

Ritz Theorem

$$R[\psi] = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}.$$

Step 1: Expand $|\psi\rangle$ in the energy eigenbasis

Because the eigenvectors $\{|n\rangle\}$ form an orthonormal basis (for the discrete part),

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle, \quad c_n = \langle n | \psi \rangle.$$

Then

$$\langle \psi | \psi \rangle = \sum_n |c_n|^2,$$

and using $H|n\rangle = E_n|n\rangle$,

$$\langle \psi | H | \psi \rangle = \sum_{m,n} c_m^* c_n \langle m | H | n \rangle = \sum_{m,n} c_m^* c_n E_m \langle m | n \rangle = \sum_n |c_n|^2 E_n.$$

So

$$R[\psi] = \frac{\sum_n |c_n|^2 E_n}{\sum_n |c_n|^2}.$$

Step 2: Prove the inequality $R[\psi] \geq E_0$

Since $E_n \geq E_0$ for all n ,

$$\sum_n |c_n|^2 E_n \geq \sum_n |c_n|^2 E_0 = E_0 \sum_n |c_n|^2.$$

Divide both sides by $\sum_n |c_n|^2 = \langle \psi | \psi \rangle$:

$$\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_0.$$

Theorem 3.3.2 — Schur's lemma for hermitian operators. Let T be an IRREP of a finite group G on a linear subspace \mathcal{V} . If there is a hermitian operator $C : \mathcal{V} \rightarrow \mathcal{V}$ such that

$$\forall g \in G \quad T(g)C = CT(g)$$

then C is proportional to the unit operator I , i.e. $C = \lambda I$, $\lambda \in \mathbb{C}$.

Proof. Given that C is an hermitian operator we can find an eigenstate $v \in \mathcal{V}$ of C such that

$$Cv = \lambda v. \quad (3.39)$$

The subspace $\text{span}\{T(G)v\}$ is an invariant subspace. We can easily see that for any vector $a = \sum_g a_g T(g)v$

$$Ca = C \sum_g a_g T(g)v = \sum_g a_g T(g)Cv = \sum_g a_g T(g)\lambda v = \lambda a. \quad (3.40)$$

Since T is an IRREP of G , $\text{span}\{T(G)v\}$ must be \mathcal{V} or the null space. As $v = T(I)v$ we conclude that $\text{span}\{T(G)v\}$ must be equal to \mathcal{V} .

Two comments: (a) This theorem is valid to any operator commuting with the group. (b) Although the proof is given for finite groups, it can be generalized for continuous but compact groups.

Conclusion, if \mathcal{V} is an IRREP invariant under the action of the hamiltonian H , and if

$$\forall g \in G \quad T(g)H = HT(g) \Leftrightarrow [T(g), H] = 0, \quad (3.41)$$

then all the states in the subspace \mathcal{V} have the same energy.

Theorem 4.2.1 The spectrum of the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{\alpha}{r^2} \quad (4.11)$$

with $\alpha > 0$, is unbounded from below if $s > 2$.

Proof. To find the constraint on s , we prepare the system in a simple spherically symmetric state characterized by radius r_0 ,

$$\Psi(r) = Ne^{-r^2/r_0^2} \quad (4.12)$$

with

$$N = \left(\frac{2}{\pi}\right)^{3/4} r_0^{-3/2}, \quad (4.13)$$

a normalization factor ensuring the normalization $\langle \Psi | \Psi \rangle = 1$.

As a result of the spherical symmetry

$$\langle x_i | = \langle p_i | = 0, \quad \text{for } i = 1, 2, 3, \quad (4.14)$$

while uncertainty relations give

$$\Delta x_i = \sqrt{\langle x_i^2 \rangle - \langle x_i \rangle^2} \sim r_0 \quad \Rightarrow \quad \Delta p_i = \sqrt{\langle p_i^2 \rangle - \langle p_i \rangle^2} = \sqrt{\langle p_i^2 \rangle} \sim \frac{\hbar}{r_0}. \quad (4.15)$$

Hence, we can write

$$\langle H \rangle = \frac{\langle p^2 \rangle}{2m} + \langle V \rangle \sim \frac{\hbar^2}{2mr_0^2} - \frac{\alpha}{r_0^2}. \quad (4.16)$$

In the above qualitative estimation, we were not careful about order one numbers as they are not going to have any impact on our discussion. Thus, for instance, we used¹

$$\begin{aligned} \langle V \rangle &= \int dr \Psi^*(r) V(r) \Psi(r) = -\frac{\alpha}{r_0^2} \left(\frac{2}{\pi}\right)^{3/2} 4\pi \int_0^{r_0} dx \frac{e^{-2x^2}}{x^{5/2} \Gamma(3/2)} \\ &= -\frac{2^{(s+2)/2} \Gamma(3/2)}{\sqrt{\pi}} \frac{\alpha}{r_0^5} \sim -\frac{\alpha}{r_0^5}. \end{aligned} \quad (4.17)$$

If $s > 2$, then one can make $\langle H \rangle$ arbitrary negative by choosing r_0 sufficiently small. This clearly indicates that the spectrum of the hamiltonian is unbounded from below and the system is unstable. A different point of view is to regard Ψ as a variational trial function, by definition $\langle H \rangle \geq E_0$, where E_0 is the lowest eigenstate of H . Thus, we deduce that $s \leq 2$. Henceforth, we take $s < 2$. The case $s = 2$ requires separate consideration, and we leave it outside the scope of these lectures.

