

Freie Universität Berlin
Tutorials for Advanced Quantum Mechanics
Wintersemester 2018/19
Sheet 4

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1. **Bosonic and Fermionic commutation relations**(3×2 points)

- (a) Recalling the quantum harmonic oscillator, it is now apparent that the ladder operators,

$$a = \frac{1}{\sqrt{2\hbar}}(x + ip), \quad a^\dagger = \frac{1}{\sqrt{2\hbar}}(x - ip) \quad (1)$$

Derive the original form of Heisenbergs uncertainty principle which states that the standard deviation product of position and momentum measurements is lower bounded as,

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad (2)$$

From lectures we know that the product of the standard deviation of two Hermitian observables is lower bounded by,

$$\Delta x \Delta p \geq \frac{1}{2} |\langle \psi | [x, p] | \psi \rangle| \quad (3)$$

Substituting from (1) gives,

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

and hence

$$\begin{aligned} [x, p] &= \frac{i\hbar}{2} [(a + a^\dagger)(a^\dagger - a) - (a^\dagger - a)(a + a^\dagger)] \\ &= \frac{i\hbar}{2} [aa^\dagger - a^2 + (a^\dagger)^2 - a^\dagger a - a^\dagger a - (a^\dagger)^2 + a^2 + aa^\dagger] \\ &= i\hbar[a, a^\dagger] \\ &= i\hbar \end{aligned} \quad (4)$$

Thus,

$$\begin{aligned} \Delta x \Delta p &\geq \frac{1}{2} |\langle \psi | i\hbar | \psi \rangle| \\ &= \frac{\hbar}{2} \end{aligned} \quad (5)$$

- (b) Starting from the fermionic anti-commutation relations

$$\{\hat{f}_j, \hat{f}_k^\dagger\} = \delta_{j,k}, \quad \{\hat{f}_j, \hat{f}_k\} = \{\hat{f}_j^\dagger, \hat{f}_k^\dagger\} = 0 \quad (6)$$

derive the action of the fermionic creation and annihilation operators on the occupation number basis states,

$$\hat{f}_j |N_1, \dots, N_j, \dots\rangle = (-1)^{\sum_{k=1}^{j-1} N_k} N_j |N_1, \dots, 1 - N_j, \dots\rangle \quad (7)$$

$$\hat{f}_j^\dagger |N_1, \dots, N_j, \dots\rangle = (-1)^{\sum_{k=1}^{j-1} N_k} (1 - N_j) |N_1, \dots, 1 - N_j, \dots\rangle \quad (8)$$

First recall the fermionic commutation relations

$$\{\hat{f}_i, \hat{f}_j\} = \{\hat{f}_i^\dagger, \hat{f}_j^\dagger\} = 0, \{\hat{f}_i, \hat{f}_j^\dagger\} = \delta_{ij} \quad (9)$$

which imply

$$\hat{f}_j^2 = (\hat{f}_j^\dagger)^2 = 0, \quad \hat{f}_j \hat{f}_{k \neq j}^\dagger = -\hat{f}_{k \neq j}^\dagger \hat{f}_j, \quad \hat{f}_j \hat{f}_j^\dagger = 1 - \hat{f}_j^\dagger \hat{f}_j \quad (10)$$

Let $\{|\lambda_n\rangle\}$ be the eigenstates satisfying $\hat{n}|\lambda_n\rangle = \hat{f}^\dagger \hat{f}|\lambda_n\rangle = \lambda_n |\lambda_n\rangle$. We can see right away that

$$\hat{n}(1 - \hat{n}) = \hat{f}^\dagger \hat{f}(1 - \hat{f}^\dagger \hat{f}) = \hat{f}^\dagger \hat{f} \hat{f} \hat{f}^\dagger = 0 \quad (11)$$

which implies that the only eigenvalues of \hat{n} must be 0 or 1. Now consider the state $\hat{f}^\dagger |\lambda_n\rangle$,

$$\hat{f}^\dagger \hat{f}(\hat{f}^\dagger |\lambda_n\rangle) = \hat{f}^\dagger (1 - \hat{f}^\dagger \hat{f}) |\lambda_n\rangle = (1 - \lambda_n) \hat{f}^\dagger |\lambda_n\rangle \quad (12)$$

which says that \hat{f}^\dagger maps $|\lambda_n\rangle$ to $|1 - \lambda_n\rangle$. This means that

$$\hat{f}^\dagger |n\rangle = c_n |1 - n\rangle \quad (13)$$

and to find the normalisation use that,

$$|c_n|^2 = \langle n | \hat{f} \hat{f}^\dagger |n\rangle = \langle n | (1 - \hat{n}) |n\rangle = (1 - n) \quad (14)$$

