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[disclaimer]

physics606 – Advanced Quantum Theory

Problem Set 13

Martin Ueding
mu@martin-ueding.de

Lino Lemmer
l2@uni-bonn.de

2015-01-22
Group 2 – Dilege Gülmez

problem number	achieved points	possible points
1		10
2		4
3		16
total		30

1 Annihilation operator in Heisenberg picture

1.1

Problem statement

Show that

$$a_j^{\mathrm{H}\dagger}(t) = \exp\left(\frac{\mathrm{i}}{\hbar} H t\right) a_j^\dagger \exp\left(\frac{\mathrm{i}}{\hbar} H t\right).$$

Hint: Take the hermitean conjugate of equation (2), remembering that $[AB]^\dagger = B^\dagger A^\dagger$.

Okay, so we start with the equation (2) that was mentioned in the problem statement. This can be found on the problem set and reads the following:

$$a_j^{\mathrm{H}}(t) = \exp\left(\frac{\mathrm{i}}{\hbar} H t\right) a_j \exp\left(-\frac{\mathrm{i}}{\hbar} H t\right).$$

We omit the parentheses around the “Heisenberg” “H” because we conform to ISO 80000-2 and set the “H” upright. Therefore it can always be distinguished from the italic Hamiltonian H.

Now we follow the lead of the hint and apply the Hermitean conjugate to this equation. To make it really clear what happens, we do not make any simplification steps up to this point.

$$\iff a_j^{\mathrm{H}\dagger}(t) = \left[\exp\left(\frac{\mathrm{i}}{\hbar}Ht\right) a_j \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)\right]^\dagger$$

It can be seen that we have added the Hermitean conjugate "†" to both sides of the previous equation. Since we have applied this to both sides, this equation is equivalent to the previous one. We need this equivalence to be able to show that equation (4) from the problem set does indeed follows from equation (2) from the problem set. Now comes the next crucial step in this derivation: We need to apply the second part of the hint, the one that said that we should remember that $[AB]^\dagger = B^\dagger A^\dagger$ holds. To make it clear which term went into which position, we will give them extra labels first.

$$= \left[\underbrace{\exp\left(\frac{\mathrm{i}}{\hbar}Ht\right)}_{A} a_j \underbrace{\exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)}_{B}\right]^\dagger$$

Now we are all set to apply the hint to this equation.

$$= \underbrace{\exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)^\dagger}_{B} a_j^\dagger \underbrace{\exp\left(\frac{\mathrm{i}}{\hbar}Ht\right)^\dagger}_{A}$$

With the extra labels, it should be visible that the terms changed their order and all got a Hermitean conjugate "†" on their own. The next step was not given in the hint. Now we have to simplify the Hermitean conjugate of the exponential function. One way to see how this works is to split up the exponential function into real and imaginary parts. The complex exponential function can be written like so:

$$\exp(\mathrm{i}\phi) = \cos(\phi) + \mathrm{i}\sin(\phi), \quad \phi \in \mathbb{R}.$$

There Hermitean conjugate will, just like the complex conjugate, switch the sign on the imaginary part. So here, the Hermitean conjugate will be given by

$$\exp(\mathrm{i}\phi)^\dagger = \cos(\phi) - \mathrm{i}\sin(\phi).$$

To write this back into the exponential form, one has to use that the cosine is symmetric, the sine is antisymmetric in its argument. So we can write this as

$$\exp(\mathrm{i}\phi)^\dagger = \cos(\phi) + \mathrm{i}\sin(-\phi).$$

However, using the above formula, we can also write this as

$$\exp(-\mathrm{i}\phi)$$

and deduce that

$$\exp(\mathrm{i}\phi)^\dagger = \exp(-\mathrm{i}\phi)$$

So for a pure imaginary number in the exponential, the sign will just flip. The Hamiltonian H is a matrix here, or can at least be thought of as a matrix. The Hermitean conjugate will also transpose the matrix. What we have to do is to apply the Hermitean conjugate to the Hamiltonian as well. Luckily, it is a self-adjoined operator, which means that $H = H^\dagger$. So we do not have to take care of this. Using all this, we can simplify the exponential functions.

$$= \exp\left(\frac{\mathrm{i}}{\hbar}Ht\right) a_j^\dagger \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)$$

And that is exactly equation (4) from the problem set.