Theorem 4.2.2 For $s < 2$ the spectrum of the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{\alpha}{r^s} \quad \alpha > 0 \quad (4.18)$$

contains infinite number of bound states.

Proof. To prove this statement we cook up a state represented by a spherically symmetric shell centred at $r = r_0$ with thickness $\Delta r = \beta r_0$. We assume that the state is very narrow, i.e. $\beta \ll 1$. As a concrete example of such state, we may consider

$$\Psi(r) = Ne^{-(r-r_0)^2/\beta^2 r_0^2} \quad (4.19)$$

where N is a normalization factor. Following our previous arguments, we may conclude this time that

$$\langle H \rangle = \frac{\langle p^2 \rangle}{2m} + \langle V \rangle \sim \frac{\hbar^2}{2m\beta^2 r_0^2} - \frac{\alpha}{r_0^s}. \quad (4.20)$$

If $s < 2$ we can make $\langle H \rangle$ negative by fine-tuning r_0 to sufficiently large values. Hence, it follows that there are stationary states of negative energy, in which the particle may be found, with a fair probability, at large distances from the origin. This means that there are levels of arbitrary small negative energy. It must be recalled that the wave functions of bound states tend to zero exponentially fast in the region of space where classical motion is forbidden, while here $\langle H \rangle$ decays according to power law.

Theorem 3.1.1 Two linear operators A and B are equal iff

$$\langle a | A | a \rangle = \langle a | B | a \rangle \quad \text{for any } |a\rangle.$$

Proof. One direction is trivial, if $A = B$ then clearly $\langle a | A | a \rangle = \langle a | B | a \rangle$. To prove the other direction we need to show that $\langle a | A | b \rangle = \langle a | B | b \rangle$ for any vectors $|a\rangle, |b\rangle$. To this end we note that by assumption the equality of the expectation values must

also hold for the states $|a\rangle = |a\rangle + |b\rangle$, and $|b\rangle = |a\rangle + i|b\rangle$, i.e.

$$\begin{aligned} (\langle a | + \langle b |) A (|a\rangle + |b\rangle) &= (\langle a | + \langle b |) B (|a\rangle + |b\rangle) \\ (\langle a | - i\langle b |) A (|a\rangle + i|b\rangle) &= (\langle a | - i\langle b |) B (|a\rangle + i|b\rangle). \end{aligned} \quad (3.7)$$

Hence, utilizing the equality of the expectation values, we get

$$\begin{aligned} \langle a | A | b \rangle + \langle b | A | a \rangle &= \langle a | B | b \rangle + \langle b | B | a \rangle \\ \langle a | A | b \rangle - \langle b | A | a \rangle &= \langle a | B | b \rangle - \langle b | B | a \rangle \end{aligned} \quad (3.8)$$

By adding and subtracting these two equations we see that $\langle a | A | b \rangle = \langle a | B | b \rangle$ for any $|a\rangle, |b\rangle$.

Theorem 3.1.2 Two linear operators A and B are equal to within a phase

$$A = e^{i\theta} B$$

iff

$$|\langle a | A | b \rangle| = |\langle a | B | b \rangle| \quad \text{for any } |a\rangle, |b\rangle.$$

" \Rightarrow "

If $A = e^{i\theta} B$ then

$$\langle a | A | b \rangle = e^{i\theta} \langle a | B | b \rangle \Rightarrow |\langle a | A | b \rangle| = |\langle a | B | b \rangle|.$$

Done.

" \Leftarrow "

$$A |b_j\rangle = e^{i\theta_j} B |b_j\rangle, \quad \theta_j := \theta(b_j).$$

Apply the same relation to $|b_1\rangle + |b_2\rangle$:

$$A(|b_1\rangle + |b_2\rangle) = e^{i\theta_{12}} B(|b_1\rangle + |b_2\rangle)$$

for some θ_{12} . But linearity gives

$$e^{i\theta_1} B |b_1\rangle + e^{i\theta_2} B |b_2\rangle = e^{i\theta_{12}} (B |b_1\rangle + B |b_2\rangle).$$

Rearrange:

$$(e^{i\theta_1} - e^{i\theta_{12}}) B |b_1\rangle + (e^{i\theta_2} - e^{i\theta_{12}}) B |b_2\rangle = 0.$$