Since a global complex phase is unobservable in quantum mechanics¹ we can choose c to be real and since $1^2 = 1$ and $0^2 = 0$ we can set $c_n = 1 - n$, meaning overall that $\hat{f}^\dagger |n\rangle = (1 - n) |1 - n\rangle$. Turning to \hat{f} we can write,

$$\hat{f}^\dagger \hat{f} \hat{f} |n\rangle = (1 - \hat{f} \hat{f}^\dagger) \hat{f} |n\rangle = (1 - n) \hat{f} |n\rangle \quad (15)$$

which means that we also have,

$$\hat{f} |n\rangle = c_n |1 - n\rangle \quad (16)$$

Again we have,

$$|c_n|^2 = \langle n | \hat{f}^\dagger \hat{f} |n\rangle = n \quad (17)$$

and again we can set $c \in \mathbb{R}$ and use that $1^2 = 1$ and $0^2 = 0$ to set $c_n = n$ so that

$$\hat{f} |n\rangle = n |1 - n\rangle \quad (18)$$

¹For any observable \hat{A} , state $|\psi\rangle$ and complex phase $e^{i\phi}$ then $\langle \psi | e^{-i\phi} \hat{A} e^{i\phi} | \psi \rangle = \langle \psi | \hat{A} | \psi \rangle$ so the phase factor cannot be observed.

The final step is to consider a multi-orbital state in the occupation representation $\hat{f}_j|N_1, N_2, \dots, N_j, \dots\rangle$ where (since these are fermions) we now know that $N_i \in \{0, 1\}$ and we can write

$$\hat{f}_j|N_1, N_2, \dots, N_j, \dots\rangle = \hat{f}_j \left(\hat{f}_1^\dagger\right)^{N_1} \left(\hat{f}_2^\dagger\right)^{N_2} \dots \left(\hat{f}_j^\dagger\right)^{N_j} \dots |\Omega\rangle \quad (19)$$

All we need to do is commute \hat{f}_j through the creation operators until we get to the j^{th} orbital where we already know it's action from above. Since by definition for all of the orbitals k to the left of j we have $k < j$ that means $\{\hat{f}_j, \hat{f}_k^\dagger\} = 0$ and so we will simply pick up a minus sign for each time that $N_k = 1$ from this we derive our final expression

$$\hat{f}_j|N_1, \dots, N_j, \dots\rangle = (-1)^{\sum_{k=1}^{j-1} N_k} N_j |N_1, \dots, 1 - N_j, \dots\rangle \quad (20)$$

and a similar argument applies to \hat{f}_j^\dagger .

- (c) Consider the single particle Hamiltonian \hat{H}_0 with eigenstates $\{|\lambda\rangle\}$ - i.e. $\hat{H}_0|\lambda\rangle = \lambda|\lambda\rangle$. Let $|\lambda_1, \dots, \lambda_N\rangle_{B(F)}$ be the corresponding bosonic (fermionic) N particle basis state in a first quantization representation. We define the number operator as $\hat{n}_\lambda = \hat{a}_\lambda^\dagger \hat{a}_\lambda$. Now, by using the second quantization representation of $|\lambda_1, \dots, \lambda_N\rangle_{B(F)}$, and the appropriate commutation relations for $\hat{a}_\lambda^\dagger, \hat{a}_\lambda$, prove that the number operator \hat{n}_λ simply counts the number of particles in state $|\lambda\rangle$ - i.e. show explicitly that for both bosonic and fermionic N particle states

$$\hat{n}_\lambda |\lambda_1, \dots, \lambda_N\rangle_{B(F)} = \sum_{i=1}^N \delta_{\lambda\lambda_i} |\lambda_1, \dots, \lambda_N\rangle_{B(F)} \quad (21)$$