1.2

The first thing that we will do is to show the identity:

$$\begin{aligned}[AB, C] &= ABC - CAB \\ &= ABC - ACB + ACB - CAB \\ &= A[B, C] + [A, C]B\end{aligned}$$

If you swap the two middle terms, you can derive this relations for anti-commutators.

Then we can solve the differential equation.

$$\dot{a}_k^{\mathrm{H}}(t) = \frac{\mathrm{i}}{\hbar}\left[H, a_k^{\mathrm{H}}(t)\right]$$

The first thing we do is to insert the unitary evolution operators.

$$= \frac{\mathrm{i}}{\hbar}\left[H, U^\dagger(t) a_k U(t)\right]$$

Since U is a analytic function of H, it will commute with H. Even the $a_j^\dagger a_j$ will, taken together as n_j, commute with H and every sufficiently well behaved function of H.

$$= \frac{\mathrm{i}}{\hbar} U^\dagger(t)[H, a_k]U(t)$$

Then we can insert H in terms of the occupation number operators.

$$= \frac{\mathrm{i}}{\hbar} U^\dagger(t) \sum_j \epsilon_j [a_j^\dagger a_j, a_k] U(t)$$

This has the form that lets us use the relation that we have shown.

$$= \frac{\mathrm{i}}{\hbar} U^\dagger(t) \sum_j \epsilon_j \left[a_j^\dagger [a_j, a_k] - [a_j^\dagger, a_k] a_j \right] U(t)$$

The first commutator is zero, the second a negative Kronecker δ. For fermions, it will have the anti-commutator here which gives the same value.

$$= \frac{\mathrm{i}}{\hbar} \epsilon_k U^\dagger(t) a_k U(t)$$

This again is the operator in the Heisenberg picture. The differential equation therefore is:

$$\dot{a}_k^{\mathrm{H}}(t) = \frac{\mathrm{i}}{\hbar} \epsilon_k a_k^{\mathrm{H}}(t).$$

With the initial condition that at $t = 0$ the Heisenberg and Schrödinger operators are the same ($a_k^{\mathrm{H}}(0) = a_k$) this can be solved by:

$$a_k^{\mathrm{H}}(t) = \exp\left(\frac{\mathrm{i}}{\hbar} \epsilon_k t \right) a_k$$

1.3

Trivial. Do the same derivation and note that the fermion anti-commutator has the same value as the boson commutator.

2 Time evolution of fermionic field operators

On problem set 12 we more or less derived the Hamiltonian in terms of the field operators. So we will continue from that and just follow the derivation from (Schwabl 2005, p. 24). So the time evolution of anything is given by

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \psi(\boldsymbol{x}, t) = -[H, \psi(\boldsymbol{x}, t)].$$

Now we write this in the Schrödinger picture for a little while and strip off the time evolution of the state. As shown in problem 1.1 in somewhat excruciating detail, they commute with the Hamiltonian. Therefore, we can move them out of the commutator.

$$= -U^\dagger(t)[H, \psi(\boldsymbol{x})]U(t)$$

Now we can plug in the Hamiltonian that we derived on problem set 12.

$$= -U^\dagger(t)\left[\int \mathrm{d}^3 y \left[\frac{\hbar^2}{2m} \boldsymbol{\nabla}\psi^\dagger(\boldsymbol{y})\boldsymbol{\nabla}\psi(\boldsymbol{y}) + U(\boldsymbol{y})\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y})\right] + \frac{1}{2}\int \mathrm{d}^3 y \; \mathrm{d}^3 z \, \psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y}, \boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})\right] U(t)$$