Take inner product with $B |b_1\rangle$ to get

$$(e^{i\theta_1} - e^{i\theta_{12}}) \|B |b_1\rangle\|^2 + (e^{i\theta_2} - e^{i\theta_{12}}) \langle B |b_1 | B |b_2 \rangle = 0.$$

Similarly inner product with $B |b_2\rangle$. Because $\langle B |b_1 | B |b_2 \rangle \neq 0$, the only way both equations hold is

$$e^{i\theta_1} = e^{i\theta_2} = e^{i\theta_{12}}.$$

So the phase does not depend on b (on the non-kernel part). Call it $e^{i\theta}$. Then for all $|b\rangle$,

$$A |b\rangle = e^{i\theta} B |b\rangle,$$

hence $A = e^{i\theta} B$.

Theorem 4.1.1 — Ritz Theorem. For an arbitrary function Ψ in our Hilbert space, the expectation value of H fulfills the relation

$$E \equiv \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_1. \quad (4.2)$$

The equality holds if and only if Ψ is the ground state wave-function of H .

Proof. As the eigenstates of H form a complete basis of the Hilbert space, Ψ may be expanded as

$$\Psi = \sum_k c_k \Phi_k. \quad (4.3)$$

It follows that

$$\frac{\langle \Psi | H - E_1 | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_{k=1}^{\infty} (E_k - E_1) |c_k|^2}{\sum_{k=1}^{\infty} |c_k|^2} \geq 0. \quad (4.4)$$

The last relation is due to the ordering of the energies, proving Ritz's theorem.

Theorem 4.1.2 — Generalized Ritz Theorem*. The expectation value of the Hamiltonian H is stationary in the neighborhood of its eigenvalues.

Proof. To prove this theorem we induce a small variation in the wave function Ψ , thus if $E(\Psi|\Psi) = \langle \Psi | H | \Psi \rangle$ then

$$\begin{aligned} \delta E(\Psi|\Psi) &= \delta(\langle \Psi | H | \Psi \rangle) - E(\langle \Psi | H - E | \Psi \rangle) \\ &= \delta\Psi | H - E | \Psi + \langle \Psi | H - E | \delta\Psi \rangle \end{aligned} \quad (4.5)$$

If we choose $\delta\Psi = \epsilon(H - E)\Psi$, then on the right hand side we get the norm of the function $\epsilon(H - E)\Psi$. It follows that E is stationary iff $(H - E)\Psi = 0$, i.e. Ψ is an exact eigenstate of H .

Let us assume that $\Psi = \Phi_n + \delta\Phi$, with $\langle \Phi_n | \delta\Phi \rangle = 0$. In this case

$$E = \frac{\langle \Phi_n + \delta\Phi | H | \Phi_n + \delta\Phi \rangle}{\langle \Phi_n + \delta\Phi | \Phi_n + \delta\Phi \rangle} = \frac{E_n \langle \Phi_n | \Phi_n \rangle + \langle \delta\Phi | H | \delta\Phi \rangle}{\langle \Phi_n | \Phi_n \rangle + \langle \delta\Phi | \delta\Phi \rangle} = E_n + O(\delta\Phi^2). \quad (4.6)$$

Thus, we conclude that the energy converge as $O(\delta\Phi^2)$. We note that all other observables converge as $O(\delta\Phi)$.

Theorem 4.1.3 — The variance theorem*. Given the variance of the energy expectation value

$$\sigma^2 \equiv \frac{\langle \Psi | (H - E)^2 | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi | H^2 | \Psi \rangle}{\langle \Psi | \Psi \rangle} - E^2, \quad (4.7)$$

there is at least one exact eigenvalue of H in the interval $[E - \sigma, E + \sigma]$.

Proof. Expanding the wave-function Ψ using the normalized eigenstates of H we can rewrite the variance as

$$\sigma^2 = \sum_{i=1}^{\infty} (E_i - E)^2 |c_i|^2. \quad (4.8)$$

Now let E_K be the eigenstates closest to E , then

$$\sum_{i=1}^{\infty} (E_i - E)^2 |c_i|^2 \geq (E_K - E)^2 \sum_{i=1}^{\infty} |c_i|^2 = (E_K - E)^2. \quad (4.9)$$

Thus $\sigma^2 \geq (E_K - E)^2$, QED.

Theorem 4.5.1 — Upper bound on the eigenvalues of J_0 . Given a Hilbert space with an orthonormal basis $\{|ab\rangle\}$ such that the states $|ab\rangle$ are eigenstates of J^2 , J_0 . If a, b are the eigenvalues of J^2, J_0

$$J^2 |ab\rangle = a |ab\rangle \quad \text{and} \quad J_0 |ab\rangle = b |ab\rangle \quad (5.60)$$

then $a \geq b^2$.

