A

Operator Method for the Harmonic Oscillator Problem

Hamiltonian

The Hamiltonian of a particle of mass $m$ moving in a one-dimensional harmonic potential is

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

The quantum mechanical operators $p$ and $x$ satisfy the commutation relation $[p, x] = -i\hbar$ where $i = \sqrt{-1}$. The Hamiltonian can be written

$$H = \frac{1}{2m} (m \omega x - ip)(m \omega + ip) + \frac{1}{2} \hbar \omega. \quad (A.2)$$

To see the equivalence of (A.1) and (A.2) one need only multiply out the product in (A.2) remembering that $p$ and $x$ are operators which do not commute. Equation (A.2) can be rewritten by

$$H = \hbar \omega \left\{ \frac{(m \omega x - ip)(m \omega + ip)}{2m \hbar \omega} + \frac{1}{2} \right\}. \quad (A.3)$$

We now define the operator $a$ and its adjoint $a^\dagger$ by the relations

$$a = \frac{m \omega x + ip}{\sqrt{2m \hbar \omega}} \quad (A.4)$$

$$a^\dagger = \frac{m \omega x - ip}{\sqrt{2m \hbar \omega}}. \quad (A.5)$$

These two equations can be solved for the operators $x$ and $p$ to give

$$x = \left( \frac{\hbar}{2m \omega} \right)^{1/2} (a^\dagger + a), \quad (A.6)$$

$$p = i \left( \frac{m \hbar \omega}{2} \right)^{1/2} (a^\dagger - a). \quad (A.7)$$
It follows from the commutation relation satisfied by $x$ and $p$ that

$$[a, a^\dagger]_- = 1, \quad \text{(A.8)}$$
$$[a, a]_- = [a^\dagger, a^\dagger]_- = 0. \quad \text{(A.9)}$$

By using the relation

$$[A, BC]_- = B [A, C]_- + [A, B]_- C, \quad \text{(A.10)}$$

it is not difficult to prove that

$$[a, a^\dagger^2]_- = 2a^\dagger, \quad [a, a^\dagger^3]_- = 3a^\dagger^2, \quad \ldots$$
$$[a, a^\dagger^n]_- = na^\dagger^{n-1}. \quad \text{(A.11)}$$

Here, $a^\dagger$ and $a$ are called as raising and lowering operators, respectively.

From (A.3)–(A.5) it can be seen that

$$H = \hbar \omega \left( a^\dagger a + \frac{1}{2} \right). \quad \text{(A.12)}$$

Now, assume that $|n>\rangle$ is an eigenvector of $H$ with an eigenvalue $\varepsilon_n$. Operate on $|n>\rangle$ with $a^\dagger$, and consider the energy of the resulting state. We can certainly write

$$H (a^\dagger|n>\rangle) = a^\dagger H |n>\rangle + [H, a^\dagger] |n>\rangle. \quad \text{(A.13)}$$

But we have assumed that $H |n>\rangle = \varepsilon_n |n>\rangle$, and we can evaluate the commutator $[H, a^\dagger]$.

$$[H, a^\dagger] = \hbar \omega [a^\dagger a, a^\dagger] = \hbar \omega a^\dagger [a, a^\dagger]$$
$$= \hbar \omega a^\dagger. \quad \text{(A.14)}$$

Therefore, (A.13) gives

$$Ha^\dagger |n>\rangle = (\varepsilon_n + \hbar \omega) a^\dagger |n>\rangle. \quad \text{(A.15)}$$

Equation (A.15) tells us that if $|n>\rangle$ is an eigenvector of $H$ with eigenvalue $\varepsilon_n$, then $a^\dagger |n>\rangle$ is also an eigenvector of $H$ with eigenvalue $\varepsilon_n + \hbar \omega$. Exactly the same technique can be used to show that

$$Ha |n>\rangle = (\varepsilon_n - \hbar \omega) a |n>\rangle. \quad \text{(A.16)}$$

Thus, $a^\dagger$ and $a$ act like raising and lowering operators, raising the energy by $\hbar \omega$ or lowering it by $\hbar \omega$. 
Ground State

