $2j$ is an integer.

Next, we choose the basis states to be normalized. Writing $J_+ |j, m\rangle = c_{j,m} |j, m+1\rangle$ we have

$$|c_{j,m}|^2 = \langle j, m|J_- J_+|j, m\rangle = \hbar^2 (j(j+1) - m(m+1)),\ \ J_+ |j, m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\, |j, m+1\rangle .$$

Similarly, writing $J_- |j, m\rangle = c_{j,m} |j, m-1\rangle$ we have

$$|c_{j,m}|^2 = \langle j, m|J_+ J_-|j, m\rangle = \hbar^2 (j(j+1) - m(m-1)),\ \ J_- |j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\, |j, m-1\rangle .$$

Orbital Angular Momentum Supposing the spatial rotation to be described by some rotation matrix R, we require $u_R |\mathbf{r}\rangle = |R\mathbf{r}\rangle$. This yields

$$\Psi'(\mathbf{r}') = \langle \mathbf{r}|u_R|\Psi\rangle \left\langle R^{-1}\mathbf{r}\middle|\Psi\right\rangle = \Psi(R^{-1}\mathbf{r}).$$

To get a better understanding of what is going on, consider a small rotation about the z-axis. Its effect on the position vector is

$$R^{-1}\mathbf{r} = \begin{bmatrix} 1 & \delta\theta & 0 \\ -\,\delta\theta & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x + \delta\theta\, y \\ y - \delta\theta\, x \\ z \end{bmatrix}.$$

Linearizing the wavefunction yields

$$\Psi(R^{-1}\mathbf{r}) \approx \Psi(\mathbf{r}) + \varepsilon \left(y\partial_x \Psi - x\partial_y \Psi \right),$$

which in the general case corresponds to Ψ being acted on by an operator $e^{-\frac{i}{\hbar}\theta_i L_i}$ where

$$L_i = \varepsilon_{ijk} x_j p_k.$$

This completes the argument that the generators of rotations are indeed angular momenta in the classical sense.

When finding the eigenfunctions of L^2 and L_z, however, the eigenvalues may only be integer multiples of $\hbar$, meaning that classical angular momentum does not by itself contain all the properties of angular momenta. It also turns out that the rest comes from spin.

Spin In addition to the transformation of coordinates, the rotation operator could also act on some non-orbital degrees of freedom. Thus we add an extra factor $D_{\mathbf{n}}(R)$. It commutes with the previously discussed operators as $e^{-i\frac{\theta}{\hbar}L}$ acts equally on all of the basis and $D_{\mathbf{n}}(R)$ is linear in the basis.

Using the machinery of Lie algebra, we may write

$$D_n(R) = e^{-\frac{i}{\hbar}\theta_i S_i}.$$

The total rotation operator is thus

$$e^{-\frac{i}{\hbar}\boldsymbol{\theta}\cdot(\mathbf{L}+\mathbf{S})},$$

prompting us to define the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$.

$\mathbf{J}$ must generate a rotation, hence $\mathbf{S}$ must satisfy the same commutation relation, implying that $\mathbf{S}$ must also be an angular momentum operator. Furthermore, it does not have the same restrictions as orbital angular momentum, and may therefore correspond to j being a half-integer. This is termed the spin.

Spin-$\frac{1}{2}$ In the particular case of $j = \frac{1}{2}$ we may construct matrices for the spin operator in the eigenbasis of S_z. The resulting matrices are $S_i = \frac{1}{2}\hbar\sigma_i$, where σ_i are the Pauli matrices. The spin factor of the rotation operator may now be written as

$$D_{\mathbf{n}}(R) = e^{-i\frac{\theta}{2}\mathbf{n}\cdot\boldsymbol{\sigma}}.$$

To simplify this, we note that

$$\begin{aligned}(\mathbf{n}\cdot\boldsymbol{\sigma})^2 &= n_i n_j \sigma_i \sigma_j \\ &= \sum_{i=j} n_i^2 \sigma_i^2 + \frac{1}{2}\sum_{i\neq j} n_i n_j (\sigma_i\sigma_j + \sigma_j\sigma_i).\end{aligned}$$

The Pauli matrices anticommute and square to identity, hence we have

$$(\mathbf{n}\cdot\boldsymbol{\sigma})^2 = 1.$$

This yields

$$\begin{aligned}D_{\mathbf{n}}(R) &= \sum_{m=0} \frac{1}{(2m)!}\left(-i\frac{\theta}{2}\right)^{2m}(\mathbf{n}\cdot\boldsymbol{\sigma})^{2m} + \frac{1}{(2m+1)!}\left(-i\frac{\theta}{2}\right)^{2m+1}(\mathbf{n}\cdot\boldsymbol{\sigma})^{2m+1} \\ &= \sum_{m=0} \frac{1}{(2m)!}(-1)^m\left(\frac{\theta}{2}\right)^{2m} - \frac{i}{(2m+1)!}(-1)^m\left(\frac{\theta}{2}\right)^{2m+1}\mathbf{n}\cdot\boldsymbol{\sigma} \\ &= \cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)\mathbf{n}\cdot\boldsymbol{\sigma}.\end{aligned}$$

Addition of Angular Momenta We would like to identify eigenstates of the total angular momentum $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$ in terms of the eigenstates of its components. The basis we are starting with is the product basis

$$|l_1, l_2; m_1, m_2\rangle = |l_1, m_1\rangle \otimes |l_2, m_2\rangle.$$

The components of the angular momentum are given by

$$J_i = (L_1)_i \otimes 1 + 1 \otimes (L_2)_i,$$

and we therefore have

$$J_z |l_1, l_2; m_1, m_2\rangle = \hbar(m_1 + m_2)|l_1, l_2; m_1, m_2\rangle.$$

As $\mathbf{J}$ is indeed an angular momentum, we may now use what we now to introduce the eigenbasis of $\mathbf{J}$ as $|l_1, l_2; j, m\rangle$. It may be expressed in terms of the previous basis as

$$|l_1, l_2; j, m\rangle = \sum_{m_1, m_2} \langle l_1, l_2; m_1, m_2 | l_1, l_2; j, m\rangle |l_1, l_2; m_1, m_2\rangle.$$

The $\langle l_1, l_2; m_1, m_2 | l_1, l_2; j, m\rangle$ are called Clebsch-Gordan coefficients, and may be found in tables.

The previously obtained eigenvalue implies $m \leq l_1 + l_2$ and $j \leq l_1 + l_2$. This allows us to identify one eigenstate

$$|l_1, l_2; l_1 + l_2, l_1 + l_2\rangle = |l_1, l_2; l_1, l_2\rangle .$$

To identify other states, one simply applies the lowering operator $J_\pm = J_x \pm iJ_y = (L_1)_- + (L_2)_-$. This will produce $2(l_1 + l_2) + 1$ new states. Next, we study the state

$$\begin{aligned} J_- |l_1, l_2; l_1 + l_2, l_1 + l_2\rangle &= \hbar(\sqrt{l_1(l_1+1) - l_1(l_1-1)}\,|l_1, l_2; l_1 - 1, l_2\rangle + \sqrt{l_2(l_2+1) - l_2(l_2-1)}\,|l_1, l_2; l_1, l_2 - 1\rangle) \\ &= \hbar(\sqrt{2l_1}\,|l_1, l_2; l_1 - 1, l_2\rangle + \sqrt{2l_2}\,|l_1, l_2; l_1, l_2 - 1\rangle). \end{aligned}$$

We thus have

$$|l_1, l_2; l_1 + l_2, l_1 + l_2 - 1\rangle = \frac{1}{\sqrt{l_1 + l_2}}(\sqrt{l_1}\,|l_1, l_2; l_1 - 1, l_2\rangle + \sqrt{l_2}\,|l_1, l_2; l_1, l_2 - 1\rangle).$$

It is orthogonal to the state

$$\frac{1}{\sqrt{l_1 + l_2}}(\sqrt{l_2}\,|l_1, l_2; l_1 - 1, l_2\rangle - \sqrt{l_1}\,|l_1, l_2; l_1, l_2 - 1\rangle).$$

To study this state, we use the fact that

$$\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2 = J_z^2 + J_+J_- - \hbar J_z.$$

Clearly the state we are working with is an eigenstate of J_z with eigenvalue $\hbar(l_1 + l_2 - 1)$, meaning that two of these terms are easily handled. The others are not as trivial, but we have

$$J_+J_- = (L_{1,+} + L_{2,+})(L_{1,-} + L_{2,-}) = L_{1,+}L_{1,-} + L_{1,+}L_{2,-} + L_{2,+}L_{1,-} + L_{2,+}L_{2,-},$$

meaning that we might be able to look at how these terms work separately.