Proof. To prove this statement we notice that

$$J^2 = J_0^2 + \frac{1}{2} (J_- J_+ + J_+ J_-) \quad (5.61)$$

and therefore

$$J^2 - J_0^2 = \frac{1}{2} (J_+ J_- + J_- J_+) \quad (5.62)$$

It follows that

$$\langle ab | J^2 - J_0^2 | ab \rangle = \langle ab | \frac{1}{2} (J_+ J_- + J_- J_+) | ab \rangle \geq 0. \quad (5.63)$$

Therefore

$$\langle ab | J^2 - J_0^2 | ab \rangle = a - b^2 \geq 0 \Rightarrow a \geq b^2. \quad (5.64)$$

Step 3: Show the same choice holds for the whole \mathcal{V}

Repeat the 2D analysis for every pair $(|m\rangle, |n\rangle)$. If one pair forced "linear" and another forced "anti-linear", you get a contradiction by considering a 3D superposition (e.g. involving $|1\rangle, |2\rangle, |3\rangle$) and comparing preserved transition probabilities in two \downarrow ways. So the choice (linear vs conjugate-linear) must be global on \mathcal{V} .

Theorem 8.2.2 — The triangular rule. The admissible values of j are limited by the triangular rule

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \quad (8.27)$$

Proof. The maximum value of m is $j_1 + j_2$. There is only one state with this value of m , the state $|j_1 j_2 j\rangle = (j_1 + j_2, m = (j_1 + j_2))$. For $m = j_1 + j_2 - 1$ there are two possible states $m_1 = j_1, m_2 = j_2 - 1$ and $m_1 = j_1 - 1, m_2 = j_2$. One of these states corresponds to the IRREP $j = j_1 + j_2$, the other to $j = j_1 + j_2 - 1$. We can go on lowering the value of m adding a new IRREP j until $m_1 = -j_1$ or $m_2 = -j_2$. Beyond this point we won't get any new j states.

Theorem 12.3.1 The operators \mathcal{S} and \mathcal{A} satisfy the following properties:

(a) \mathcal{S} and \mathcal{A} are Hermitian operators: $\mathcal{S}^\dagger = \mathcal{S}$, $\mathcal{A}^\dagger = \mathcal{A}$.

(b) \mathcal{S} and \mathcal{A} commute with P_g for all $g \in S_N$,

$$P_g \mathcal{S} = \mathcal{S} P_g = \mathcal{S}, \\ P_g \mathcal{A} = \mathcal{A} P_g = \text{sign}(g) \mathcal{A}. \quad (12.24)$$

(c) \mathcal{S} and \mathcal{A} are projectors to orthogonal subspaces of \mathcal{H}_{tot} i.e.

$$\mathcal{S}^2 = \mathcal{S}, \quad \mathcal{A}^2 = \mathcal{A}, \quad \mathcal{S}\mathcal{A} = \mathcal{A}\mathcal{S} = 0. \quad (12.25)$$

Proof. (a) By definition

$$\mathcal{S}^\dagger = \frac{1}{N!} \sum_{g \in S_N} P_g^\dagger = \frac{1}{N!} \sum_{g \in S_N} P_g^{-1} = \frac{1}{N!} \sum_{g \in S_N} P_g = \mathcal{S}, \quad (12.26)$$

where 2nd equality follows from unitarity of representation $P_g^\dagger = P_g^{-1}$, the 3rd equality rests on $P_g^{-1} = P_{g^{-1}}$ which follows from (12.22). Finally, the last equality is because inverse operation is a bijection from S_N to itself. The proof of $\mathcal{A}^\dagger = \mathcal{A}$ is almost identical. We only need to note that since $g^{-1}g = I$ and $\text{sign}(I) = 1$ we must have $\text{sign}(g^{-1}) = \text{sign}(g)$.

(b) We have

$$P_g \mathcal{A} = \frac{1}{N!} \sum_{g' \in S_N} \text{sign}(g') P_g P_{g'} = \frac{1}{N!} \sum_{g' \in S_N} \text{sign}(g)^2 \text{sign}(g') P_{g'} \\ = \frac{\text{sign}(g)}{N!} \sum_{g' \in S_N} \text{sign}(gg') P_{g'} = \text{sign}(g) \mathcal{A}, \quad (12.27)$$

where in the 2nd equality we used (12.22) and $\text{sign}(g)^2 = 1$, $\forall g \in S_N$, whereas in the 1st equality of the second line we substituted $\text{sign}(g)\text{sign}(g') = \text{sign}(gg')$. Finally, last equality rests on the bijective nature of the map $g' \rightarrow gg'$. The proof for \mathcal{S} follow suit.