Since $V(x) \geq 0$ everywhere, the energy must be greater than or equal to zero. Suppose the ground state of the system is denoted by $|0 >$. Then, by applying the operator $a$ to $|0 >$ we generate a state whose energy is lower by $\hbar \omega$, i.e.,

$$H a |0 > = (\varepsilon_0 - \hbar \omega) a |0 > .$$  \hspace{1cm} (A.17)

The only possible way for (A.17) to be consistent with the assumption that $|0 >$ was the ground state is to have $a |0 >$ give zero. Thus, we have

$$a |0 >= 0 .$$  \hspace{1cm} (A.18)

If we use the position representation where $\Psi_0(x)$ is the ground state wavefunction and $p$ can be represented by $p = -i \hbar \partial / \partial x$, (A.18) becomes a simple first-order differential equation

$$\left( \frac{\partial}{\partial x} + \frac{m \omega}{\hbar} x \right) \Psi_0(x) = 0 .$$  \hspace{1cm} (A.19)

One can see immediately see that the solution of (A.19) is

$$\Psi_0(x) = N_0 e^{-\frac{1}{2} \alpha^2 x^2} ,$$  \hspace{1cm} (A.20)

where $N_0$ is a normalization constant, and $\alpha^2 = \frac{m \omega}{\hbar}$. The normalization constant is given by $N_0 = \alpha^{1/2} \pi^{-1/4}$. The energy is given by $\varepsilon_0 = \frac{\hbar \omega}{2}$, since $a^\dagger a |0 > = 0$.

Excited States

We can generate all the excited states by using the operator $a^\dagger$ to raise the system to the next higher energy level, i.e., if we label the $n$th excited state by $|n >$,

$$| 1 > \propto a^\dagger |0 > , \quad \varepsilon_1 = \hbar \omega \left( 1 + \frac{1}{2} \right) ,$$

$$| 2 > \propto a^\dagger^2 |0 > , \quad \varepsilon_2 = \hbar \omega \left( 2 + \frac{1}{2} \right) ,$$

$$\vdots$$

$$| n > \propto a^\dagger^n |0 > , \quad \varepsilon_n = \hbar \omega \left( n + \frac{1}{2} \right) .$$  \hspace{1cm} (A.21)

Because $a^\dagger$ creates one quantum of excitation and $a$ annihilates one, $a^\dagger$ and $a$ are often called creation and annihilation operators, respectively.

If we wish to normalize the eigenfunctions $|n >$ we can write

$$|n > = C_n a^\dagger^n |0 > .$$  \hspace{1cm} (A.22)
Assume that $|0\rangle$ is normalized (see (A.20)). Then, we can write
\[ \langle n|n \rangle = |C_n|^2 \left \langle 0 \left | a^n a^\dagger^n \right | 0 \right \rangle. \] (A.23)

Using the relations given by (A.12) allows one to show that
\[ a^n a^\dagger^n |0\rangle = n! |0\rangle. \] (A.24)

So that
\[ |n\rangle = \frac{1}{\sqrt{n!}} a^\dagger^n |0\rangle \] (A.25)
is the normalized eigenfunction for the \(n\)th excited state.

One can use \(\Psi_0(x) = \alpha^{1/2} \pi^{-1/4} e^{-\frac{1}{2} \alpha^2 x^2} \) and express \(a^\dagger^n\) in terms of \(p\) and \(x\) to obtain
\[ \Psi_n(x) = \frac{1}{\sqrt{n!}} \left [ -i (-i \hbar \partial/\partial x) + m\omega x \right ]^n \frac{\alpha^{1/2}}{\pi^{1/4}} e^{-\frac{\alpha^2 x^2}{2}}, \] (A.26)

This can be simplified a little to the form
\[ \Psi_n(x) = \frac{(\alpha/\sqrt{\pi})^{1/2} (-)^n}{\alpha^n (2^n n!)^{1/2}} \left ( \frac{\partial}{\partial x} - \alpha^2 x \right )^n e^{-\frac{\alpha^2 x^2}{2}}. \] (A.27)

Summary

The Hamiltonian of the simple harmonic oscillator can be written
\[ H = \hbar \omega \left ( a^\dagger a + \frac{1}{2} \right ). \] (A.28)

and \(H|n\rangle = \hbar \omega (n + \frac{1}{2})|n\rangle\). The excited eigenkets can be written
\[ |n\rangle = \frac{1}{\sqrt{n!}} a^\dagger^n |0\rangle \] (A.29)