We consider the effect on the left-hand term, as the effect on the other is obtained by simply switching the numbers 1 and 2. The first and last terms can be rewritten nicely as

$$L_{1,+}L_{1,-} = \mathbf{L}_1^2 - L_{1,z}^2 + \hbar L_{1,z},$$

meaning

$$\begin{aligned} L_{1,+}L_{1,-}\,|l_1, l_2; l_1 - 1, l_2\rangle &= \hbar^2(l_1(l_1+1) - (l_1-1)^2 + l_1 - 1)\,|l_1, l_2; l_1 - 1, l_2\rangle \\ &= \hbar^2(l_1^2 + 2l_1 - 1 - (l_1^2 - 2l_1 + 1))\,|l_1, l_2; l_1 - 1, l_2\rangle \\ &= 2\hbar^2(2l_1 - 1)\,|l_1, l_2; l_1 - 1, l_2\rangle , \\ L_{2,+}L_{2,-}\,|l_1, l_2; l_1 - 1, l_2\rangle &= \hbar^2(l_2(l_2+1) - l_2^2 + l_2)\,|l_1, l_2; l_1 - 1, l_2\rangle \\ &= 2\hbar^2 l_2\,|l_1, l_2; l_1 - 1, l_2\rangle . \end{aligned}$$

The other two are not so nice, but let us try anyway. We have

$$\begin{aligned} L_{1,+}L_{2,-}\,|l_1, l_2; l_1 - 1, l_2\rangle &= \hbar\sqrt{l_2(l_2+1) - l_2(l_2-1)}L_{1,+}\,|l_1, l_2; l_1 - 1, l_2 - 1\rangle \\ &= \hbar^2\sqrt{l_1(l_1+1) - (l_1-1)l_1}\sqrt{l_2(l_2+1) - l_2(l_2-1)}L_{1,+}\,|l_1, l_2; l_1, l_2 - 1\rangle \\ &= 2\hbar^2\sqrt{l_1 l_2}\,|l_1, l_2; l_1, l_2 - 1\rangle , \\ L_{2,+}L_{1,-}\,|l_1, l_2; l_1 - 1, l_2\rangle &= 0. \end{aligned}$$

The latter comes from me skipping to the fun part of raising the second spin, which returns 0.

Let us now look at what we have. We write the total angular momentum operator as

$$\mathbf{J}^2 = J_z^2 - \hbar J_z + L_{1,+}L_{1,-} + L_{2,+}L_{2,-} + L_{1,+}L_{2,-} + L_{2,+}L_{1,-}.$$

Let us first consider its effect on the term $|l_1, l_2; l_1 - 1, l_2\rangle$. All operators but the last two have this state as an eigenvector, and the total eigenvalue is

$$\begin{aligned} \hbar^2\left((l_1 + l_2 - 1)^2 - (l_1 + l_2 - 1) + 2(2l_1 - 1) + 2l_2\right) &= \hbar^2\left((l_1 + l_2 - 1)(l_1 + l_2 - 2) + 4l_1 - 2 + 2l_2\right) \\ &= \hbar^2\left((l_1 + l_2 - 1)(l_1 + l_2) + 2l_1\right). \end{aligned}$$

Next, the total eigenvalue from acting on $|l_1, l_2; l_1, l_2 - 1\rangle$ is

$$\begin{aligned}\hbar^2\left((l_1+l_2-1)^2-(l_1+l_2-1)+2l_1+2(2l_2-1)\right) &= \hbar^2\left((l_1+l_2-1)(l_1+l_2-2)+2(l_1+2l_2-1)\right)\\ &= \hbar^2\left((l_1+l_2-1)(l_1+l_2)+2l_2\right).\end{aligned}$$

Collecting the terms of the first kind nets us the coefficient

$$\begin{aligned}\sqrt{\frac{l_2}{l_1+l_2}}\hbar^2\left((l_1+l_2-1)(l_1+l_2)+2l_1\right)-2\sqrt{\frac{l_1}{l_1+l_2}}\hbar^2\sqrt{l_1 l_2} &= \sqrt{\frac{l_2}{l_1+l_2}}\hbar^2\left((l_1+l_2-1)(l_1+l_2)+2l_1-2l_1\right)\\ &= \sqrt{\frac{l_2}{l_1+l_2}}\hbar^2(l_1+l_2-1)(l_1+l_2).\end{aligned}$$

Next, collecting the terms of the second kind nets us

$$\begin{aligned}2\sqrt{\frac{l_2}{l_1+l_2}}\hbar^2\sqrt{l_1 l_2}-\sqrt{\frac{l_1}{l_1+l_2}}\hbar^2\left((l_1+l_2-1)(l_1+l_2)+2l_2\right) &= \sqrt{\frac{l_1}{l_1+l_2}}\hbar^2\left(2l_2-(l_1+l_2-1)(l_1+l_2)-2l_2\right)\\ &= -\sqrt{\frac{l_1}{l_1+l_2}}\hbar^2(l_1+l_2-1)(l_1+l_2),\end{aligned}$$

meaning that we have identified an eigenstate of $\mathbf{J}^2$ with eigenvalue $\hbar^2(l_1+l_2)(l_1+l_2-1)$. How nice. This is the recipe for obtaining all the states.

As a final sanity check, how many states are there? We may without loss of generality assume that $l_1 > l_2$, meaning that the lowest eigenvalue of $\mathbf{J}^2$ that is found should be $l_1 - l_2$. Hence the total nunber of states is

$$\begin{aligned}N &= \sum_{n=l_1-l_2}^{l_1+l_2} 2n+1\\ &= \frac{1}{2}(l_1+l_2-(l_1-l_2)+1)\left(2(l_1-l_2)+1+2(l_1+l_2)+1\right)\\ &= (2l_1+1)\left(2l_1+1\right),\end{aligned}$$

as expected.

Spatial Inversion Next, we require that rotations and inversions commute (that this must be is clear as the matrix representation of a rotation is diagonal). Hence we obtain

$$\Pi\mathbf{J}\Pi^\dagger = \mathbf{J}$$

by a similar procedure. Notably, this is true for spin as well - a result which we could only arrive at by enforcing these requirements.

Time Reversal Requiring that rotations and time reversal commute will yield that angular momentum is odd under time reversal, just as was shown for momentum.

Time Reversal of Non-Integral Spin While our requirement is satisfied for integral spin, we do not really know how time reversal acts on non-integral spin. To help with this, we factorize the time reversal as $T = uK$, where u is unitary and K is complex conjucation. For spin-$\frac{1}{2}$, we have $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$, and we must thus have

$$uK\boldsymbol{\sigma}u^\dagger K = -\boldsymbol{\sigma}.$$

The complex conjugation in this basis produces the complex conjugate of the Pauli matrices We write $T = uK$, hence the problem is now to find an operator such that σ_x and σ_z change sign, while σ_y is unaltered. The answer turns out to be

$$u = e^{i\frac{\pi}{2}\sigma_y} = i\sigma_y.$$

We thus have time reversal on non-integral spin as $T = i\sigma_y K$. The general case is $u = e^{i\frac{\pi}{\hbar}S_y}$.