(c) Using the definition of \mathcal{S} and (b), yields

$$\mathcal{S}^2 = \frac{1}{N!} \sum_{g \in S_N} P_g \mathcal{S} = \frac{1}{N!} \sum_{g \in S_N} \mathcal{S} = \mathcal{S}. \quad (12.28)$$

Similarly,

$$\mathcal{A}^2 = \frac{1}{N!} \sum_{g \in S_N} \text{sign}(g) P_g \mathcal{A} = \frac{1}{N!} \sum_{g \in S_N} \text{sign}(g)^2 \mathcal{A} = \mathcal{A}. \quad (12.29)$$

Now for $\mathcal{S}\mathcal{A}$ see that

$$\mathcal{S}\mathcal{A} = \mathcal{S}(P_g^{-1}P_g)\mathcal{A} = (\mathcal{S}P_g^{-1})(P_g\mathcal{A}) = \mathcal{S}\text{sign}(g)\mathcal{A}, \quad (12.30)$$

and choosing an odd parity g we much have $\mathcal{S}\mathcal{A} = 0$. ■

$$\begin{aligned} & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \end{aligned}$$

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$$\begin{aligned} & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \end{aligned}$$

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$$\begin{aligned} & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \end{aligned}$$

$$\begin{aligned} & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \end{aligned}$$

$$\mathcal{A} = -g^2 \mathbf{E}^2$$

Theorem 13.9.1 — The Optical theorem. The optical theorem states that

$$\text{Im } f_{\text{tot}}(k) = \frac{4\pi}{k} \text{Im } f_k(0). \quad (13.59)$$

Proof. To prove the optical theorem we use the T -matrix

$$f_k(0) = f(k, k) = -\frac{m}{2\pi\hbar^2} (2\pi\hbar)^3 \langle k | T | k \rangle. \quad (13.60)$$

Now using the Lippmann-Schwinger equation (13.24) and (13.43) we have

$$\begin{aligned} \text{Im } \langle k | T | k \rangle &= \text{Im } \langle k | V | \Psi_k^{in} \rangle \\ &= \text{Im } \left[\left(\langle \Psi_k^{in} | \Psi_k^{in} \rangle - \frac{1}{E - E_0 + i\epsilon} \right) V | \Psi_k^{in} \rangle \right]. \end{aligned} \quad (13.61)$$

To proceed we recall the definition of the principle value integral

$$\text{Pr} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0} = \lim_{\delta \rightarrow 0} \left[\int_{-\infty}^{-\delta} dx \frac{f(x)}{x - x_0} + \int_{\delta}^{\infty} dx \frac{f(x)}{x - x_0} \right], \quad (13.62)$$

and note that

$$\begin{aligned} \int_{-\infty}^{\infty} dE \frac{f(E)}{E - E_0 + i\epsilon} &= \lim_{\delta \rightarrow 0} \left[\int_{-\infty}^{-\delta} dE \frac{f(E)}{E - E_0 + i\epsilon} + \int_{\delta}^{\infty} dE \frac{f(E)}{E - E_0 + i\epsilon} \right] \\ &= \text{Pr} \int_{-\infty}^{\infty} dE \frac{f(E)}{E - E_0 + i\epsilon} + i\pi f(E_0), \end{aligned} \quad (13.63)$$

where c stands for integration over a semicircle from $-\delta$ to δ , see Fig. 13.2.

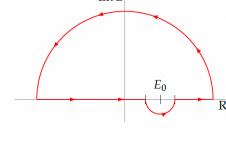


Figure 13.2: A principle value integral.

It follows that

$$\frac{1}{E - E_0 + i\epsilon} = \text{Pr} \left(\frac{1}{E - E_0} \right) + i\pi \delta(E - E_0). \quad (13.64)$$

Utilizing this relation we see that

$$\begin{aligned} \text{Im } \langle k | T | k \rangle &= \text{Im} \left[\langle \Psi_k^{in} | V | \Psi_k^{in} \rangle - \text{Pr} \left(\frac{1}{E - E_0} \right) V | \Psi_k^{in} \rangle \right] \\ &\quad - i\pi \langle \Psi_k^{in} | V \delta(E - E_0) | V | \Psi_k^{in} \rangle \end{aligned} \quad (13.65)$$

Due to the hermiticity of V and H_0 the first two term are real, hence

$$\text{Im } \langle k | T | k \rangle = -\pi \langle \Psi_k^{in} | V \delta(E - E_0) | V | \Psi_k^{in} \rangle. \quad (13.66)$$

Utilizing once more the relation (13.43) between V and T we get

$$\begin{aligned} \text{Im } \langle k | T | k \rangle &= -\pi \langle k | T \delta(E - E_0) | T | k \rangle \\ &= -\pi \int \hbar^2 dk' \langle k | T | k' \rangle \langle k' | T | k \rangle \delta \left(E - \frac{\hbar^2 k'^2}{2m} \right) \\ &= -\pi \int \hbar^2 dk' \frac{mk}{\hbar^2} | \langle k' | T | k \rangle |^2, \end{aligned} \quad (13.67)$$

where in the last step we have used $dK' = \hbar^2 dE' / (dk' \delta E')$. With a little help form (13.46) we can rewrite this result in terms of the total cross-section,

$$\begin{aligned} \text{Im } \langle k | T | k \rangle &= -\pi \left(\frac{2\pi\hbar^2}{m(2\pi\hbar)^3} \right)^2 \int dk' \hbar m k | \langle k' | T | k \rangle |^2, \\ &= -\pi \left(\frac{2\pi\hbar^2}{m(2\pi\hbar)^3} \right)^2 \hbar m k \sigma_{\text{tot}}. \end{aligned} \quad (13.68)$$