Now that is some long expression. And it is really hard to see that the outer square bracket is a commutator. Well, it should be clear *now*, then. A lot can be pulled out of the commutator right here, so that might simplify it a bit. Now it does not even fit on a single line in landscape, but that does not really hurt that much.

$$\begin{aligned} &= -U^\dagger(t)\int \mathrm{d}^3 y \left[\frac{\hbar^2}{2m}[\boldsymbol{\nabla}\psi^\dagger(\boldsymbol{y})\boldsymbol{\nabla}\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] + U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]\right] U(t) \\ &\quad - U^\dagger(t)\frac{1}{2}\int \mathrm{d}^3 y \; \mathrm{d}^3 z \, [\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y}, \boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]U(t) \end{aligned}$$

We start with the first commutator, the one with the kinetic energy. There we can use the $[AB, C]$ commutator relation. Because we can, we will do this derivation for both fermions and bosons and denote this with a $\pm$, where the upper sign is for fermions. The (anti-)commutator for $\phi(\boldsymbol{y})$ and $\psi(\boldsymbol{x})$ is always zero, so that is not interesting. And we directly drop that term before we write it down.

$$
\begin{aligned}
&= -U^\dagger(t) \int \mathrm{d}^3 y \left[\mp \frac{\hbar^2}{2m} [\boldsymbol{\nabla}\psi^\dagger(\boldsymbol{y}), \psi(\boldsymbol{x})]_\pm \boldsymbol{\nabla}\psi(\boldsymbol{y}) + U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] \right] U(t) \\
&\quad - U^\dagger(t) \frac{1}{2} \int \mathrm{d}^3 y \; \mathrm{d}^3 z \, [\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z}) V(\boldsymbol{y}, \boldsymbol{z}) \psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] U(t)
\end{aligned}
$$

Since the partial derivative is supposed to act on $\boldsymbol{y}$ only—maybe we should have mentioned that earlier, sorry—we can pull it out of the commutator.

$$
\begin{aligned}
&= -U^\dagger(t) \int \mathrm{d}^3 y \left[\mp \frac{\hbar^2}{2m} \boldsymbol{\nabla}[\psi^\dagger(\boldsymbol{y}), \psi(\boldsymbol{x})]_\pm \boldsymbol{\nabla}\psi(\boldsymbol{y}) + U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] \right] U(t) \\
&\quad - U^\dagger(t) \frac{1}{2} \int \mathrm{d}^3 y \; \mathrm{d}^3 z \, [\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z}) V(\boldsymbol{y}, \boldsymbol{z}) \psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] U(t)
\end{aligned}
$$

Then this (anti-)commutator is just a negative δ-distribution.

$$
\begin{aligned}
&= -U^\dagger(t) \int \mathrm{d}^3 y \left[\pm \frac{\hbar^2}{2m} \boldsymbol{\nabla}\delta^{(3)}(\boldsymbol{x} - \boldsymbol{y}) \boldsymbol{\nabla}\psi(\boldsymbol{y}) + U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] \right] U(t) \\
&\quad - U^\dagger(t) \frac{1}{2} \int \mathrm{d}^3 y \; \mathrm{d}^3 z \, [\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z}) V(\boldsymbol{y}, \boldsymbol{z}) \psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] U(t)
\end{aligned}
$$

We use partial integration to move the gradient from the δ-distribution to the field operator. This will give us yet another minus sign that we have to take into account.

$$
\begin{aligned}
&= -U^\dagger(t) \int \mathrm{d}^3 y \left[\mp \frac{\hbar^2}{2m} \delta^{(3)}(\boldsymbol{x} - \boldsymbol{y}) \triangle \psi(\boldsymbol{y}) + U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] \right] U(t) \\
&\quad - U^\dagger(t) \frac{1}{2} \int \mathrm{d}^3 y \; \mathrm{d}^3 z \, [\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z}) V(\boldsymbol{y}, \boldsymbol{z}) \psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})] U(t)
\end{aligned}
$$

