# Physics 127c: Statistical Mechanics

# Second Quantization

## Ladder Operators in the SHO

It is useful to first review the use of ladder operators in the simple harmonic oscillator. Here I present the bare bones—review your favorite Quantum textbook for more details.

The Hamiltonian for the SHO is

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

For this section only, I will scale variables so that $m = 1$, $K = 1$,and also $\hbar = 1$, to save writing. So the Hamiltonian is

$$H = \frac{1}{2}p + \frac{1}{2}x^2 \tag{2}$$

and using $p = -i\partial/\partial x$ (remember $\hbar = 1$) Schrodinger's equation $H\psi = E\psi$ gives eigenstates $\psi_n$ and energy eigenvalues $\varepsilon_n$

$$-\frac{1}{2}\frac{d^2}{dx^2}\psi_n(x) + \frac{1}{2}x^2\psi_n(x) = \varepsilon_n\psi(x). \tag{3}$$

This differential equation can be solved with all the technology of orthogonal polynomials to find the eigenvalues $\varepsilon_n = n + \frac{1}{2}$, etc.

We can instead solve the problem algebraically by introducing up and down ladder operators $b^+$ and $b$

$$b = \frac{1}{\sqrt{2}}(p - ix) \tag{4}$$

$$b^+ = (b)^+ = \frac{1}{\sqrt{2}}(p + ix) \tag{5}$$

where the $+$ superscript denotes the Hermitian conjugate. We know that the *commutator*

$$[x, p] \equiv [xp - px] = i \tag{6}$$

is equivalent to the coordinate representation $p \to -i\partial/\partial x$, and so it is natural to look at the commutation properties of $b$, $b^+$:

$$[b, b^+] = \frac{1}{2}[p - ix, p + ix] \tag{7}$$

$$= -i[x, p] = 1. \tag{8}$$

The Hamiltonian is

$$H = b^+b + \frac{1}{2}, \tag{9}$$

and we are led to look at

$$[b, b^+b] = bb^+b - b^+bb \tag{10}$$

$$= [b, b^+]b = b, \tag{11}$$

and

$$[b^+, b^+b] = b^+b^+b - b^+bb^+ \tag{12}$$

$$= -b^+[b, b^+] = -b^+. \tag{13}$$

Collecting the results:

$$[b, b^+] = 1, \tag{14a}$$
$$[b, b^+b] = b, \tag{14b}$$
$$[b^+, b^+b] = -b^+. \tag{14c}$$

Since $H$ is the sum of squares, the eigenvalues must be positive, and so there is lowest energy $\varepsilon_0$ and corresponding normalized eigenfunction $\psi_0$. Let's consider the state $b\psi_0$, and ask how the Hamiltonian acts on this state using the commutation rules to transfer the action of $H$ onto $\psi_0$:

$$H(b\psi_0) = (b^+b + \frac{1}{2})b\psi_0 \tag{15}$$
$$= [b(b^+b + \frac{1}{2}) - b]\psi_0 \tag{16}$$
$$= (\varepsilon_0 - 1)(b\psi_0). \tag{17}$$

This suggests that $b\psi_0$ is an eigenfunction with energy $\varepsilon_0 - 1$, but since $\varepsilon_0$ was defined as the lowest energy this is not possible, and the only way out is

$$b\psi_0 = 0. \tag{18}$$

Thus *the ground state eigenfunction is defined by the action of the down ladder operator $b$ giving zero*.

Similarly

$$H(b^+\psi_0) = (\varepsilon_0 + 1)(b^+\psi_0) \tag{19}$$

so that $b^+\psi_0$ is an eigenfunction with energy $\varepsilon_0 + 1$. Continuing in this way we find a "ladder" of eigenstates

$$\psi_n = (b^+)^n\psi_0 \quad \text{with energy} \quad \varepsilon_n = n + \frac{1}{2}. \tag{20}$$

We can argue that this generates the complete set of states, etc., etc. (see your Quantum text book). Note that

$$b^+b\psi_n = n\psi_n \tag{21}$$

so the operator $b^+b$ acts as a level counter.