Now

$$\begin{aligned} \text{Im } f_k(0) &= -\frac{m}{2\pi\hbar^2} (2\pi\hbar)^3 (-\pi) \left(\frac{2\pi\hbar^2}{m(2\pi\hbar)^3} \right)^2 \hbar m k \sigma_{\text{tot}} \\ &= \pi \left(\frac{2\pi\hbar^2}{m(2\pi\hbar)^3} \right)^2 \hbar m k \sigma_{\text{tot}} = \frac{k}{4\pi} \sigma_{\text{tot}}, \end{aligned} \quad (13.69)$$

which concludes our proof. ■

$$\begin{aligned} & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \\ & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \\ & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \\ & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \\ & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - g(\mathbf{B} \cdot \nabla)^2 - g^2 \mathbf{E}^2) \\ & = \frac{1}{2m} \left(-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - g^2 \mathbf{E}^2 \right) \\ & = \frac{1}{2m} \left(-\hbar^2 \nabla^2 + (-\hbar^2 \mathbf{B}^2 - g^2 \mathbf{E}^2) \right) = -g^2 \mathbf{E}^2 \\ & \mathcal{A} = -g^2 \mathbf{E}^2 \\ & \text{Left side: } \text{sign}(g) P_g \mathcal{A} = \text{sign}(g) \text{sign}(g) \mathcal{A} = \mathcal{A} \\ & \text{Right side: } P_g^{-1} P_g \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \mathcal{A} \mathcal{A} \rightarrow \mathcal{A} = \mathcal{A} \\ & \mathcal{A} = \frac{1}{2m} (-\hbar^2 \nabla^2 - 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$$\nabla \cdot \gamma(x^2 - y^2) \quad \text{gradient operator} \quad \text{divergence of vector field}$$

$$[L_0, A_{\mu}^{(0)}] = i \mu A_{\mu}^{(0)}$$

$$[L_{\pm}, A_{\mu}^{(0)}] = \pm \sqrt{(A_{\mu}^{(0)})} (A_{\mu+1}^{(0)} - A_{\mu-1}^{(0)})$$

$$[\delta_2, z] = 1$$

$$[\delta_{x,y}, z] = 0$$

$$z = \Theta_0^2 = \Theta_0'$$

$$L_x = i(y\partial_x - z\partial_y), \quad L_y = -i(z\partial_x - x\partial_z), \quad L_z = L_x + iL_y$$

$$[L_z, z^2] = 0 \Rightarrow f = 0$$

for $\mu = 0$ we have $L_z = 0$

$$[L_z, z^2] = -i(y\partial_x - z\partial_y) - (z\partial_x - x\partial_z) = -iz\partial_x - zx\partial_z$$

$$[L_z, (x+iy)^2] = -i(y\partial_x - z\partial_y) + (z\partial_x - x\partial_z) = (x+iy)^2$$

$$[L_z, (x+iy)^2] = -i(y\partial_x - z\partial_y) + (z\partial_x - x\partial_z) = 0 \Rightarrow \boxed{\mu=0}$$

$$[L_z, z^2] = \sqrt{x(x+1) + y(y+1)} \quad \Theta_1^2 = -iz\partial_x - zx\partial_z$$

$$[L_z, z^2] = \sqrt{x(x+1) - y(y+1)} \quad \Theta_2^2 = 2 \quad S_2^2 = (x+iy)^2$$

$$[L_z, z^2] = \sqrt{x(x+1) + y(y+1)} \quad \Theta_3^2 = 2 \quad S_3^2 = (x-iy)^2$$

$$\vdots$$

$$\Theta_{-2}^2 = \frac{1}{2}(x-iy)^2 = \frac{1}{2}(x^2 - iy^2 - y^2)$$

$$\Theta_2^2 = \frac{1}{2}(x+iy)^2 = \frac{1}{2}(x^2 + iy^2 - y^2)$$

$$\vdots$$

$$\nabla = \Theta_2^2 + \Theta_{-2}^2$$

$$|\lambda \gamma \mu l'm| = 12m \quad \text{from above}$$

$$m = m' + j_n \rightarrow m = m' + 2 \quad \Theta_2^2 \rightarrow -2$$

$$1 \geq l' \leq l \leq \mu + l' \rightarrow 12 - l' \leq l \leq 12 + l'$$

$$\text{since } l' \neq 0 \quad \text{and } l' \neq 12$$

$$<1'm| x^2 | 1'm> = <1'm| x^2 x^2 x^2 | 1'm> = (-1)^{l+l'} <1'm| x | 1'm>$$

$$\vdots$$

$$l+l' = \text{even}$$

$$|1'm>$$

$$\nabla = \gamma \cdot \begin{pmatrix} 1211 & 210 & 211 & 200 \\ 12102 & 0 & 0 & \alpha^* & 0 \\ 12112 & 0 & 0 & 0 & 0 \\ 12002 & 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \Theta_2^2 \quad \Theta_{-2}^2$$