Great, now we can integrate over it to eliminate it.

$$= -U^\dagger(t)\left[\pm\frac{\hbar^2}{2m}\triangle\psi(\boldsymbol{x}) + \int \mathrm{d}^3y\, U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]\right]U(t)$$
$$- U^\dagger(t)\frac{1}{2}\int \mathrm{d}^3y\ \mathrm{d}^3z\,[\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]U(t)$$

To finalize the kinetic energy, we sandwich the time evolution operators back onto it. That will make it a Heisenberg field operator again.

$$= \mp\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) - U^\dagger(t)\int \mathrm{d}^3y\, U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]U(t)$$
$$- \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\,[\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]U(t)$$

One down, two more to go. Next up is the scalar potential term. Here the same think with the $[AB, C]$ formula applies as well.

$$= -\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) - U^\dagger(t)\int \mathrm{d}^3y\, U(\boldsymbol{y})[\psi^\dagger(\boldsymbol{y}), \psi(\boldsymbol{x})]_\pm\psi(\boldsymbol{y})U(t)$$
$$- \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\,[\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]U(t)$$

As before, the (anti-)commutator is a negative δ-distribution. Then we can integrate over that as well and get rid of it. Now we can finally go back to writing this expression on a single line. It will probably not last very long, however.

$$= -\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) + U^\dagger(t)U(\boldsymbol{x})\psi(\boldsymbol{x})U(t) - \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\,[\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}), \psi(\boldsymbol{x})]U(t)$$

Now we did not want to make too many steps without an explanation in between. So the second term can now be written a Heisenberg state.

$$= -\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) - U(\boldsymbol{x})\psi(\boldsymbol{x},t) - \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\ \left[\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z})V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y}),\psi(\boldsymbol{x})\right]U(t)$$

This leaves the last summand for us to work on. Of course, we use the same trusty (anti-)commutator relation that has served us so well in the course of this problem. But first of all, we move everything out of the commutator that commuted with $\psi(\boldsymbol{x})$ anyway.

$$= -\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) - U(\boldsymbol{x})\psi(\boldsymbol{x},t) - \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\ \left[\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{z}),\psi(\boldsymbol{x})\right]V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y})U(t)$$

Without much further ado, we use the $[AB,C]$ relation. However, it is going to be in two lines again since it is so long because neither (anti-)commutator vanishes in this particular case here.

$$\begin{aligned}&= -\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) - U(\boldsymbol{x})\psi(\boldsymbol{x},t)\\ &\quad - \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\ \left[\psi^\dagger(\boldsymbol{y})\left[\psi^\dagger(\boldsymbol{z}),\psi(\boldsymbol{x})\right]_\pm \mp \left[\psi^\dagger(\boldsymbol{y}),\psi(\boldsymbol{x})\right]_\pm \psi^\dagger(\boldsymbol{z})\right]V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y})U(t)\end{aligned}$$

Those (anti-)commutators are again δ-distributions—surprise!—and can be integrated away. Since this derivation is not long enough yet we will include those steps. It would not be consistent either. So we expand the square bracket—the one which is not a commutator.

$$\begin{aligned}&= -\frac{\hbar^2}{2m}\triangle\psi^{\mathrm{H}}(\boldsymbol{x},t) - U(\boldsymbol{x})\psi(\boldsymbol{x},t) - \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\,\psi^\dagger(\boldsymbol{y})\left[\psi^\dagger(\boldsymbol{z}),\psi(\boldsymbol{x})\right]_\pm V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y})U(t)\\ &\quad \pm \frac{1}{2}U^\dagger(t)\int \mathrm{d}^3y\ \mathrm{d}^3z\ \left[\psi^\dagger(\boldsymbol{y}),\psi(\boldsymbol{x})\right]_\pm \psi^\dagger(\boldsymbol{z})V(\boldsymbol{y},\boldsymbol{z})\psi(\boldsymbol{z})\psi(\boldsymbol{y})U(t)\end{aligned}$$