We have not addressed the normalization of the $\psi_n$ created in this way. The normalization of the $\psi_n$ can be related:

$$\langle\psi_n|\psi_n\rangle = \left\langle\psi_{n-1}|bb^+|\psi_{n-1}\right\rangle = \left\langle\psi_{n-1}|b^+b + 1|\psi_{n-1}\right\rangle = n\,\langle\psi_{n-1}|\psi_{n-1}\rangle\,. \tag{22}$$

Since $\psi_0$ is normalized, this gives $\langle\psi_n|\psi_n\rangle = n!$. Then the functions

$$u_n = (n!)^{-1/2}\psi_n \tag{23}$$

are normalized eigenfunctions, $\langle u_n|u_n\rangle = 1$.

Rewriting the effect of the ladder operators on $\psi_n$ in terms of the normalized states $u_n$ gives

$$b^+u_n = \sqrt{n+1}u_{n+1} \tag{24}$$
$$bu_n = \sqrt{n}u_{n-1} \tag{25}$$
$$b^+bu_n = nu_n. \tag{26}$$

Remembering that the level $n$ can be thought of as $n$ bosons in the single particle state of energy 1 we therefore have the following dictionary. We have introduced a raising operator or boson creation operator $b^+$, and a lowering operator or boson annihilation operator $b$. The operator $b^+b = n$ counts the level or the

number of bosons. The Hamiltonian is just $b^+b$ plus a constant. (Going back to unscaled units, it would be $b^+b$ times the harmonic oscillator energy $\hbar\omega$, plus a constant.) The lowering or annihilation operator gives zero when acting on the lowest or zero particle state. The analysis in terms of ode theory has been replaced by an analysis in terms of the algebra of the $b, b^+$ operators, a considerable simplification.

Other expectation values can also be calculated e.g.

$$\langle u_0|x^2|u_0\rangle = -\frac{1}{2}\langle u_0|(b^+ - b)(b^+ - b)|u_0\rangle \tag{27}$$

$$= -\frac{1}{2}\langle u_0|(b^+b^+ - b^+b - bb^+ + bb|u_0\rangle \tag{28}$$

$$= \frac{1}{2}\langle u_0|(bb^+|u_0\rangle = \frac{1}{2} \tag{29}$$

where $b\,|u_0\rangle = 0 = \langle u_0|\,b^+$ has been used. Again this is considerably easier than integrating over the Gaussian form of $u_0(x)$.

## Many Particle Systems

### Occupation number representation

For a many particle system we choose as the basis any symmetrized (bosons) or antisymmetrized (fermions) product of complete orthonormal set of single particle states $\phi_i$. Often these will be chosen as momentum states, position states, or eigenstates of the noninteracting Hamiltonian.

**Bosons:** The $N$ particle basis state is

$$\psi_B(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N) = C\sum_P \phi_1(P\,\vec{r}_1)\phi_1(P\,\vec{r}_2)\ldots\phi_1(P\,\vec{r}_{n_1})\ldots\phi_Q(P\,\vec{r}_N) \tag{30}$$

where $\phi_q, q = 1\ldots Q$ occurs $n_q$ times ("$n_q$ particles in the state $\phi_q$"). The sum runs over $N!$ permutations $P$ and the normalization constant is

$$C = (N!n_1!n_2!\ldots n_Q!)^{-1/2}. \tag{31}$$

Last term we introduced the *occupation number representation* where this state is represented

$$\psi_B = \left|n_1 n_2 \ldots n_Q \ldots\right\rangle \tag{32}$$

where all the $n_q$ are zero for the empty states $q > Q$. We define boson creation operator $b_q^+$ and annihilation operator $b_q$ that adds or subtracts one particle from the single particle state $\phi_q$

$$b_q^+\left|n_1 n_2 \ldots n_q \ldots n_Q\right\rangle = (n_q+1)^{1/2}\left|n_1 n_2 \ldots (n_q+1)\ldots n_Q\right\rangle, \tag{33a}$$

$$b_q\left|n_1 n_2 \ldots n_q \ldots n_Q\right\rangle = (n_q)^{1/2}\left|n_1 n_2 \ldots (n_q-1)\ldots n_Q\right\rangle. \tag{33b}$$