$$\nabla = \gamma \cdot \begin{pmatrix} 0 & 0 & \alpha^* & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\text{only } \alpha^* \text{ is non-zero}$$

$$\alpha = <21-1 | x^2 - y^2 | 2111> = \int \nabla_{211}^* (x^2 - y^2) \nabla_{211} dx dy$$

$$\text{using } \nabla = \gamma \text{ we get} \quad \nabla = -i(\partial_x - \partial_y) \quad \alpha = \text{real part}$$

gradient operator

$$\nabla(x) = \begin{cases} F_0 x & 0 < x < T \\ 0 & \text{otherwise} \end{cases}$$

$$x = \int_{2m\pi}^{\frac{\pi}{L}} (\omega + \omega_0^2) \quad \omega_0 = \tan(\frac{1}{2}\alpha + \frac{1}{2})$$

$$\nabla(t) = F_0 X(t) = F_0 \int_{2m\pi}^{\frac{\pi}{L}} (\omega + \omega_0^2) \quad \equiv g$$

$$|\psi_{nlm}> = \sum c_{nlm} e^{\frac{i\omega_{nlm} t}{\hbar}} |t> = \sum c_{nlm} e^{-i\omega_{nlm} t} |t>$$

$$|t> = |\psi>$$

$$\text{use } \nabla$$

$$c_{nlm} = 1$$

$$m=0$$

$$C_n^{(0)}(t) = -\frac{i}{\hbar} \sum_{m=1}^n c_{nm}(t_0) \int_{t_0}^t dt' e^{i\omega_{nm} t'} \nabla_{nm}(t') e^{i\omega_{nm} t'} \nabla_{nm}(t')$$

$$\nabla_{nm} = g <01010111> = g <\text{colat1}> \times g$$

$$C_n^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^t dt' e^{i\omega_{n1} t'} \nabla_{n1}(t') (1 - e^{i\omega_{n1} t'})$$

$$\nabla_m = g <1101111> \rightarrow g <01010111> \quad n=0$$

$$g <2101111> + \sqrt{2} g \quad n=2$$

$$C_2^{(2)} = -\frac{i\sqrt{2}}{\hbar} \int_{t_0}^t dt' e^{i\omega_{21} t'} (1 - e^{i\omega_{21} t'}) = \frac{i\sqrt{2}}{\hbar} \left(\frac{e^{i\omega_{21} t} - 1}{i\omega_{21}} - \frac{e^{i(\omega_{21} + \omega_{10}) t} - 1}{i(\omega_{21} + \omega_{10})} \right)$$

$$C_0^{(2)} = -\frac{i\sqrt{2}}{\hbar} \int_{t_0}^t dt' e^{i\omega_{01} t'} (1 - e^{i\omega_{01} t'}) = \frac{i\sqrt{2}}{\hbar} \left(\frac{e^{i\omega_{01} t} - 1}{i\omega_{01}} - \frac{e^{i(\omega_{01} + \omega_{10}) t} - 1}{i(\omega_{01} + \omega_{10})} \right)$$

$$C_n^{(0)} = \frac{i}{\hbar} \sum_{m=1}^n c_{nm}(t_0) \int_{t_0}^t dt' e^{i\omega_{nm} t'} \nabla_{nm}(t') \quad \text{use } \nabla$$

$$= -\frac{1}{\hbar} \int_{t_0}^t dt' e^{i\omega_{n1} t'} \nabla_{n1}(t')$$

$$\nabla_{n1}(t) = g \cdot <111 (0+0^2) 10> + g <110 010> = g$$

$$\text{use } \nabla \quad n=1 \quad \uparrow$$

$$C_1^{(0)}(t) = -\frac{i}{\hbar} \int_{t_0}^t dt' e^{i\omega_{10} t'} = \frac{g}{\hbar \omega_{10}} (1 - e^{i\omega_{10} t})$$