In the previous question you derived the action of the fermionic creation and annihilation operators on eigenstates of $\hat{n}_\lambda = a_j^\dagger \lambda a_j$. We call this the *number* operator because when acted on a multi-particle state it counts the number of particles in mode j . We are now going to prove this property, since the RHS of (21) is precisely counting how many times $\lambda_i = \lambda$ and returning that many copies of the state. First recall that we can write a many particle state using creation operators in the first quantisation picture as

$$|\lambda_1, \dots, \lambda_N\rangle_{B(F)} = \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a_{\lambda_N}^\dagger \dots a_{\lambda_1}^\dagger |\Omega\rangle = |\lambda_1, \lambda_2, \dots, \lambda_N\rangle \quad (22)$$

where operators are either fermionic or bosonic, the product is over all orbitals λ and n_λ is the number of instances where $\lambda_i = \lambda$. Now, our plan is to commute the \hat{n}_λ operator through the $\hat{a}_{\lambda_i}^\dagger$ operators until it reaches the vacuum state, (where it will vanish since $a_\lambda|\Omega\rangle = 0|\Omega\rangle \forall \lambda$). For bosons we have,

$$\begin{aligned} [\hat{a}_\lambda^\dagger \hat{a}_\lambda, \hat{a}_{\lambda_i}^\dagger] &= \hat{a}_\lambda^\dagger [\hat{a}_\lambda, \hat{a}_{\lambda_i}^\dagger] + [\hat{a}_\lambda^\dagger, \hat{a}_{\lambda_i}^\dagger] \hat{a}_\lambda \\ &= \delta_{\lambda, \lambda_i} \hat{a}_\lambda^\dagger = \delta_{\lambda, \lambda_i} \hat{a}_{\lambda_i}^\dagger \\ \Rightarrow \hat{a}_\lambda^\dagger \hat{a}_\lambda \hat{a}_{\lambda_i}^\dagger &= \delta_{\lambda, \lambda_i} \hat{a}_{\lambda_i}^\dagger + \hat{a}_{\lambda_i}^\dagger \hat{a}_\lambda^\dagger \hat{a}_\lambda \end{aligned} \quad (23)$$

where the last equality is simply because given the action of the δ function we are free to change the index on the creation operator in the first term. Now we can write,

$$\begin{aligned}\hat{n}_\lambda|\lambda_1, \dots, \lambda_N\rangle_B &= \frac{1}{\sqrt{\prod_\lambda n_\lambda!}}(\delta_{\lambda, \lambda_N} \hat{a}_{\lambda_N}^\dagger + \hat{a}_{\lambda_N}^\dagger \hat{a}_\lambda^\dagger \hat{a}_\lambda^\dagger) \hat{a}_{\lambda_{N-1}}^\dagger \dots \hat{a}_{\lambda_1}^\dagger |\Omega\rangle \\ &= \delta_{\lambda, \lambda_N} |\lambda_1, \dots, \lambda_N\rangle_B + \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} \hat{a}_{\lambda_N}^\dagger \hat{a}_\lambda^\dagger \hat{a}_\lambda^\dagger \hat{a}_{\lambda_{N-1}}^\dagger \dots \hat{a}_{\lambda_1}^\dagger |\Omega\rangle\end{aligned}\quad (24)$$

Iterating this through the other $N - 1$ creation operators we will arrive at,

$$\hat{n}_\lambda|\lambda_1, \dots, \lambda_N\rangle_{B(F)} = \sum_{i=1}^N \delta_{\lambda \lambda_i} |\lambda_1, \dots, \lambda_N\rangle_B + \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a_{\lambda_N}^\dagger \dots a_{\lambda_1}^\dagger \hat{n}_\lambda |\Omega\rangle \quad (25)$$

where the last term vanishes to give the desired result.