The eigenfunctions (A.29) form a complete orthonormal set, i.e.,
\[ \langle n|m \rangle = \delta_{nm}, \] (A.30)

and
\[ \sum_n |n\rangle \langle n| = 1. \] (A.31)

The creation and annihilation operators satisfy the commutation relation
\[ [a, a^\dagger] = 1. \]

Problems

A.1. Prove that \([\hat{A}, \hat{B} \hat{C}]_- = \hat{B}[\hat{A}, \hat{C}]_- + [\hat{A}, \hat{B}]_- \hat{C},\) where \(\hat{A}, \hat{B},\) and \(\hat{C}\) are quantum mechanical operators.

A.2. Prove that \([\hat{a}, (\hat{a}^\dagger)^n]_- = n(\hat{a}^\dagger)^{n-1} \).
Neutron Scattering

A beam of neutrons interacts with a crystal through a potential

\[ V(\mathbf{r}) = \sum_{\mathbf{R}_i} v(\mathbf{r} - \mathbf{R}_i), \quad (B.1) \]

where \( \mathbf{r} \) is the position operator of the neutron, and \( \mathbf{R}_i \) is the position operator of the \( i^{th} \) atom in the crystal. It is common to write \( v(\mathbf{r} - \mathbf{R}_i) \) in terms of its Fourier transform \( v(\mathbf{r}) = \sum_k v_k e^{ik \cdot \mathbf{r}} \). Then, (B.1) can be rewritten

\[ V(\mathbf{r}) = \sum_{k, \mathbf{R}_i} v_k e^{ik \cdot (\mathbf{r} - \mathbf{R}_i)}. \quad (B.2) \]

The potential \( v(\mathbf{r}) \) is very short-range, and \( v_k \) is almost independent of \( k \). The \( k \)-independent coefficient \( v_k \) is usually expressed as

\[ v_k = \frac{2\pi}{\bar{\hbar}} \frac{1}{a M_n}, \]

where \( a \) is defined as the scattering length and \( M_n \) is the mass of the neutron.

The initial state of the system can be expressed as

\[ \Psi_i(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{r}) = V^{-1/2} e^{i\mathbf{p} \cdot \mathbf{r}} |n_1, n_2, \ldots, n_N\rangle. \quad (B.3) \]

Here, \( V^{-1/2} e^{i\mathbf{p} \cdot \mathbf{r}} \) is the initial state of a neutron of momentum \( \mathbf{p} \). The ket \( |n_1, n_2, \ldots, n_N\rangle \) represents the initial state of the crystal, with \( n_i \) phonons in mode \( i \). The final state, after the neutron is scattered, is

\[ \Psi_f(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{r}) = V^{-1/2} e^{i\mathbf{p'} \cdot \mathbf{r}} |m_1, m_2, \ldots, m_N\rangle. \quad (B.4) \]

The transition rate for going from \( \Psi_i \) to \( \Psi_f \) can be calculated from Fermi’s golden rule.

\[ R_{i\rightarrow f} = \frac{2\pi}{\hbar} |\langle \Psi_f | V | \Psi_i \rangle|^2 \delta(E_f - E_i). \quad (B.5) \]

Here, \( E_i \) and \( E_f \) are the initial and final energies of the entire system. Let us write \( \varepsilon_i = E_i - \frac{p^2}{2M_n} \) and \( \varepsilon_f = E_f - \frac{p'^2}{2M_n} \). The total rate of scattering out of
initial state $\Psi_i$ is given by

$$R_{\text{out of } i} = \frac{2\pi}{\hbar} \sum_f \delta (\varepsilon_f - \varepsilon_i - \hbar \omega) |\langle \Psi_f | V | \Psi_i \rangle|^2,$$

(B.6)

where $\hbar \omega = \frac{p'^2 - p^2}{2M_n}$ is the change in energy of the neutron. If we write $p' = p + \hbar k$, where $\hbar k$ is the momentum transfer, the matrix element becomes

$$\sum_{i,k} \langle m_1, m_2, \ldots, m_N | v_k e^{-i k \cdot R_i} | n_1, n_2, \ldots, n_N \rangle.$$