A More General Case The general case is in fact that T^2 produces a minus sign when acting on half-integer spins and a plus sign otherwise.

Kramer's Degeneracy Consider a system which is invariant under time reversal. It would seem that for any eigenvector $|E\rangle$, there must also exist an eigenvector $T|E\rangle$. However, in cases with spin-$\frac{1}{2}$, for which $T^2 = -1$, we have

$$\langle E|T|E\rangle = (\langle TE|)(|T^2 E\rangle)^\star = -(\langle TE|)(|E\rangle)^\star = -\langle E|T|E\rangle,$$

implying the two vectors are orthogonal. This is called Kramer's degeneracy.

4 Approximation Methods

Time-Independent Perturbation Theory Consider a Hamiltonian of the form

$$H = H_0 + \lambda V,$$

where λ is a dimensionless parameter, and suppose that we know the eigenstates $|n_0\rangle$ of H_0. We are then interested in the eigenstates

$$H|n(\lambda)\rangle = E_n(\lambda)|n(\lambda)\rangle.$$

To do this we expand the new eigenstates as

$$|n(\lambda)\rangle = |n_0\rangle + \lambda|n_1\rangle + \lambda^2|n_2\rangle + \dots$$

and the new eigenvalues as

$$E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

and obtain

$$(H_0 + \lambda V)\left(|n_0\rangle + \lambda|n_1\rangle + \lambda^2|n_2\rangle + \dots\right) = \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots\right)\left(|n_0\rangle + \lambda|n_1\rangle + \lambda^2|n_2\rangle + \dots\right).$$

We may now identify terms, one order at a time. The zeroth-order terms are trivial. The first-order terms are

$$H_0|n_1\rangle + V|n_0\rangle = E_n^{(0)}|n_1\rangle + E_n^{(1)}|n_0\rangle.$$

To simplify this, we must first say something about the states. We first require $\langle n_0|n_i\rangle$ to be real. Requiring orthonormality for the new eigenvectors, we obtain

$$\langle n_0|n_0\rangle + 2\lambda\langle n_0|n_1\rangle + \dots = 1,$$

meaning $\langle n_0|n_1\rangle = 0$. Using this, we obtain

$$E_n^{(1)} = \langle n_0|V|n_0\rangle.$$

Next, we ty to identify the expansion coefficients by projecting onto some other state $|m_0\rangle$, yielding

$$E_m^{(0)}\langle m_0|n_1\rangle + \langle m_0|V|n_0\rangle = E_n^{(0)}\langle m_0|n_1\rangle,$$

and thus

$$\langle m_0|n_1\rangle = \frac{\langle m_0|V|n_0\rangle}{E_n^{(0)} - E_m^{(0)}}.$$

Hence we have

$$|n_1\rangle = \sum_{m\neq n}\frac{\langle m_0|V|n_0\rangle}{E_n^{(0)} - E_m^{(0)}}|m_0\rangle.$$

This causes certain issues if any eigenvalue is degenerate. In such a case, you should for each degenerate subspace choose a basis such that the perturbation is diagonal. This will produce the same formula in the end.

Next we collect the second-order terms. We have

$$H_0|n_2\rangle + V|n_1\rangle = E_n^{(0)}|n_2\rangle + E_n^{(1)}|n_1\rangle + E_n^{(2)}|n_0\rangle.$$

Orthonormality yields

$$\langle n_0|n_0\rangle + 2\lambda \langle n_0|n_1\rangle + \lambda^2(2\langle n_0|n_2\rangle + \langle n_1|n_1\rangle) = 1,$$

and thus

$$\langle n_0|n_2\rangle = -\frac{1}{2}\langle n_1|n_1\rangle .$$

The second-order expression from earlier then yields

$$E_n^{(2)} = \langle n_0|V|n_1\rangle = \sum_{m\neq n} \frac{\langle m_0|V|n_0\rangle}{E_n^{(0)} - E_m^{(0)}} \langle n_0|V|m_0\rangle = \sum_{m\neq n} \frac{|\langle m_0|V|n_0\rangle|^2}{E_n^{(0)} - E_m^{(0)}}.$$

We may now compute the second-order state in a similar manner.

The Variational Principle Any state $|\Psi\rangle$ produces a limit on the ground-state energy of a system according to

$$E_0 \leq \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}.$$

This is easily shown by the fact that

$$|\Psi\rangle = \sum_n c_n |E_n\rangle ,$$

yielding

$$\langle\Psi|H|\Psi\rangle = \sum_n E_n|c_n|^2 \leq E_0 \sum_n |c_n|^2 = E_0 \langle\Psi|\Psi\rangle .$$

The variational principle uses this to approximate the ground state energy. The trick is to introduce a family of states parametrized by some set of parameters $\boldsymbol{\alpha}$ and minimize the expression

$$\frac{\langle\Psi(\boldsymbol{\alpha})|H|\Psi(\boldsymbol{\alpha})\rangle}{\langle\Psi(\boldsymbol{\alpha})|\Psi(\boldsymbol{\alpha})\rangle}$$

with respect to these parameters.

Time-Dependent Perturbation Theory Suppose we have a Hamiltonian of the form

$$H = H_0 + V(t),$$

where H_0 has known eigenstates $|n\rangle$ with eigenvalues E_n. We write a general time-dependent state as

$$|\Psi\rangle = \sum_n c_n(t) e^{-i\frac{E_n}{\hbar}t} |n\rangle .$$

This is useful as all the information about the time dependence of the Hamiltonian is contained in the expansion coefficients. Inserting this into the Schrödinger equation yields

$$\begin{aligned} i\hbar \sum_n \left(\frac{\mathrm{d}c_n}{\mathrm{d}t} e^{-i\frac{E_n}{\hbar}t} - i\frac{E_n}{\hbar} c_n(t) e^{-i\frac{E_n}{\hbar}t} \right) |n\rangle &= \sum_n (E_n + V) c_n(t) e^{-i\frac{E_n}{\hbar}t} |n\rangle , \\ i\hbar \sum_n \frac{\mathrm{d}c_n}{\mathrm{d}t} e^{-i\frac{E_n}{\hbar}t} |n\rangle &= \sum_n V c_n(t) e^{-i\frac{E_n}{\hbar}t} |n\rangle . \end{aligned}$$

This may be projected onto any basis state, implying

$$i\hbar \frac{\mathrm{d}c_n}{\mathrm{d}t} = \sum_m c_m(t) e^{-i\frac{(E_m - E_n)}{\hbar}t} \langle n|V|m\rangle .$$

Integrating this yields

$$c_n(t) = c_n - \frac{i}{\hbar} \int_0^t \mathrm{d}\tau \sum_m c_m(t) e^{-i\frac{(E_m - E_n)}{\hbar}\tau} \langle n|V|m\rangle$$

This only gives an implicit solution for the expansion coefficients.