For fermions we now have an anti-commutation relation so that

$$\begin{aligned}\{\hat{f}_\lambda^\dagger \hat{f}_\lambda, \hat{f}_{\lambda_i}^\dagger\} &= \hat{f}_\lambda^\dagger \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger + \hat{f}_{\lambda_i}^\dagger \hat{f}_\lambda^\dagger \hat{f}_\lambda \\ &= \hat{f}_\lambda^\dagger \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger - \hat{f}_{\lambda_i}^\dagger \hat{f}_\lambda^\dagger \hat{f}_\lambda \\ &= \hat{f}_\lambda^\dagger \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger - \hat{f}_{\lambda_i}^\dagger (\delta_{\lambda, \lambda_i} - \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger) \\ &= 2\hat{f}_\lambda^\dagger \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger - \delta_{\lambda, \lambda_i} \hat{f}_{\lambda_i}^\dagger\end{aligned}\quad (26)$$

Equating the first and last lines of the above expression and subtracting $\hat{f}_\lambda^\dagger \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger$ from both sides gives,

$$\hat{f}_\lambda^\dagger \hat{f}_\lambda \hat{f}_{\lambda_i}^\dagger = \delta_{\lambda, \lambda_i} \hat{f}_{\lambda_i}^\dagger + \hat{f}_{\lambda_i}^\dagger \hat{f}_\lambda^\dagger \hat{f}_\lambda = \delta_{\lambda, \lambda_i} \hat{f}_{\lambda_i}^\dagger + \hat{f}_{\lambda_i}^\dagger \hat{f}_\lambda^\dagger \hat{f}_\lambda \quad (27)$$

which is the same as (23) for bosons so the rest of the proof follows.

2. Observables in second quantisation (2×2 points)

- (a) Consider a system of N particles, and a one-body operator $\hat{O}_1 = \sum_{j=1}^N \hat{o}_j$, where \hat{o}_j is an ordinary single particle operator acting on the j 'th particle. Furthermore, using the same notation as (1c), assume that \hat{O}_1 is diagonal in the $\{|\lambda\rangle\}$ basis, i.e. $\hat{o} = \sum_\lambda o_\lambda |\lambda\rangle\langle\lambda|$. Show that a second quantization representation of \hat{O}_1 , with respect to the $\{|\lambda\rangle\}$ basis, is given by

$$\hat{O}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} \langle\lambda|\hat{o}|\lambda\rangle \hat{a}_\lambda^\dagger \hat{a}_\lambda \quad (28)$$

Writing a one body operator in the form $\hat{O}_1 = \sum_{j=1}^N \hat{o}_j$ might seem a bit strange at first in the sense that any two quantum particles are indistinguishable. But this is already taken care of by the (anti-)symmetrisation of the (fermionic) bosonic state. For example, for a two particle state we would have $\hat{O}_1 = \hat{o}_1 + \hat{o}_2 = \hat{o} \otimes \mathbb{I} + \mathbb{I} \otimes \hat{o}$. Consider acting this on a state with one particle in mode λ_1 and another in mode λ_2 . This would be

$|\lambda_1, \lambda_2\rangle_{B(F)} = \frac{1}{\sqrt{2}} (|\lambda_1\rangle_1 |\lambda_2\rangle_2 \pm |\lambda_2\rangle_1 |\lambda_1\rangle_2)$ where the subscripts on the kets are labelling the particle, so then

$$\begin{aligned}\hat{O}_1 |\lambda_1, \lambda_2\rangle_{B(F)} &= (\hat{o} \otimes \mathbb{I} + \mathbb{I} \otimes \hat{o}) \frac{1}{\sqrt{2}} (|\lambda_1\rangle_1 |\lambda_2\rangle_2 \pm |\lambda_2\rangle_1 |\lambda_1\rangle_2) \\ &= \frac{1}{\sqrt{2}} [o_{\lambda_1} |\lambda_1\rangle_1 |\lambda_2\rangle_2 \pm o_{\lambda_2} |\lambda_2\rangle_1 |\lambda_1\rangle_2 \\ &\quad + o_{\lambda_2} |\lambda_1\rangle_1 |\lambda_2\rangle_2 \pm o_{\lambda_1} |\lambda_2\rangle_1 |\lambda_1\rangle_2] \\ &= (o_{\lambda_1} + o_{\lambda_2}) |\lambda_1, \lambda_2\rangle_{B(F)}\end{aligned}\tag{29}$$

For N particles we will simply find that

$$\hat{O}_1 |\lambda_1, \lambda_2, \dots, \lambda_N\rangle = \sum_{i=1}^N o_{\lambda_i} |\lambda_1, \lambda_2, \dots, \lambda_N\rangle\tag{30}$$