Now we insert the δ-distributions. Note that the signs flip again.

$$
\begin{aligned}
&= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x})\psi(\boldsymbol{x}, t) + \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \; \mathrm{d}^3 z \, \psi^\dagger(\boldsymbol{y}) \delta^{(3)}(\boldsymbol{z} - \boldsymbol{x}) V(\boldsymbol{y}, \boldsymbol{z}) \psi(\boldsymbol{z}) \psi(\boldsymbol{y}) U(t) \\
&\quad \mp \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \; \mathrm{d}^3 z \, \delta^{(3)}(\boldsymbol{y} - \boldsymbol{x}) \psi^\dagger(\boldsymbol{z}) V(\boldsymbol{y}, \boldsymbol{z}) \psi(\boldsymbol{z}) \psi(\boldsymbol{y}) U(t)
\end{aligned}
$$

With the δ-distributions in place, we can finally carry out the integration and remove the number of variables in this expression.

$$
\begin{aligned}
&= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x})\psi(\boldsymbol{x}, t) + \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{y}, \boldsymbol{x}) \psi(\boldsymbol{x}) \psi(\boldsymbol{y}) U(t) \\
&\quad \mp \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 z \, \psi^\dagger(\boldsymbol{z}) V(\boldsymbol{x}, \boldsymbol{z}) \psi(\boldsymbol{z}) \psi(\boldsymbol{x}) U(t)
\end{aligned}
$$

In the last integration, we rename the integration variable from z to y to match the other integral.

$$
\begin{aligned}
&= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x})\psi(\boldsymbol{x}, t) + \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{y}, \boldsymbol{x}) \psi(\boldsymbol{x}) \psi(\boldsymbol{y}) U(t) \\
&\quad \mp \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{y}) \psi(\boldsymbol{x}) U(t)
\end{aligned}
$$

Since V is symmetric in its arguments, we can switch those in the first term.

$$
\begin{aligned}
&= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x})\psi(\boldsymbol{x}, t) + \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{x}) \psi(\boldsymbol{y}) U(t) \\
&\quad \mp \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{y}) \psi(\boldsymbol{x}) U(t)
\end{aligned}
$$

Now the use that the (anti-)commutator for the field annihilation operators vanishes for the two kinds of particles, respectively, and switch the very last two field operators in the last term. That will also let us get rid of the plus-minus-sign.

$$
\begin{aligned}
&= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x}) \psi(\boldsymbol{x}, t) + \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{x}) \psi(\boldsymbol{y}) U(t) \\
&\quad + \frac{1}{2} U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{x}) \psi(\boldsymbol{y}) U(t)
\end{aligned}
$$

Now we can combine those identical terms.

$$
= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x}) \psi(\boldsymbol{x}, t) + U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{x}) \psi(\boldsymbol{y}) U(t)
$$

As a last step, we can insert ones in the manifestation of $U(t) U^\dagger(t)$ between all the field operators.

$$
= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x}) \psi(\boldsymbol{x}, t) + U^\dagger(t) \int \mathrm{d}^3 y \, \psi^\dagger(\boldsymbol{y}) U(t) U^\dagger(t) V(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{x}) U(t) U^\dagger(t) \psi(\boldsymbol{y}) U(t)
$$

Then we can write all the field operators as Heisenberg operators.

$$
= -\frac{\hbar^2}{2m} \triangle \psi^{\mathrm{H}}(\boldsymbol{x}, t) - U(\boldsymbol{x}) \psi(\boldsymbol{x}, t) + \int \mathrm{d}^3 y \, \psi^{\mathrm{H}\dagger}(\boldsymbol{y}, t) V(\boldsymbol{x}, \boldsymbol{y}) \psi^{\mathrm{H}}(\boldsymbol{x}, t) \psi^{\mathrm{H}}(\boldsymbol{y}, t)
$$

Except for the sign error in the last term, this worked out.