To proceed, we imagine that we do a series expansion in the strength of V with a corresponding expansion of c_n. The first-order terms will yield

$$c_n^{(1)}(t) = c_n - \frac{i}{\hbar} \int_0^t \mathrm{d}\tau \sum_m c_m e^{-i\frac{(E_m - E_n)}{\hbar}\tau} \langle n|V|m\rangle .$$

We can iterate this to obtain higher-order terms. For instance,

$$c_n^{(2)}(t) = c_n - \frac{i}{\hbar} \int_0^t \mathrm{d}\tau \sum_m e^{-i\frac{(E_m - E_n)}{\hbar}\tau} \langle n|V|m\rangle \left(c_m - \frac{i}{\hbar} \int_0^\tau \mathrm{d}\tau' \sum_k c_k e^{-i\frac{(E_k - E_m)}{\hbar}\tau'} \langle m|V|k\rangle \right) .$$

A Typical Example In a typical setup a system is prepared in some state i and the perturbation is turned on at $t = 0$. This yields

$$\begin{aligned} c_n^{(1)}(t) &= \delta_{ni} - \frac{i}{\hbar} \int_0^t \mathrm{d}\tau \sum_m \delta_{mi} e^{-i\frac{(E_m - E_n)}{\hbar}\tau} \langle n|V|m\rangle \\ &= \delta_{ni} - \frac{i}{\hbar} \int_0^t \mathrm{d}\tau\, e^{-i\frac{(E_i - E_n)}{\hbar}\tau} \langle n|V|i\rangle . \end{aligned}$$

This allows us to exclude certain transitions depending on the properties of the potential.

Harmonic Perturbations Let us use a harmonic perturbation

$$V(t) = V\left(e^{i\omega t} + e^{-i\omega t}\right) .$$

In the typical case previously described, we obtain

$$c_n^{(1)}(t) = \delta_{ni} - \frac{i}{\hbar} \int_0^t \mathrm{d}\tau\, e^{-i\frac{(E_i - E_n)}{\hbar}\tau} \langle n|V|i\rangle .$$

Introducing

$$\omega_{in} = \frac{(E_i - E_n)}{\hbar},$$

we obtain

$$\begin{aligned} c_n^{(1)}(t) &= \delta_{ni} - \frac{i}{\hbar} \langle n|V|i\rangle \int_0^t \mathrm{d}\tau\, e^{-i\omega_{in}\tau} \left(e^{i\omega\tau} + e^{-i\omega\tau}\right) \\ &= \delta_{ni} - \frac{i}{\hbar} \langle n|V|i\rangle \int_0^t \mathrm{d}\tau\, e^{i(\omega - \omega_{in})\tau} + e^{i(-\omega - \omega_{in})\tau}. \end{aligned}$$

This is sharply peaked around the two cases $\omega = \pm\omega_{in}$. The perturbation is independent of the sign of ω, hence we may take it to be positive. This means that the peaks are found where an energy quantum is either absorbed or emitted.

Consider now some $n \neq i$. For this case we obtain

$$c_n^{(1)}(t) = -\frac{1}{\hbar} \langle n|V|i\rangle \left(\frac{e^{i(\omega-\omega_{in})t} - 1}{(\omega - \omega_{in})} - \frac{e^{i(-\omega-\omega_{in})t} - 1}{\omega + \omega_{in}} \right).$$

In the limit of large times, one obtains

$$P(i \to n) = \frac{2\pi}{\hbar} |\langle n|V|i\rangle|^2 \delta(E_n - E_i - \hbar\omega),$$

which is called Fermi's golden rule.

Adiabatic Evolution Consider some time-dependent Hamiltonian. Imagining that we can diagonalize the Hamiltonian at any time, energy levels obtained may or may not cross as a function of time. For two energy levels to cross, there can be no coupling in the Hamiltonian between the corresponding states. A general state may now be written as

$$|\Psi(t)\rangle = \sum_n c_n(t) |n(t)\rangle .$$

Inserted into the Schrödinger equation, we obtain

$$i\hbar \sum_n \frac{\mathrm{d}c_n}{\mathrm{d}t} |n(t)\rangle + c_n(t) \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle = \sum_n c_n(t) E_n(t) |n(t)\rangle .$$

Projecting onto some particular state $|m(t)\rangle$ yields

$$i\hbar \left(\frac{\mathrm{d}c_m}{\mathrm{d}t} + \sum_n c_n(t) \langle m| \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle \right) = c_m(t) E_m(t).$$

The Schrödinger equation may not be used on the basis states due to how they are defined (I should say more about this). However, we have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}(H|n(t)\rangle) &= \frac{\mathrm{d}}{\mathrm{d}t}(E_n(t)|n(t)\rangle), \\ \frac{\mathrm{d}H}{\mathrm{d}t} |n(t)\rangle + H \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle &= \frac{\mathrm{d}E_n}{\mathrm{d}t} |n(t)\rangle + E_n(t) \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle . \end{aligned}$$

Projecting onto the state $|m\rangle$ (with suppressed time dependence) yields

$$\langle m| \frac{\mathrm{d}H}{\mathrm{d}t} |n\rangle + E_m(t) \langle m| \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle = \frac{\mathrm{d}E_n}{\mathrm{d}t} \delta_{mn} + E_n(t) \langle m| \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle .$$

For $m \neq n$ we thus have

$$\langle m| \frac{\mathrm{d}}{\mathrm{d}t} |n(t)\rangle = -\frac{\langle m| \frac{\mathrm{d}H}{\mathrm{d}t} |n\rangle}{E_m - E_n}.$$

Inserted into our previous expression we obtain

$$i\hbar \left(\frac{\mathrm{d}c_m}{\mathrm{d}t} + c_m(t) \langle m| \frac{\mathrm{d}}{\mathrm{d}t} |m\rangle - \sum_{n \neq m} c_n(t) \frac{\langle m| \frac{\mathrm{d}H}{\mathrm{d}t} |n\rangle}{E_m - E_n} \right) = c_m(t) E_m(t)$$

This means that we may ignore contribution from states such that the potential varies sufficiently slowly that the above matrix elements are much smaller than the energy differences. These are the states causing crossings, meaning that in the limit of very slowly varying potentials the above equation is diagonal in c_m, and if one starts in $|m\rangle$, one will stay there.

Berry Phase Dropping non-diagonal terms we obtain

$$i\hbar\left(\frac{\mathrm{d}c_m}{\mathrm{d}t}+c_m(t)\left\langle m\right|\frac{\mathrm{d}}{\mathrm{d}t}\left|m\right\rangle\right)=c_m(t)E_m(t),$$

with the solution

$$c_m(t)=c_m(0)e^{-\frac{i}{\hbar}\int\limits_0^t\mathrm{d}\tau E(\tau)+i\gamma(t)}.$$

γ is termed the Berry phase, and given by

$$\gamma(t)=i\int\limits_0^t\mathrm{d}\tau\left\langle m\right|\frac{\mathrm{d}}{\mathrm{d}t}\left|m\right\rangle.$$

We find that it is imaginary, as

$$\langle m|m\rangle=1\to 2\,\mathrm{Re}(\left\langle m\right|\frac{\mathrm{d}}{\mathrm{d}t}\left|m\right\rangle)=0.$$

The Berry phase has a geometric interpretation. To understand it, construct a vector $\mathbf{R}(t)$ of parameters entering into the Hamiltonian. The eigenvalues of the instantaneous eigenstates are thus functions of these parameters. The Berry phase is given by

$$\begin{aligned}\gamma&=i\int\limits_0^t\mathrm{d}\tau\left\langle m\right|\frac{\mathrm{d}}{\mathrm{d}t}\left|m\right\rangle\\&=i\int\limits_0^t\mathrm{d}\tau\left\langle m\middle|\vec{\boldsymbol{\nabla}}_{\mathbf{R}}m\right\rangle\cdot\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\\&=i\int\mathrm{d}\mathbf{R}\cdot\left\langle m\middle|\vec{\boldsymbol{\nabla}}_{\mathbf{R}}m\right\rangle,\end{aligned}$$

where the integral is now converted to a curve integral in parameter space. This is the geometric interpretation.