But the sum of the eigenvalue o_{λ_i} over of the λ_i 's for all particles in a particular state, each of which are in one of the orbitals labelled by λ , is the same as asking how many particles are in orbital λ , multiplying by the eigenvalue for that orbital and summing over all the orbitals. In other words, it is necessarily true that $\sum_{i=1}^N o_{\lambda_i} |\lambda_1, \lambda_2, \dots, \lambda_N\rangle = \sum_{\lambda} \hat{n}_{\lambda} o_{\lambda} |\lambda_1, \lambda_2, \dots, \lambda_N\rangle$. Thus,

$$\begin{aligned}\langle \lambda'_1, \lambda'_2, \dots, \lambda'_N | \hat{O}_1 |\lambda_1, \lambda_2, \dots, \lambda_N\rangle &= \langle \lambda'_1, \lambda'_2, \dots, \lambda'_N | \sum_{i=1}^N o_{\lambda_i} |\lambda_1, \lambda_2, \dots, \lambda_N\rangle \\ &= \langle \lambda'_1, \lambda'_2, \dots, \lambda'_N | \sum_{\lambda} \hat{n}_{\lambda} o_{\lambda} |\lambda_1, \lambda_2, \dots, \lambda_N\rangle\end{aligned}$$

Since this holds true for all basis states $|\lambda_1, \lambda_2, \dots, \lambda_N\rangle$ and $\langle \lambda'_1, \lambda'_2, \dots, \lambda'_N |$ it follows that $\hat{O}_1 = \sum_{\lambda} \hat{n}_{\lambda} o_{\lambda}$.

- (b) What is the second quantized representation of \hat{O}_1 in a different basis $\{|\mu\rangle\}$, in which \hat{O}_1 is not diagonal?

Any set of orbitals forms a basis for the single-particle Hilbert space so $\sum_{\lambda} |\lambda\rangle \langle \lambda| = \mathbb{I}$ and using the definitions $\hat{a}_{\lambda}^{\dagger} |\Omega\rangle = |\lambda\rangle$ and $\hat{a}_{\mu}^{\dagger} |\Omega\rangle = |\mu\rangle$ we can see

$$\begin{aligned}\hat{a}_{\lambda}^{\dagger} |\Omega\rangle &= |\lambda\rangle = \sum_{\mu} |\mu\rangle \langle \mu | \lambda \rangle = \sum_{\mu} \langle \mu | \lambda \rangle \hat{a}_{\mu}^{\dagger} |\Omega\rangle \\ \Rightarrow \hat{a}_{\lambda}^{\dagger} &= \sum_{\mu} \langle \mu | \lambda \rangle \hat{a}_{\mu}^{\dagger}, \quad \hat{a}_{\lambda} = \sum_{\mu} \langle \lambda | \mu \rangle \hat{a}_{\mu}\end{aligned}\tag{31}$$

Remember we can also think of these inner products between basis elements as elements of the unitary matrix that transforms between the bases, i.e. $U_{\lambda\mu} = \langle \lambda | \mu \rangle$. Now rewriting,

$$\begin{aligned}\hat{O}_1 &= \sum_{\lambda} \langle \lambda | \hat{o} | \lambda \rangle \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda} \\ &= \sum_{\lambda\mu\nu} \langle \lambda | \hat{o} | \lambda \rangle \langle \nu | \lambda \rangle \hat{a}_{\nu}^{\dagger} \langle \lambda | \mu \rangle \hat{a}_{\mu} \\ &= \sum_{\lambda\mu\nu} \langle \nu | \lambda \rangle \langle \lambda | \hat{o} | \lambda \rangle \langle \lambda | \mu \rangle \hat{a}_{\nu}^{\dagger} \hat{a}_{\mu} \\ &= \sum_{\mu\nu} \langle \nu | \hat{o} | \mu \rangle \hat{a}_{\nu}^{\dagger} \hat{a}_{\mu}\end{aligned}\tag{32}$$

where we again used $\sum_{\lambda} |\lambda\rangle\langle\lambda| = \mathbb{I}$. For continuous degrees of freedom the sums are replaced by integrals.

- (c) Consider a single particle in one-dimensional system of length L with periodic boundary conditions. Write down the basis transformations between \hat{a}_p and $\hat{a}(x)$ - i.e. the operators which annihilate a particle at a fixed momentum or position.