(B.7)

But we can take $v_k = v$ outside the sum since it is a constant. In addition, we can write $R_j = R^0_j + u_j$ and

$$u_j = \sum_{q\lambda} \left( \frac{\hbar}{2MN\omega_{q\lambda}} \right)^{1/2} e^{i q \cdot R^0_j} \tilde{\epsilon}_{q\lambda} (a_{q\lambda} - a_{-q\lambda}^\dagger).$$

(B.8)

The matrix element of $e^{i q \cdot u_j}$ between harmonic oscillator states $|n_1, n_2, \ldots, n_N\rangle$ and $|m_1, m_2, \ldots, m_N\rangle$ is exactly what we evaluated earlier in studying the Mössbauer effect. By using our earlier results and then summing over the atoms in the crystal, one can obtain the transition rate. The cross-section is related to the transition rate divided by the incident flux.

One can find the following result for the cross-section:

$$\frac{d\sigma}{d\Omega d\omega} = \frac{p'}{p} N \frac{a^2}{\hbar} S(q, \omega),$$

(B.9)

where $d\Omega$ is solid angle, $d\omega$ is energy transfer, $N$ is the number of atoms in the crystal, $a$ is the scattering length, and $S(q, \omega)$ is called the dynamic structure factor. It is given by

$$S(q, \omega) = N^{-1} \sum_f \left| \sum_j \langle m_1, \ldots, m_N | e^{i q \cdot u_j} | n_1, \ldots, n_N \rangle \right|^2 \delta (\varepsilon_f - \varepsilon_i - \hbar \omega).$$

(B.10)

Again, there is an elastic scattering part of $S(q, \omega)$, corresponding to no-phonon emission or absorption in the scattering process. For that case $S(q, \omega)$ is given by

$$S_0(q, \omega) = e^{-2W} \delta(\omega) N \sum_{K} \delta_{q,K}.$$

(B.11)

Here, $e^{-2W}$ is the Debye–Waller factor. $W$ is proportional to

$$\left[ \langle n_1, \ldots, n_N | q \cdot u_0 | n_1, \ldots, n_N \rangle \right]^2.$$
From (B.11) we see that there are Bragg peaks. In the harmonic approximation
the peaks are $\delta$-functions [because of $\delta(\omega)$] due to energy conservation. The
peaks occur at momentum transfer $\mathbf{p}' - \mathbf{p} = \mathbf{K}$, a reciprocal lattice vector.

In the early days of X-ray scattering there was some concern over whether
the motion of the atoms (both zero point and thermal motion) would broaden
the $\delta$-function peaks and make X-ray diffraction unobservable. The result,
in the harmonic approximation, is that the $\delta$-function peaks are still there,
but their amplitude is reduced by the Debye–Waller factor $e^{-2W}$.

For the one-phonon contribution to the cross-section, we obtain

$$
\frac{d\sigma}{d\Omega d\omega} = N e^{-2W} \frac{p'}{p} \sum_{\lambda} \frac{(\mathbf{q} \cdot \hat{\mathbf{q}}_\lambda)^2}{2M\omega_{q\lambda}} \{ (1 + n_{q\lambda}) \delta(\omega + \omega_{q\lambda}) + n_{q\lambda} \delta(\omega - \omega_{q\lambda}) \}.
$$

(B.12)

There are still unbroadened $\delta$-function peaks at $\varepsilon_f \pm \hbar \omega_{q\lambda} = \varepsilon_i$, corresponding
to the emission or absorption of a phonon. The peaks occur at a scattering
angle determined from $\mathbf{p}' - \mathbf{p} = \mathbf{q} + \mathbf{K}$ where $\mathbf{K}$ is a reciprocal lattice vector.
The amplitude again contains the Debye–Waller factor $e^{-2W}$. Inelastic neutron scattering allows a experimentalist to determine the phonon frequencies
$\omega_{q\lambda}$ as a function of $\mathbf{q}$ and of $\lambda$.

The broadening of the $\delta$-function peaks occurs only when anharmonic
terms are included in the calculation. Anharmonic forces lead to phonon–phonon scattering and to finite phonon lifetimes.
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