Imagine now that we vary the parameters periodically with period T. The Berry phase then contains an integral over a closed curve. By introducing the Berry connection

$$\mathbf{A}_m=\left\langle m\middle|\vec{\boldsymbol{\nabla}}_{\mathbf{R}}m\right\rangle,$$

which indeed satisfies

$$i\left\langle m\middle|\vec{\boldsymbol{\nabla}}_{\mathbf{R}}m\right\rangle=\mathbf{A},$$

we may also introduce the Berry curvature

$$\boldsymbol{\Omega}=\vec{\boldsymbol{\nabla}}\times\mathbf{A},$$

the flux of which may equally well determine the Berry phase.

Prior to Berry's paper, it was believed that the Berry phase could be eliminated. Namely, by modifying the phase of the basis states by

$$\left|n\right\rangle\to e^{i\chi(\mathbf{R})}\left|n\right\rangle,$$

the Berry connection would be transformed to

$$\mathbf{A}\to\mathbf{A}-\vec{\boldsymbol{\nabla}}_{\mathbf{R}}\chi.$$

For non-periodic paths through parameter space, this would indeed be the case. However, for a closed path, we may instead compute the Berry phase using a flux integral of the Berry curvature. As the Berry curvature is unchanged by this change of phase, the Berry phase is also left unchanged.

5 Quantum Mechanics for Many-Body Physics

Identical Particles For different particles the total Hilbert space may be constructed as the tensor product of the Hilbert spaces describing the individual particles. For identical particles, swapping the states of the particles seems to produce a different states. This does not match with experiments, which indicate identical particles to be indistinguishable. Hence only parts of the total product space is physical.

We introduce the permutation operator P_{12} for two particles such that

$$P_{12} \left|\alpha\right\rangle \otimes \left|\beta\right\rangle = \left|\beta\right\rangle \otimes \left|\alpha\right\rangle.$$

This operator satisfies

$$P_{12}^2 = 1,\ P_{12}^\dagger = P_{12}.$$

In addition, as identical particles are indistinguishable, it should not modify expectation values. Hence

$$\left\langle\Psi\middle|A\middle|\Psi\right\rangle = \left\langle\Psi\middle|P_{12}^\dagger A P_{12}\middle|\Psi\right\rangle = \left\langle\Psi\middle|P_{12} A P_{12}\middle|\Psi\right\rangle.$$

This implies that $P_{12}AP_{12} = A$ and that P_{12} commutes with any operator. Furthermore, the permutation operator has eigenvalues ± 1, hence we may change introduce basis states

$$\left|\alpha\beta\right\rangle_{\text{S}} = \frac{1}{\sqrt{2}}(\left|\alpha\beta\right\rangle + \left|\beta\alpha\right\rangle),\ \left|\alpha\beta\right\rangle_{\text{A}} = \frac{1}{\sqrt{2}}(\left|\alpha\beta\right\rangle - \left|\beta\alpha\right\rangle)$$

and write Hilbert space as the direct sum of the subspaces spanned by these basis states.

Similarly, for multiple particles we have states $\left|\alpha_1, \alpha_2, \ldots, \alpha_N\right\rangle$ and introduce permutation operators P_{ijk}, which cyclically permute the corresponding particles. Such permutations constitute a non-Abelian discrete group, and its generators are permutations of two particles. For such operators we may also introduce a sign of a permutation, equal to -1 to the power of the number of generators involved. As the permutation operators do not commute, one cannot simultaneously diagonalize them. However, one can find subspaces of Hilbert space which are invariant under any permutation. These may be constructed from single product kets using the symmetrizer and antisymmetrizer, defined as

$$S = \frac{1}{N!}\sum_p P_p,\ A = \frac{1}{N!}\sum_p \text{sgn}(P)P_p.$$

These operators are projectors, and are therefore their own squares. While they are self-adjoint, they do not add to the identity. Hence Hilbert space must be constructed as a direct sum of the eigenbases of S and A, as well as other states.

Note that on these subspaces, where the physical states exist according to our postulates, the permutation operators are multiples of identity. This explains why there is no observable corresponding to them.

The Spin-Statistics Theorem Particles with half-integer spins are called fermions, and particles with integer spins are called bosons.

Many-Body Operators Many-body operators may be constructed from adding single-particle operators or by adding operators containing interactions.

Second Quantization Rather than working with many-body wavefunctions, Slater determinants and the like, we will introduce a new formalism based on creation and annihilation operators for particles. This process is called second quantization.

Fock Space Let $\mathcal{F}_N$ denote the space of physical states for a many-body system of N particles. Fock space is defined using these spaces according to

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}_n.$$

Basis states in any space $\mathcal{F}_N$ may now be re-labelled from individual quantum numbers to occupation numbers according to

$$\left|\alpha_1\alpha_2\right\rangle_\pm = \left|n_{\alpha_1} = 1, n_{\alpha_2} = 1, \ldots\right\rangle$$

where the left-hand side is a symmetrized or antisymmetrized kets. For fermions any occupation number is either 0 or 1, whereas for bosons they may be any non-negative integer.

Creation and Annihilation Operators For fermions we define

$$c_\alpha^\dagger |0\rangle = |\alpha\rangle\,,\ c_\alpha |0\rangle = 0,\ c_\alpha^\dagger c_\beta^\dagger |0\rangle = |\alpha,\beta\rangle_- = -c_\beta^\dagger c_\alpha^\dagger |0\rangle\,.$$

We would like to study the commutation relations between the creation operators. Starting with some state $|\alpha_1,\ldots,\alpha_N\rangle_-$ we have

$$c_\alpha^\dagger c_\beta^\dagger |\alpha_1,\ldots,\alpha_N\rangle_- = |\alpha,\beta,\alpha_1,\ldots,\alpha_N\rangle_- = -c_\beta^\dagger c_\alpha^\dagger |\alpha_1,\ldots,\alpha_N\rangle_-\,,$$

implying that the two operators anti-commute. Thus the anti-symmetry of the state is incorporated into the operators. Hermitian conjugation yields that the annihilation operators also anti-commute. The anti-symmetry of the states also imply $(c_\alpha^\dagger)^2 = (c_\alpha)^2 = 0$. We can also show that $c_\alpha^\dagger c_\beta + c_\beta^\dagger c_\alpha = 0$.

Next we have

$$c_\alpha^\dagger c_\alpha |0\rangle = 0,\ c_\alpha c_\alpha^\dagger |0\rangle = |0\rangle\,.$$

For any non-zero state we also have

$$\begin{aligned} c_\alpha^\dagger c_\alpha |\alpha,\alpha_1,\ldots,\alpha_N\rangle_- = |\alpha,\alpha_1,\ldots,\alpha_N\rangle_-\,,\ c_\alpha c_\alpha^\dagger |\alpha,\alpha_1,\ldots,\alpha_N\rangle_- = 0, \\ (c_\alpha^\dagger c_\alpha + c_\alpha c_\alpha^\dagger) |\beta,\alpha_1,\ldots,\alpha_N\rangle_- = |\beta,\alpha_1,\ldots,\alpha_N\rangle_-\,, \end{aligned}$$

implying

$$\left\{c_\alpha^\dagger, c_\beta\right\} = \delta_{\alpha,\beta}.$$

To create some particular state defined by some occupation numbers, we use the fact that

$$|n_{\alpha_1}, n_{\alpha_2},\ldots\rangle = (c_{\alpha_1}^\dagger)^{n_{\alpha_1}} (c_{\alpha_2}^\dagger)^{n_{\alpha_2}} \ldots |0\rangle\,.$$

This expression also defines the order of the quantum numbers in the corresponding anti-symmetric state, which was previously unclear. We therefore generally have

$$c_{\alpha_i}^\dagger |n_{\alpha_1}, n_{\alpha_2},\ldots,0,\ldots\rangle = (-1)^{\sum\limits_{j=1}^{i-1} n_j} |n_{\alpha_1}, n_{\alpha_2},\ldots,1,\ldots\rangle\,,$$

with a similar result for the annihilation operator.