You have seen previously that the position wavefunction for a 1D system with periodic boundary conditions, namely $\psi_p(x) = \frac{e^{-ixp}}{\sqrt{L}} = \langle x|p\rangle$, where p takes only discrete values. So we have,

$$\hat{a}_p = \int_0^L dx \frac{e^{ipx}}{\sqrt{L}} \hat{a}(x), \quad \hat{a}_p^\dagger = \int_0^L dx \frac{e^{-ipx}}{\sqrt{L}} \hat{a}^\dagger(x), \quad (33)$$

$$\hat{a}(x) = \sum_p \frac{e^{-ipx}}{\sqrt{L}} \hat{a}_p, \quad \hat{a}^\dagger(x) = \sum_p \frac{e^{ipx}}{\sqrt{L}} \hat{a}_p^\dagger \quad (34)$$

- (d) Now consider a many-particle finite one-dimensional system of length L with periodic boundary conditions. The single particle kinetic energy operator is given by $\hat{T} = \sum_j \hat{p}_j^2/2m$. Show that the second quantized representation of this operator is given by

$$\hat{T} = \int_0^L dx \hat{a}^\dagger(x) \frac{p^2}{2m} \hat{a}(x) \quad (35)$$

[Hint: Use the strategy developed in (a) and (b), with the tools from (c) - ie. first express the kinetic energy operator in the basis in which it is diagonal, obtain the second quantized representation in this basis, and then transform into the co-ordinate basis carefully.]

Since the operator is a sum of one-body terms diagonal in the p -basis it can be conveniently re-written as we saw above as $\sum_p o_p a_p^\dagger a_p$ or

$$\hat{T} = \sum_p \langle p|\hat{p}^2/2m|p\rangle a_p^\dagger a_p = \sum_p \frac{p^2}{2m} a_p^\dagger a_p \quad (36)$$

Transforming the second operator to the position basis we have,

$$\hat{T} = \frac{1}{\sqrt{L}} \sum_p a_p^\dagger \int_0^L dx \frac{p^2}{2m} e^{ipx} a(x) \quad (37)$$

Recall that the momentum operator can be written (we have here set $\hbar = 1$) $\hat{p} = -i \frac{\partial}{\partial x}$ hence we have,

$$\frac{\hat{p}^2}{2m} e^{ipx} = \frac{-1}{2m} \frac{\partial^2}{\partial x^2} e^{ipx} = \frac{p^2}{2m} e^{ipx} \quad (38)$$

So we may write

$$\hat{T} = \frac{1}{\sqrt{L}2m} \sum_p a_p^\dagger \int_0^L dx \frac{\partial^2}{\partial x^2} e^{ipx} a(x) \quad (39)$$

Now using the product rule² we have,

$$\begin{aligned}\int_0^L dx \frac{\partial^2}{\partial x^2} e^{ipx} a(x) &= - \int_0^L dx \frac{\partial}{\partial x} e^{ipx} \frac{\partial}{\partial x} a(x) + \frac{\partial}{\partial x} e^{ipx} a(x) \Big|_0^L \\ &= \int_0^L dx e^{ipx} \frac{\partial^2}{\partial x^2} a(x) + e^{ipx} \frac{\partial}{\partial x} a(x) \Big|_0^L + \frac{\partial}{\partial x} e^{ipx} a(x) \Big|_0^L\end{aligned}$$

where the last two terms will vanish due to the periodic boundary conditions (i.e. $a(0) = a(L)$). Substituting back gives,

$$\begin{aligned}\hat{T} &= \frac{1}{\sqrt{L}} \sum_p a_p^\dagger \int_0^L dx e^{ipx} \frac{1}{2m} \frac{\partial^2}{\partial x^2} a(x) \\ &= \int_0^L dx \sum_p \frac{e^{ipx}}{\sqrt{L}} a_p^\dagger \frac{\hat{p}}{2m} a(x) \\ &= \int_0^L dx a^\dagger(x) \frac{\hat{p}}{2m} a(x)\end{aligned}\tag{40}$$

where we again used the Fourier relation between position and momentum in the last line.