The prefactors are motivated by the ladder-operator results, and can be checked to preserve the normalization. Of course if $n_q = 0$, the second result is just zero, consistent with the action of $b$ on a zero particle state. It is easy to check that $b, b^+$ satisfy

$$[b_r, b_s^+] = \delta_{rs}, \tag{34}$$

$$[b_r, b_s] = [b_r^+, b_s^+] = 0. \tag{35}$$

**Fermions** The antisymmetrized Fermi basis state is the Slater determinant

$$\psi_F(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N) = C \sum_P (-1)^P \phi_1(P\,\vec{r}_1)\phi_2(P\,\vec{r}_2)\ldots\phi_N(P\,\vec{r}_N) \tag{36}$$

where now all the $\phi_i$ have to be different for a nonzero wave function (equivalent to the Pauli exclusion principle). The normalization constant is

$$C = (N!)^{-1/2}. \tag{37}$$

The occupation number representation is

$$\psi_F = |n_1 n_2 \ldots\rangle \tag{38}$$

where each $n_i$ is one if the state appears in the Slater determinant and zero otherwise. Note that the order of the states affects the overall sign through the $(-1)^P$, so we must have some convention for ordering the list of one particle states. What are the appropriate creation and annihilation operators?

First consider the single particle state. Possible occupation numbers are 0, 1, i.e. the states $|0\rangle$ and $|1\rangle$. Define creation operator $a^+$ and annihilation operator $a$ such that

$$\begin{array}{ll} a^+|0\rangle = |1\rangle & a^+|1\rangle = 0 \\ a|0\rangle = 0 & a|1\rangle = |0\rangle\,. \end{array} \tag{39}$$

(Take care of the difference between 0 and $|0\rangle$.) It is easy to check that $a$, $a^+$ satisfy *anticommutation rules*

$$\left\{a, a^+\right\} = 1 \tag{40a}$$

$$\{a, a\} = 0 = \left\{a^+, a^+\right\} \tag{40b}$$

where

$$\{A, B\} = AB + BA. \tag{41}$$

For a multiparticle system

$$a_s|n_1 n_2 \ldots n_s \ldots\rangle = \begin{cases} (-1)^S |n_1 n_2 \ldots 0_s \ldots\rangle & \text{if } n_s = 1 \\ 0 & \text{if } n_s = 0 \end{cases} \tag{42a}$$

$$a_s^+|n_1 n_2 \ldots n_s \ldots\rangle = \begin{cases} 0 & \text{if } n_s = 1 \\ (-1)^S |n_1 n_2 \ldots 1_s \ldots\rangle & \text{if } n_s = 0 \end{cases} \tag{42b}$$

where

$$S = n_1 + n_2 + \cdots n_{s-1} \tag{43}$$

is to keep track of the ordering convention. The full algebra is then

$$\left\{a_r, a_s^+\right\} = \delta_{rs}, \tag{44a}$$

$$\{a_r, a_s\} = 0 = \left\{a_r^+, a_s^+\right\}. \tag{44b}$$

Note, for example that

$$a_1^+ a_2^+ |0, 0, \ldots\rangle = -a_2^+ a_1^+ |0, 0, \ldots\rangle \tag{45}$$

consistent with the definition in terms of Slater determinants.

In either case the number operator that counts the number of particles is the same

$$n_s = \begin{cases} b_s^+ b_s & \text{BOSONS} \\ a_s^+ a_s & \text{FERMIONS} \end{cases} \tag{46}$$

and has eigenvalues corresponding to the possible occupation numbers of the state $s$ ($0, 1$ for Fermions, $0, 1, \ldots$ for Bosons). It follows from the commutation or anticommutation rules that in either case

$$[n_s, n_r] = 0 \tag{47}$$

so that the set $\{n_r\}$ are simultaneously diagonalizable, as we expect from the definition of occupation number states.

A general many particle wave function $\psi$ can be expressed as a linear combination of the occupation number basis states. The expectation value $\langle \psi \,|n_s|\, \psi \rangle$ may then be nonintegral.

We have replaced complicated symmetric product or determinant wave functions by states in the simpler occupation number representation, and have developed the algebra of operators connecting these states. Any occupation number state can be generated by acting on the no-particle state $|0\rangle$ (the "vacuum state") with appropriate combinations of creation operators $c^+$. This notation is called "second quantization" as opposed to the original "first quantization" notation. It is the notation of quantum field theory. The next task is to write *physical* operators in terms of these elementary operators.

**Physical Operators**

We are usually interested in few-body operators, i.e. those involving a few particle coordinates in the "usual" first quantization notation, such as the kinetic energy $T = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2$ or the potential energy $V = \sum_{i<j} u(\vec{r}_i - \vec{r}_j)$.