Number Operators We next introduce number operators such that

$$\hat{n}_\alpha |n_{\alpha_1}, n_{\alpha_2},\ldots\rangle = n_\alpha |n_{\alpha_1}, n_{\alpha_2},\ldots\rangle\,.$$

We propose that $n_\alpha = c_\alpha^\dagger c_\alpha$. To verify this, we have

$$\left[c_\alpha^\dagger c_\alpha, c_\alpha^\dagger\right] = c_\alpha^\dagger \left\{c_\alpha, c_\alpha^\dagger\right\} - \left\{c_\alpha^\dagger, c_\alpha^\dagger\right\} c_\alpha = c_\alpha^\dagger,$$

and similarly

$$\left[c_\alpha^\dagger c_\alpha, c_\alpha\right] = -c_\alpha.$$

Next we have

$$n_\alpha^2 = c_\alpha^\dagger (1 - c_\alpha^\dagger c_\alpha) c_\alpha = n_\alpha.$$

This implies that n_α has 0 and 1 as its eigenvalues, which is a good sign.

The action of this operator on some state is given by

$$\begin{aligned} n_\alpha |\alpha\rangle = c_\alpha^\dagger c_\alpha c_\alpha^\dagger |0\rangle = c_\alpha^\dagger (1 - c_\alpha^\dagger c_\alpha) |0\rangle = |\alpha\rangle\,, \\ n_\alpha |0\rangle = 0, \end{aligned}$$

which is exactly what we wanted to show.

We may now proceed to define a total number operator

$$N = \sum_\alpha n_\alpha.$$

Creation and Annihilation Operators for Bosons For bosons we may repeat the procedure to obtain

$$\left[b_\alpha^\dagger, b_\beta^\dagger\right] = [b_\alpha, b_\beta] = 0, \ \left[b_\alpha, b_\beta^\dagger\right] = \delta_{\alpha,\beta}.$$

The occupation number states are defined according to

$$|n_{\alpha_1}, n_{\alpha_2}, \dots\rangle = (b_{\alpha_1}^\dagger)^{n_{\alpha_1}} (b_{\alpha_2}^\dagger)^{n_{\alpha_2}} \dots |0\rangle .$$

The action of the operators add constants $\sqrt{n_\alpha + 1}$ and $\sqrt{n_\alpha}$ to the new states.

Change of Basis Consider some change of basis. We will do this generically, and thus write the creation and annihilation operators as a. We have

$$a_{\alpha'}^\dagger |0\rangle = |\alpha'\rangle = \sum_\alpha |\alpha\rangle \langle\alpha|\alpha'\rangle = \sum_\alpha a_\alpha^\dagger |0\rangle \langle\alpha|\alpha'\rangle ,$$

which implies

$$a_{\alpha'}^\dagger = \sum_\alpha \langle\alpha|\alpha'\rangle a_\alpha^\dagger, \ a_{\alpha'} = \sum_\alpha \langle\alpha'|\alpha\rangle a_\alpha.$$

Such transformations preserve both the commutation relations and the total number operator.

One-Body Operators A one-body operator is of the form

$$T0 \sum T_i,$$

where T_i operates on a single factor in the product state. Re-introducing the anti-symmetrization operator A, with which T must commute, we have

$$\begin{aligned}
TA\,|\alpha_1, \alpha_2, \dots\rangle &= AT\,|\alpha_1, \alpha_2, \dots\rangle \\
&= A \sum_i \sum_{\alpha,\beta} (T_i)_{\alpha\beta} \langle\beta|\alpha_i\rangle |\alpha_1, \alpha_2, \dots, \alpha_{i-1}, \alpha, \alpha_{i+1}, \dots\rangle \\
&= \sum_{\alpha,\beta} \sum_i (T_i)_{\alpha\beta} \delta_{\beta,\alpha_i} A\,|\alpha_1, \alpha_2, \dots, \alpha_{i-1}, \alpha, \alpha_{i+1}, \dots\rangle \\
&= \sum_{\alpha,\beta} \sum_i (T_i)_{\alpha\beta} \delta_{\beta,\alpha_i} c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger \dots c_{\alpha_{i-1}}^\dagger c_\alpha^\dagger c_{\alpha_{i+1}}^\dagger \dots |0\rangle \\
&= \sum_{\alpha,\beta} \sum_i (T_i)_{\alpha\beta} \delta_{\beta,\alpha_i} c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger \dots c_{\alpha_{i-1}}^\dagger c_\alpha^\dagger c_{\alpha_i} c_{\alpha_i}^\dagger c_{\alpha_{i+1}}^\dagger \dots |0\rangle .
\end{aligned}$$

Neither operator in the product $c_\alpha^\dagger c_{\alpha_i}$ occur to the left of where it is found, hence these operators may be commuted through to the left. This also adds no sign due to the fact that we are moving two operators. Thus we obtain

$$TA\,|\alpha_1, \alpha_2, \dots\rangle = \sum_{\alpha,\beta} \sum_i (T_i)_{\alpha\beta} \delta_{\beta,\alpha_i} c_\alpha^\dagger c_{\alpha_i} A\,|\alpha_1, \alpha_2, \dots\rangle .$$

Assuming that all T_i work the same on the individual bodies we have

$$TA\,|\alpha_1, \alpha_2, \dots\rangle = \sum_{\alpha,\beta} T_{\alpha\beta} \sum_i \delta_{\beta,\alpha_i} c_\alpha^\dagger c_{\alpha_i} A\,|\alpha_1, \alpha_2, \dots\rangle .$$

Now, there are two cases which occur here: $\alpha_i = \beta$ or not. For the term where this is true we may switch the index of the annihilation operator. For the term where this is not true the annihilation operator will cause the corresponding contribution to be zero. Hence we have

$$TA\,|\alpha_1, \alpha_2, \dots\rangle = \sum_{\alpha,\beta} T_{\alpha\beta} c_\alpha^\dagger c_\beta A\,|\alpha_1, \alpha_2, \dots\rangle ,$$

and thus the operator identity

$$T = \sum_{\alpha,\beta} T_{\alpha\beta} c_\alpha^\dagger c_\beta.$$

The expression is the same for bosons.

Diagonalization of Two-Body Operators We may always (I think) identify some change of basis caused by a unitary operator u such that T is diagonal. We thus have

$$\begin{aligned} T &= \sum_{\alpha,\beta,\gamma} ((u^\dagger)_{\alpha\gamma}\tilde{T}_{\gamma\gamma}u_{\gamma\beta})c^\dagger_\alpha c_\beta \\ &= \sum_{\alpha,\beta,\gamma} \tilde{T}_{\gamma\gamma}(u^\dagger)_{\alpha\gamma}c^\dagger_\alpha u_{\gamma\beta}c_\beta \\ &= \sum_\gamma \tilde{T}_{\gamma\gamma}\tilde{c}^\dagger_\gamma \tilde{c}_\beta. \end{aligned}$$

Two-Body Operators As can be shown, the corresponding relation for two-body operators is

$$T = \sum_{\alpha,\beta,\gamma,\delta} T_{\alpha\beta\gamma\delta}c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma.$$

Quantum Field Operators I make brief mention of quantum field operators, which are in essence everything we have seen performed in the coordinate basis. These may be written as

$$\Psi^\dagger(\mathbf{r}) = \sum_\alpha \langle\alpha|\mathbf{r}\rangle\, a^\dagger_\alpha = \sum_\alpha \Psi^\star_\alpha a^\dagger_\alpha,\ \ \Psi(\mathbf{r}) = \sum_\alpha \Psi_\alpha a_\alpha.$$

The commutation (or anti-commutation) relation is

$$\left[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\right] = \sum_{\alpha,\beta} \Psi_\alpha(\mathbf{r})\Psi^\star_\beta(\mathbf{r}')\left[c_\alpha, c^\dagger_\beta\right] = \sum_\alpha \Psi_\alpha(\mathbf{r})\Psi^\star_\alpha(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}').$$