- (e) Consider a bosonic Hamiltonian $H = \sum_{i,j} h_{i,j} \hat{b}_i^\dagger \hat{b}_j$, with $\hat{b}_i^\dagger, \hat{b}_j$ the usual bosonic creation and annihilation operators. Prove that the Heisenberg picture evolved creation and annihilation operators are given by:

$$\hat{b}_i(t) = \sum_j (e^{-ith})_{i,j} \hat{b}_j\tag{41}$$

$$\hat{b}_i^\dagger(t) = \sum_j (e^{ith})_{i,j} \hat{b}_j^\dagger\tag{42}$$

[Hint: Again it helps to consider a basis in which the Hamiltonian is diagonal.] Begin by writing the Hamiltonian in a basis in which it is diagonal, say, $H = \sum_\alpha \lambda_\alpha c_\alpha^\dagger c_\alpha$ which are related to the initial operators via,

$$\begin{aligned}c_\alpha &= \sum_j U_{\alpha j} b_j & \rightarrow b_j &= \sum_\alpha U_{j\alpha}^\dagger c_\alpha \\ c_\alpha^\dagger &= \sum_j U_{j\alpha}^\dagger b_j^\dagger & \rightarrow b_j^\dagger &= \sum_\alpha U_{\alpha j} c_\alpha^\dagger\end{aligned}\tag{43}$$

where we have applied the transformation equations (31) writing the coefficients as elements of the transformation unitary. Now the time evolution of a specific annihilation operator from that basis set can be calculated either via the Heisenberg equations of motion,

$$\begin{aligned}\frac{d}{dt} c_\beta(t) &= i[H, c_\beta(t)] \\ &= e^{iHt} i \left[\sum_\alpha \lambda_\alpha c_\alpha^\dagger c_\alpha, c_\beta \right] e^{-iHt} = e^{iHt} i \lambda_\beta \underbrace{\left[c_\beta^\dagger c_\beta, c_\beta \right]}_{-c_\beta} e^{-iHt} \\ &= -i \lambda_\beta c_\beta(t) \\ \Rightarrow c_\beta(t) &= e^{-i\lambda_\beta t} c_\beta\end{aligned}\tag{44}$$

² $\int_a^b dx \frac{\partial f}{\partial x} g = - \int_a^b dx \frac{\partial g}{\partial x} f + fg \Big|_a^b$

where we used the fact that operators in different orbitals commute and that $c_\beta(0) = c_\beta$. The calculation can also be done in the Schrödinger picture via

$$\begin{aligned}
c_\alpha(t) &= e^{iHt} c_\alpha e^{-iHt} \\
&= e^{it \sum_\beta \lambda_\beta c_\beta^\dagger c_\beta} c_\alpha e^{-it \sum_\gamma \lambda_\gamma c_\gamma^\dagger c_\gamma} \\
&= e^{it \lambda_\alpha c_\alpha^\dagger c_\alpha} c_\alpha e^{-it \lambda_\alpha c_\alpha^\dagger c_\alpha} \\
&= c_\alpha + \underbrace{it \lambda_\alpha [c_\alpha^\dagger c_\alpha, c_\alpha]}_{-c_\alpha} + \underbrace{(it \lambda_\alpha)^2 \frac{1}{2} [c_\alpha^\dagger c_\alpha, [c_\alpha^\dagger c_\alpha, c_\alpha]]}_{c_\alpha} + \dots \\
&= \left[\sum_m \frac{(-1)^m}{m!} (it \lambda_\alpha)^m \right] c_\alpha = e^{-it \lambda_\alpha} c_\alpha
\end{aligned} \tag{45}$$

where in the penultimate line we used the identity (that follows from the Baker-Campbell-Hausdorff Lemma) $e^A B e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \dots$. Now, we can find the time evolution of the b_j operators simply via basis transformations

$$\begin{aligned}
b_i(t) &= \sum_\alpha U_{i\alpha}^\dagger c_\alpha(t) = \sum_\alpha U_{i\alpha}^\dagger e^{-it \lambda_\alpha} c_\alpha \\
&= \sum_{\alpha j} U_{i\alpha}^\dagger e^{-it \lambda_\alpha} U_{\alpha j} b_j = \sum_j (e^{-itH})_{ij} b_j
\end{aligned} \tag{46}$$

This equation says that an operator non in the diagonalising basis of the Hamiltonian will in general evolve into a combination of operators of different orbitals in it's own basis over time (i.e. the initial b_i operator evolves into a sum over all the b_j).