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

Due date: 10:15 16/11/2018 J. Eisert

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

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

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

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

   $$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{2}$$

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

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

   Substituting from (1) gives,

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

   and hence

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

   Thus,

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

   (b) Starting from the fermionic anti-commutation relations

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

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

$$\hat{f}_j|N_1,\ldots,N_j,\ldots\rangle = (-1)^{\sum_{k=1}^{j-1}N_k}N_j|N_1,\ldots,1-N_j,\ldots\rangle \quad (7)$$
$$\hat{f}_j^\dagger|N_1,\ldots,N_j,\ldots\rangle = (-1)^{\sum_{k=1}^{j-1}N_k}(1-N_j)|N_1,\ldots,1-N_j\ldots\rangle \quad (8)$$

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

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

Let $\{|\lambda_n\rangle\}$ be the eigenstates satisfying $\hat{n}|\lambda_n\rangle = \hat{f}^\dagger f|\lambda_n\rangle = \lambda_n|\lambda_n\rangle$. 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 $\hat{f}^\dagger|\lambda_n\rangle$,

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

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 mechanics[1] 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

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

[1]For 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 $\hat{f}_j|N_1, N_2, ..N_j, ..\rangle$ where (since these are fermions) we now know that $N_i \in \{0, 1\}$ and we can write

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

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

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

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 $|\lambda_1, \ldots \lambda_N\rangle_{B(F)}$ 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 $|\lambda_1, \ldots \lambda_N\rangle_{B(F)}$, and the appropriate commutation relations for $\hat{a}_\lambda^\dagger, \hat{a}_\lambda$, prove that the number operator $\hat{n}_\lambda$ simply counts the number of particles in state $|\lambda\rangle$ - i.e. show explicitly that for both bosonic and fermionic N particle states

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

In the previous question you derived the action of the fermionic creation and annihilation operators on eigenstates of $\hat{n}_\lambda = a_j^\dagger \lambda a_j \lambda$. 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

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

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 $\hat{n}_\lambda$ 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,

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

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,

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

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

$$\hat{n}_\lambda|\lambda_1,\ldots\lambda_N\rangle_{B(F)}=\sum_{i=1}^{N}\delta_{\lambda\lambda_i}|\lambda_1,\ldots\lambda_N\rangle_B+\frac{1}{\sqrt{\prod_\lambda n_\lambda!}}a^\dagger_{\lambda_N}\cdots a^\dagger_{\lambda_1}\hat{n}_\lambda|\Omega\rangle \tag{25}$$

where the last term vanishes to give the desired result.
For fermions we now have an anti-commutation relation so that

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

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

$$\hat{f}^\dagger_\lambda\hat{f}_\lambda\hat{f}^\dagger_{\lambda_i} = \delta_{\lambda,\lambda_i}\hat{f}^\dagger_\lambda+\hat{f}^\dagger_{\lambda_i}\hat{f}^\dagger_\lambda\hat{f}_\lambda=\delta_{\lambda,\lambda_i}\hat{f}^\dagger_{\lambda_i}+\hat{f}^\dagger_{\lambda_i}\hat{f}^\dagger_\lambda\hat{f}_\lambda \tag{27}$$

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

$$\hat{O}_1=\sum_{\lambda=0}^{\infty}o_\lambda\hat{n}_\lambda=\sum_{\lambda=0}^{\infty}\langle\lambda|\hat{o}|\lambda\rangle\hat{a}^\dagger_\lambda\hat{a}_\lambda \tag{28}$$

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 $\hat{O}_1=\hat{o}_1+\hat{o}_2=\hat{o}\otimes\mathbb{I}+\mathbb{I}\otimes 2$. 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

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

For N particles we will simply find that

$$\hat{O}_1|\lambda_1, \lambda_2, .., \lambda_N\rangle = \sum_{i=1}^{N} o_{\lambda_i}|\lambda_1, \lambda_2, .., \lambda_N\rangle \qquad (30)$$

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 $\sum_{i=1}^{N} o_{\lambda_i}|\lambda_1, \lambda_2, .., \lambda_N\rangle = \sum_\lambda \hat{n}_\lambda o_\lambda|\lambda_1, \lambda_2, .., \lambda_N\rangle$. Thus,

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

Since this holds true for all basis states $|\lambda_1, \lambda_2, .., \lambda_N\rangle$ and $\langle\lambda'_1, \lambda'_2, .., \lambda'_N|$ 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 $\hat{a}^\dagger_\lambda|\Omega\rangle = |\lambda\rangle$ and $\hat{a}^\dagger_\mu|\Omega\rangle = |\ u\rangle$ we can see

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

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,

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

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 discree values. So we have,

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

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

(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

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

[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

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

Transforming the second operator to the position basis we have,

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

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

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

So we may write

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

Now using the product rule[2] we have,

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

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

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

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,

$$\begin{array}{ll} c_\alpha = \sum_j U_{\alpha j} b_j & \to b_j = \sum_\alpha U_{j\alpha}^\dagger c_\alpha \\ c_\alpha^\dagger = \sum_j U_{j\alpha}^\dagger b_j^\dagger & \to b_j = \sum_\alpha U_{\alpha j} c_\alpha^\dagger \end{array} \tag{43}$$

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,

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

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

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

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

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

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

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).