6 Applications

The Harmonic Oscillator The Hamiltonian of the harmonic oscillator is

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

To diagonalize it we introduce the lowering operator

$$a = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{i}{\sqrt{m\omega\hbar}}p\right)$$

and its adjoint, the raising operator. Their commutator is

$$\begin{aligned} \left[a, a^\dagger\right] &= \left[\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{i}{\sqrt{m\omega\hbar}}p\right), \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \frac{i}{\sqrt{m\omega\hbar}}p\right)\right] \\ &= \left[\frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}x, -\frac{1}{\sqrt{2}}\frac{i}{\sqrt{m\omega\hbar}}p\right] + \left[\frac{1}{\sqrt{2}}\frac{i}{\sqrt{m\omega\hbar}}p, \frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}x\right] \\ &= \frac{1}{2}\frac{i}{\hbar}\left([x,-p] + [p,x]\right) \\ &= 1. \end{aligned}$$

The definition of the raising and lowering operators may be inverted to obtain

$$x = \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}(a^\dagger + a),\ \ p = \frac{i}{\sqrt{2}}\sqrt{m\omega\hbar}(a^\dagger - a).$$

The Hamiltonian may now be written in terms of these operators as

$$\begin{aligned} H &= \frac{1}{2m}\cdot -\frac{1}{2}m\omega\hbar(a^\dagger - a)^2 + \frac{1}{2}m\omega^2\frac{1}{2}\frac{\hbar}{m\omega}(a^\dagger + a)^2 \\ &= -\frac{1}{4}\hbar\omega(a^\dagger - a)^2 + \frac{1}{4}\hbar\omega(a^\dagger + a)^2 \\ &= \frac{1}{4}\hbar\omega\left((a^\dagger)^2 + a^\dagger a + aa^\dagger + a^2 - \left((a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2\right)\right) \\ &= \frac{1}{2}\hbar\omega\left(a^\dagger a + aa^\dagger\right) \\ &= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right). \end{aligned}$$

We now define the operator $n = a^\dagger a$. It is Hermitian, meaning that an orthonormal basis of its eigenvectors exists (fortunately, as it constitutes the Hamiltonian). These eigenvectors must be studied next. To do this, we use the commutation relations[1]

$$[n,a] = a^\dagger[a,a] + \left[a^\dagger, a\right]a = -a, \ \left[n, a^\dagger\right] = a^\dagger\left[a, a^\dagger\right] + \left[a^\dagger, a^\dagger\right]a = a^\dagger$$

applied to some eigenvector $|\nu\rangle$ with eigenvalue ν to obtain

$$na\,|\nu\rangle = (an - a)\,|\nu\rangle = (\nu - 1)a\,|\nu\rangle\,.$$

Hence, if some eigenvalue ν exists, we can repeat this argument to show that $\nu-1,\ \nu-2,\dots$ are also eigenvalues, assuming no value in this sequence is zero. The length of these eigenvectors is given by

$$\langle\nu|a^\dagger a|\nu\rangle = \nu\,\langle\nu|\nu\rangle \geq 0,$$

where the latter is due to the positivity of the inner product. In order for this to work, no negative eigenvalues may exist. This only fits with the previous sequence of eigenvalues if $\nu = 0$ is an eigenvalue.

Having established that, we rename the eigenvalues to n. Next, we have

$$na^\dagger\,|n\rangle = (a^\dagger n + a^\dagger)\,|n\rangle = (n+1)a^\dagger\,|n\rangle\,.$$

Hence the sequence $n+1, n+2, \dots$ also consists of eigenvalues of n. The length of such vectors is

$$\langle n|aa^\dagger|n\rangle = \langle n|a^\dagger a + 1|n\rangle = (n+1)\,\langle n|n\rangle > 0.$$

Now the eigenvalues of the Hamiltonian are found to be

$$H_n = \hbar\omega\left(n + \frac{1}{2}\right),\ H\,|n\rangle = H_n\,|n\rangle\,.$$

With respect to degeneracy, suppose there is a set of eigenvectors denoted by the index k such that $a\,|0,k\rangle = 0$. In the coordinate basis we obtain

$$\left\langle x\middle|\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{i}{\sqrt{m\omega\hbar}}p\right)\middle|0,k\right\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \sqrt{\frac{\hbar}{m\omega}}\frac{\mathrm{d}}{\mathrm{d}x}\right)\Psi_{0,k} = 0.$$

The solution to this differential equation is unique, hence the ground state is non-degenerate. The linearity of the raising operator therefore implies that the other eigenvalues are non-degenerate as well.

With respect to normalization, we may require all states to be normalized. Then

$$\begin{aligned}
a^\dagger\,|n\rangle &= c_{n+1}\,|n+1\rangle\,, \\
|c_{n+1}|^2 &= \langle n|aa^\dagger|n\rangle = \langle n|n+1|n\rangle = n+1, \\
c_n &= \sqrt{n}.
\end{aligned}$$

Next we have

$$\begin{aligned}
aa^\dagger\,|n-1\rangle &= \sqrt{n}a\,|n\rangle \\
n\,|n-1\rangle &= \sqrt{n}a\,|n\rangle\,, \\
a\,|n\rangle &= \sqrt{n}\,|n-1\rangle\,.
\end{aligned}$$

Finally, the excited states may be found according to

$$|n\rangle = \frac{1}{\sqrt{n}}a^\dagger\,|n-1\rangle = \dots = \frac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle\,,$$

which when applied to the ground state will reproduce some special function.

[1]What might inspire this? A suggestion might be the fact that if n and the raising and lowering operators commuted, we would find that they share eigenvectors.

Quantum Hall Effect The Hamiltonian of a charged particle in a magnetic field is

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2.$$

We recall that gauge transformations of the electromagnetic field are defined according to $A^\mu \to A^\mu - \partial^\mu \chi$ for some function χ. While Maxwell's equations are gauge invariant, Schrödinger's equation is not. We try to remedy this by combining the gauge transformation with a transformation

$$|\Psi\rangle \to e^{i\frac{q}{\hbar}\chi}|\Psi\rangle.$$

The inverse transformation yields

$$(\mathbf{p} - q\mathbf{A})|\Psi\rangle = (\mathbf{p} - q(\mathbf{A} - \vec{\boldsymbol{\nabla}}\chi))e^{-i\frac{q}{\hbar}\chi}|\Psi\rangle,$$

which is given by

$$(\mathbf{p} - q(\mathbf{A} - \vec{\boldsymbol{\nabla}}\chi))e^{-i\frac{q}{\hbar}\chi}|\Psi\rangle = e^{i\frac{q}{\hbar}\chi}(\mathbf{p} - q\vec{\boldsymbol{\nabla}}\chi - q(\mathbf{A} - \vec{\boldsymbol{\nabla}}\chi))|\Psi\rangle = e^{-i\frac{q}{\hbar}\chi}(\mathbf{p} - q\mathbf{A})|\Psi\rangle,$$

implying that the transformation does not change the Schrödinger equation.