For a one body operator $O_1 = \sum f_i$ the second quantized expression is

$$O_1 = \sum_{r,s} \langle \phi_r \,|f|\, \phi_s \rangle \, c_r^+ c_s \tag{48}$$

where $\langle \phi_r \,|f|\, \phi_s \rangle$ is the matrix element

$$\langle \phi_r \,|f|\, \phi_s \rangle = \int d^3r \, \phi_r^*(\vec{r}) f(\vec{r}) \phi_s(\vec{r}) \tag{49}$$

and $c$ represents $a$ for Fermions and $b$ for Bosons.

For a two body operator $O_2 = \sum_{ij} f(\vec{r}_i, \vec{r}_j)$ the second quantized form is

$$O_2 = \sum_{pqrs} f_{pqrs} c_p^+ c_q^+ c_s c_r \tag{50}$$

with

$$f_{pqrs} = \int d^3r d^3r' \, \phi_p^*(\vec{r}) \phi_q^*(\vec{r}') f(\vec{r}, \vec{r}') \phi_r(\vec{r}) \phi_s(\vec{r}'). \tag{51}$$

Note carefully for Fermions the ordering of the $c$ operators in Eq. (50)— this ordering does not matter for bosons because the operators commute. These expressions are the same for both Bosons and Fermions.

We will prove these results for the more difficult Fermion case, first the one particle operator. In first quantized notation we consider

$$R = \sum_s f(\vec{r}_s) A[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\ldots\phi_N(\vec{r}_N)] \tag{52}$$

with $A$ the antisymmetrization operation. Since $\sum f$ is unchanged by particle permutation we can put it inside the $A$ operation. We then use completeness of the $\phi_s$

$$f(\vec{r})\phi_s(\vec{r}) = \sum_r \langle \phi_r \,|\, f \,|\, \phi_s \rangle \, \phi_r(\vec{r}) \tag{53}$$

so that $R$ becomes the sum, with weights $\langle \phi_r \,|\, f \,|\, \phi_s \rangle$, of antisymmetrized products in which the $s$th basis state $\phi_s$ is replaced by $\phi_r$. This is the content of the second quantized expression, since $c_r^+ c_s$ has precisely this effect. For a two particle operator the analogous result holds, i.e. we replace basis functions $r, s$ with basis functions $p, q$ with weight $f_{pqrs}$. The ordering of the $c$ operators arises because

$$(c_p^+ c_q^+ c_s c_r)(c_r^+ c_s^+) \,|0\rangle = c_p^+ c_q^+ \,|0\rangle \tag{54}$$

which is the required transformation (check from the (anti)commutation rules).

**Examples**

A common choice of basis is plane wave states in a volume $\Omega = L^3$

$$\phi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}, \quad \vec{k} = \frac{2\pi}{L}(l, m, n). \tag{55}$$

(If there is spin, as must be the case for Fermions, we would use plane wave states for each spin state, i.e. $\phi_{\vec{k}\sigma}$, and the sums over $\vec{k}$ below would be enlarged to sums over $\vec{k}$ and $\sigma$.) The kinetic energy is $T = \sum_{\vec{k},\vec{k}'} T_{\vec{k}\vec{k}'} c_{\vec{k}}^+ c_{\vec{k}'}$ with

$$T_{\vec{k}\vec{k}'} = \frac{1}{\Omega} \int d^3r e^{-i\vec{k}\cdot\vec{r}} \left( -\frac{\hbar^2}{2m} \nabla^2 \right) e^{i\vec{k}'\cdot\vec{r}} \tag{56}$$

giving

$$T = \sum_{\vec{k}} \varepsilon_k c_{\vec{k}}^+ c_{\vec{k}} \quad \text{with} \quad \varepsilon_k = \frac{\hbar^2 k^2}{2m}. \tag{57}$$

The potential energy involves the matrix element

$$V_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4} = \frac{1}{\Omega^2} \int\int d^3r d^3r' \, e^{-i\vec{k}_1\cdot\vec{r}} e^{-i\vec{k}_2\cdot\vec{r}'} u(\vec{r} - \vec{r}') e^{i\vec{k}_3\cdot\vec{r}} e^{i\vec{k}_4\cdot\vec{r}'} \tag{58a}$$

$$= \frac{1}{\Omega^2} \int d^3r \, e^{i(-\vec{k}_1 - \vec{k}_2 + \vec{k}_3 + \vec{k}_4)\cdot\vec{r}} \int d^3R \, e^{i(-\vec{k}_2 + \vec{k}_4)\cdot\vec{R}} \, u(\vec{R}) \tag{58b}$$

$$= \frac{1}{\Omega} \delta_{-\vec{k}_1 - \vec{k}_2 + \vec{k}_3 + \vec{k}_4} \tilde{u}(\vec{k}_2 - \vec{k}_4) \tag{58c}$$

writing $\vec{R} = \vec{r} - \vec{r}'$ and in the last expression

$$\tilde{u}(\vec{q}) = \int d^3R \, u(\vec{R}) e^{-\vec{q}\cdot\vec{r}}. \tag{59}$$