100% use ∇ to get ∇ from ∇

$$\nabla(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) x$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

$$\Psi_{nm} = \nabla(x) \cdot \nabla(z) \cdot \nabla(y) = \frac{2}{L} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \chi_{spin}$$

$$E_{nm} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + \frac{\hbar^2 \pi^2 m^2}{2mL^2} + \frac{\hbar^2 \pi^2 l^2}{2mL^2}$$

use ∇

$n=1, m=1$

$$\Psi_{111} = \nabla(x) \cdot \nabla(z) \cdot \nabla(y) = \frac{2}{L} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \chi_{spin}$$

$$E_{111} = \frac{\hbar^2 \pi^2}{mL^2} \quad \leftarrow \text{use } \nabla$$

$$S = S_1 S_2$$

$$1S_1 S_2 \leftarrow S \leq S_1 S_2$$

$$0 \leq S \leq 2$$

$$S=0 \quad S=1 \quad S=2$$

$$S=1-1,0-1 \quad S=3 \quad S=5$$

$$S=2-1,0-1,1-2 \quad S=5 \quad S=7$$

$$P_1 |S, M> = (-1)^{S+1} |S, M> \quad S \geq 1$$

$$P_2 |S, M> = |S, M> \quad \text{use } \nabla$$

$$P_3 |S, M> = -1 |S, M> \quad \text{use } \nabla$$

$$P_4 |S, M> = 1 |S, M> \quad \text{use } \nabla$$

$$(S=2, S=0) \quad 6 \quad \text{use } \nabla$$

$$100 \text{ or } \text{use } \nabla \text{ to get } S=2 \quad \text{use } \nabla$$

$$100 \text{ or } \text{use } \nabla \text{ to get } S=0 \quad \text{use } \nabla$$

$$S=0, 2 \quad \Psi_{111} = \frac{1}{\sqrt{2}} [\chi_{+}(x) \chi_{+}(y) + \chi_{-}(x) \chi_{-}(y)] \cdot \chi_{spin}$$

$$S=1 \quad \Psi_{111} = \frac{1}{\sqrt{2}} [\chi_{+}(x) \chi_{-}(y) - \chi_{-}(x) \chi_{+}(y)] \cdot \chi_{spin}$$

$$S=3 \quad \text{use } \nabla$$

$$E = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + \chi_{spin}$$

(nonzero for $S=3$ since ∇ is zero)

$$E = \hbar \omega (n+\frac{1}{2})$$

$$: \text{use } \nabla \text{ to get } S=3$$

$$\nabla(x) = \left(\frac{\pi x}{L}\right)^{\frac{3}{2}} e^{-\frac{\pi x}{L}}$$

$$E_0 = \hbar \omega (n+\frac{1}{2}) = \frac{1}{2} \hbar \omega$$

nonzero for $S=3$ since ∇ is zero

$$E = \hbar \omega (n_1 + n_2 + n_3 + \frac{3}{2}) = \hbar \omega (6 + 0 + 1 + \frac{3}{2}) = \frac{5}{2} \hbar \omega$$

nonzero for $S=3$ since ∇ is zero

$$\Psi_0 = \Psi_{111} \Psi_{222} \Psi_{333} = \left(\frac{\pi x_1}{L}\right)^{\frac{3}{2}} \left(\frac{\pi y_1}{L}\right)^{\frac{3}{2}} \left(\frac{\pi z_1}{L}\right)^{\frac{3}{2}} e^{-\frac{\pi x_1}{L}} e^{-\frac{\pi y_1}{L}} e^{-\frac{\pi z_1}{L}}$$

$$E_0 = \hbar \omega (n_1 + n_2 + n_3 + \frac{3}{2}) = \frac{3}{2} \hbar \omega$$

$$n_1 = n_2 = n_3 = 0$$

$$E = \hbar \omega (n_1 + n_2 + n_3 + \frac{3}{2}) = \hbar \omega (6 + 0 + 1 + \frac{3}{2}) = \frac{5}{2} \hbar \omega$$

$$\Psi_0 = \frac{1}{\sqrt{3!}} \det \begin{pmatrix} \chi_{+}(x_1) \chi_{+}(y_1) \chi_{+}(z_1) & \chi_{+}(x_1) \chi_{+}(y_1) \chi_{-}(z_1) & \chi_{+}(x_1) \chi_{-}(y_1) \chi_{+}(z_1) \\ \chi_{+}(x_2) \chi_{+}(y_2) \chi_{+}(z_2) & \chi_{+}(x_2) \chi_{+}(y_2) \chi_{-}(z_2) & \chi_{+}(x_2) \chi_{-}(y_2) \chi_{+}(z_2) \\ \chi_{+}(x_3) \chi_{+}(y_3) \chi_{+}(z_3) & \chi_{+}(x_3) \chi_{+}(y_3) \chi_{-}(z_3) & \chi_{+}(x_3) \chi_{-}(y_3) \chi_{+}(z_3) \end{pmatrix}$$

$$E = \hbar \omega (n_1 + n_2 + n_3 + \frac{3}{2}) = \hbar \omega (6 + 0 + 1 + \frac{3}{2}) = \frac{5}{2} \hbar \omega$$