We will start by studying two-dimensional motion in a rectangular domain with a constant magnetic field in the z-direction. In the Landau gauge we choose the vector potential $\mathbf{A} = Bx\mathbf{e}_x$. The Hamiltonian is thus

$$H = \frac{1}{2m}\left(p_x^2 + (p_y - qBx)^2\right).$$

We see that the Hamiltonian commutes with p_y, but not with p_x, implying that the solution is of the form

$$\Psi(\mathbf{x}) = \frac{1}{\sqrt{2\pi\hbar}}e^{-ik_y y}f(x),$$

where $k_y = \frac{1}{\hbar}p_y$ may be taken to have a definite value. We are thus left with

$$H = \frac{1}{2m}\left(p_x^2 + \hbar^2\left(k_y - \frac{1}{l_B^2}x\right)^2\right),\ l_B^2 = \frac{\hbar}{qB}.$$

We solve this by introducing raising and lowering operators

$$a_{k_y} = \frac{1}{\sqrt{2}}\left(\frac{x - k_y l_B^2}{l_B} + i\frac{l_B}{\hbar}p_x\right)$$

such that

$$H = \hbar\omega(a_{k_y}^\dagger a_{k_y} + \frac{1}{2}),$$

yielding a harmonic oscillator with the classical cyclotron frequency

$$\omega = \frac{\hbar}{ml_B^2} = \frac{eB}{m}.$$

The energy levels of this harmonic oscillator are called Landau levels.

To study the degeneracy, we impose periodic boundary conditions in the y-direction, implying

$$k_y = \frac{2\pi}{L_y}m.$$

If you have a large but finite sample of length L_x in the x-direction, the fact that the state is localized around $k_y l_B^2$ implies that the maximum value of m is

$$N = \frac{L_x}{l_B^2\frac{2\pi}{L_y}} = \frac{qBA}{h}.$$

In particular, for $q = e$ we have

$$H = \frac{\Phi}{\Phi_0},$$

where $\Phi_0 = \frac{h}{e}$ is the flux quantum.

To study samples at the edge of the sample, add a potential to represent the edge and assume that it varies slowly when compared to the length scale l_B. In this case the eigenvalues are modified to

$$E_n = \hbar\omega(n + \frac{1}{2}) + V(x == -k_y l_B^2)$$

The edge states (perhaps) carry the current, meaning that such systems that we have studied will display steps in their Hall coefficient. This is the quantum Hall effect.

Aharanov-Bohm Effect To demonstrate the principle, consider a metal ring connected to two terminals with magnetic flux through the middle and suppose that current flows from one terminal to the other. The vector potential is non-zero in the ring, and may in fact be written as $\mathbf{A} = \vec{\boldsymbol{\nabla}} f$ here. Performing a gauge transformation preserves the Schrödinger equation, as before. Now, as we may write

$$f = \int\limits_{\gamma} \mathrm{d}\mathbf{x} \cdot \mathbf{A},$$

this implies that the phase of the state is determined by the path taken. Combining this with our knowledge of path integrals yields the transmittion probability

$$T = |t_{\text{upper}}|^2 + |t_{\text{lower}}|^2 + 2\,\mathrm{Re}\left(t_{\text{upper}} t^{\star}_{\text{upper}} e^{iq\left(\int\limits_{\gamma_{\text{lower}}} \mathrm{d}\mathbf{x}\cdot\mathbf{A} - \int\limits_{\gamma_{\text{upper}}} \mathrm{d}\mathbf{x}\cdot\mathbf{A}\right)} \right) = |t_{\text{upper}}|^2 + |t_{\text{lower}}|^2 + 2\,\mathrm{Re}\left(t_{\text{upper}} t^{\star}_{\text{upper}} e^{-iq\Phi} \right).$$

This oscillating transmission probability is the Aharanov-Bohm effect.

Entanglement Suppose you prepare a system of two particles with two possible states in some state $\frac{1}{\sqrt{2}}(|ab\rangle - |ba\rangle)$ and introduce some operator $O_A = O \otimes 1$ in the frame of some observer A. The projection onto the a eigenstates is given by

$$P_a = \sum_{\alpha} |\langle a\alpha|\Psi\rangle|^2 = \frac{1}{2} = P_b.$$

The same turns out to be true for any non-degenerate operator. Hence making any measurement only in frame A does not reveal everything about the state.

To work around this, we introduce the reduced density matrix. Suppose the state is of the form

$$|\Psi\rangle = \sum_{\sigma_A, \sigma_B} \Psi_{\sigma_A \sigma_B} |\sigma_A \sigma_B\rangle .$$

The expectation value of an operator of the form O_A is given by

$$\begin{aligned} \langle O_A \rangle &= \sum_{\sigma_A, \sigma_B, \sigma'_A, \sigma'_B} \Psi^{\star}_{\sigma_A \sigma_B} \Psi_{\sigma'_A \sigma'_B} \langle \sigma_A | O | \sigma'_A \rangle \langle \sigma_B | \sigma'_B \rangle \\ &= \sum_{\sigma_A, \sigma_B, \sigma'_A} \Psi^{\star}_{\sigma_A \sigma_B} \Psi_{\sigma'_A \sigma_B} \langle \sigma_A | O | \sigma'_A \rangle \\ &= \sum_{\sigma'_A} \langle \sigma'_A | \sum_{\sigma_A, \sigma_B, \sigma''_A} \Psi^{\star}_{\sigma_A \sigma_B} \Psi_{\sigma''_A \sigma_B} | \sigma''_A \rangle \langle \sigma_A | O | \sigma'_A \rangle . \end{aligned}$$

This defines the reduced density matrix

$$\rho_A = \mathrm{tr}(\rho)_B,$$

allowing us to write

$$\langle O_A \rangle = \mathrm{tr}(\rho_A A)_A.$$

For the given state we have

$$\begin{aligned} \langle a|\rho_A|a\rangle &= \sum_d \Psi^{\star}_{ad} \Psi_{ad} = \frac{1}{2}, \\ \langle a|\rho_A|b\rangle &= \sum_d \Psi^{\star}_{ad} \Psi_{bd} = 0, \\ \langle b|\rho_A|b\rangle &= \sum_d \Psi^{\star}_{bd} \Psi_{bd} = \frac{1}{2}. \end{aligned}$$

Note that such density matrices do not necessarily correspond to pure states. One case that does, however, is when the product state is a single tensor product.

We now introduce the von Neumann entanglement entropy

$$S = -\operatorname{tr}(\rho_A \log(\rho_A))_A = -\operatorname{tr}(\rho_B \log(\rho_B))_B.$$

By expanding the density matrix in terms of its eigenvalues and eigenkets, one obtains

$$S = -\sum_i \lambda_i \log(\lambda_i).$$

For a pure state, we thus have $S = 0$. Hence the von Neumann entropy is a measure of how separable the states are.

Bell's Inequalities Suppose the two observers measure two entangled particles in two (generally different) directions $\mathbf{a}$ and $\mathbf{b}$, and denote the correlation between the measurements as $C(\mathbf{a}, \mathbf{b})$. Bell's inequality states that if the measurement is an outcome of a classical distribution, then

$$\left|C(\mathbf{a}, \mathbf{b}) - C(\mathbf{a}, \mathbf{b}')\right| + \left|C(\mathbf{a}', \mathbf{b}') + C(\mathbf{a}', \mathbf{b})\right| \leq 2.$$

Experiments have been performed on quantum systems where values greater than 2 have been observed. This disproves the statement that quantum mechanics is merely classical mechanics described by some so-called hidden variables.

Quantum Computing A single qubit is a two-level system, denoted as

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,.$$

In a quantum computer you have a set of these which interact with some Hamiltonian. A quantum computation is simply evolving the qubits with some unitary operator and measuring them.

Numbers are represented according to

$$x = q_1 2^0 + q_2 2^1 + \ldots, \quad |x\rangle = |q_1, q_2, \ldots\rangle\,.$$

Suppose now that there exists some operator U_f such that $U_f\,|x\rangle = |f(x)\rangle$. Then if you prepare a state

$$|\Psi_0\rangle = \sum_{x=0}^{N} |x\rangle\,,$$

you have

$$U_f\,|\Psi_0\rangle = \sum_{x=0}^{N} |f(x)\rangle\,.$$

Hence by performing a single operation, an exponential number of computations has been performed. However, the question remains about how to extract the results.

The solution to this problem is the Deutsch algorithm.