This gives for the second quantized operator

$$V = \frac{1}{2\Omega} \sum_{\vec{k},\vec{k}',\vec{q}} \tilde{u}(\vec{q}) c_{\vec{k}+\vec{q}}^+ c_{\vec{k}'-\vec{q}}^+ c_{\vec{k}'} c_{\vec{k}}. \tag{60}$$

In the case of spins, we usually are concerned with a spin-independent interaction, and then

$$V = \frac{1}{2\Omega} \sum_{\substack{\vec{k},\vec{k}',\vec{q} \\ \sigma,\sigma'}} \tilde{u}(\vec{q}) c_{\vec{k}+\vec{q},\sigma}^+ c_{\vec{k}'-\vec{q},\sigma'}^+ c_{\vec{k}',\sigma'} c_{\vec{k},\sigma}. \tag{61}$$

Another common choice is the position basis, e.g. for the $i$th particle to be at position $\vec{r}$

$$\phi(\vec{r}_i) = \delta(\vec{r}_i - \vec{r}). \tag{62}$$

With this basis, the creation and annihilation operators are usually written $\psi^+(\vec{r})$ and $\psi(\vec{r})$. They satisfy the algebras:

**Bosons:**

$$[\psi(\vec{r}), \psi^+(\vec{r}')] = \delta(\vec{r} - \vec{r}') \tag{63a}$$
$$[\psi(\vec{r}), \psi(\vec{r}')] = 0 = [\psi^+(\vec{r}), \psi^+(\vec{r}')] \tag{63b}$$

**Fermions:**

$$\left\{\psi(\vec{r}), \psi^+(\vec{r}')\right\} = \delta(\vec{r} - \vec{r}') \tag{64a}$$
$$\left\{\psi(\vec{r}), \psi(\vec{r}')\right\} = 0 = \left\{\psi^+(\vec{r}), \psi^+(\vec{r}')\right\} \tag{64b}$$

The kinetic and potential energies are

$$T = \int d^3r\, \psi^+(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi(\vec{r}) \tag{65a}$$
$$V = \frac{1}{2}\int\int d^3r d^3r' u(\vec{r} - \vec{r}')\psi^+(\vec{r})\psi^+(\vec{r}')\psi(\vec{r}')\psi(\vec{r}) \tag{65b}$$

or with spin (and spin independent interaction)

$$T = \sum_\sigma \int d^3r\, \psi^+_\sigma(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi_\sigma(\vec{r}) \tag{66a}$$
$$V = \frac{1}{2}\sum_{\sigma,\sigma'}\int\int d^3r d^3r' u(\vec{r} - \vec{r}')\psi^+_\sigma(\vec{r})\psi^+_{\sigma'}(\vec{r}')\psi_{\sigma'}(\vec{r}')\psi_\sigma(\vec{r}) \tag{66b}$$

These two choices of creation and annihilation operators are related by

$$\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}}\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}\, c_{\vec{q}}, \tag{67a}$$
$$\psi^+(\vec{r}) = \frac{1}{\sqrt{\Omega}}\sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{r}}\, c^+_{\vec{q}}, \tag{67b}$$

and the inverse

$$c_{\vec{q}} = \frac{1}{\sqrt{\Omega}}\int d^3r\, e^{-i\vec{q}\cdot\vec{r}}\psi(\vec{r}), \tag{68a}$$
$$c^+_{\vec{q}} = \frac{1}{\sqrt{\Omega}}\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\psi^+(\vec{r}), \tag{68b}$$

as can be verified by constructing the plane wave state $c^+_q|0\rangle$.

## Further Reading

Consult your favorite Quantum textbook for harmonic oscillator ladder operators. *Pathria* §10.1 discusses the formalism of second quantization, as do a number of the books on reserve for the class.