Side question

How do the four points that can be achieved in the problem related to the two points that can be achieved in problem 1.1? Problem 1.1 was utterly trivial, this is not trivial. Except when one would just say that it is the same relation as for the bosons since all the commutators just get replaced with anti-commutators in the relation used in 1.2 and 1.3 and is done with it. Was *that* asked here?

3 Hubbard model

3.1

The diagonal terms in the energy can be computed with the usual methods.

$$t_i j = \langle i|T|j\rangle$$

We insert two complete sets of position eigenstates.

$$= \int \mathrm{d}^3x\ \mathrm{d}^3y\ \langle i|\boldsymbol{x}\rangle \langle \boldsymbol{x}|T|\boldsymbol{y}\rangle \langle \boldsymbol{y}|j\rangle$$

Now making the connection between $\boldsymbol{x} = \boldsymbol{n}_i a$ and the same for y, we get position eigenstates. The kinetic energy operator is now given in position space.

$$= -\frac{\hbar^2}{2m} \int \mathrm{d}^3x\, \phi(\boldsymbol{x}) \triangle \phi(\boldsymbol{x})$$

At this point we insert equation (10) from the problem set.

$$= -\frac{\hbar^2}{2m\Delta^3\pi^{3/2}} \int \mathrm{d}^3x \, \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right) \triangle \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right)$$

We compute the derivatives.

$$= -\frac{\hbar^2}{2m\Delta^3\pi^{3/2}} \int \mathrm{d}^3x \, \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right) \left[-\frac{1}{2\Delta^2} + \boldsymbol{x}^2 \frac{1}{4\Delta^4}\right] \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right)$$

Factor stuff out.

$$= \frac{\hbar^2}{4m\Delta^5\pi^{3/2}} \left[\int \mathrm{d}^3x \, \exp\left(-\frac{\boldsymbol{x}^2}{\Delta^2}\right) - \frac{1}{2\Delta^2} \int \mathrm{d}^3x \, \boldsymbol{x}^2 \exp\left(-\frac{\boldsymbol{x}^2}{\Delta^2}\right)\right]$$

Now we have the Gaussian integrals back. We thought that we would not see them again, but mistaken! Since they are in three dimensions—as the hint did not want us to forget—we get the results cubed out of them.

$$\begin{aligned} &= \frac{\hbar^2}{4m\Delta^5\pi^{3/2}} \left[\left[\Delta\sqrt{\pi}\right]^3 - \left[\frac{1}{2}\Delta^3\sqrt{\pi}\right]^3\right] \\ &= \frac{\hbar^2}{4m\Delta^2} - \frac{\hbar^2}{4m\Delta^5\pi^{3/2}} \left[\frac{1}{2}\Delta^3\sqrt{\pi}\right]^3 \end{aligned}$$

3.2

Do it all again, just with a shift.

$$\begin{aligned} \langle \phi(a\hat{\boldsymbol{e}}_x) | T | \phi(\boldsymbol{0}) \rangle &= -\frac{\hbar}{2m} \frac{1}{\Delta^3\pi^{3/2}} \int \mathrm{d}^3x \, \exp\left(-\frac{[\boldsymbol{x} - a\hat{\boldsymbol{e}}_x]^2}{2\Delta^2}\right) \triangle \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right) \\ &= -\frac{\hbar}{2m} \frac{1}{\Delta^3\pi^{3/2}} \int \mathrm{d}^3x \, \exp\left(-\frac{\boldsymbol{x}^2 - 2ax + a^2}{2\Delta^2}\right) \triangle \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right) \end{aligned}$$

Linear term will cancel in symmetric integral, pull a^2 term out.

$$\begin{aligned} &= -\frac{\hbar}{2m} \frac{1}{\Delta^3\pi^{3/2}} \exp\left(-\frac{a^2}{2\Delta^2}\right) \int \mathrm{d}^3x \, \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right) \triangle \exp\left(-\frac{\boldsymbol{x}^2}{2\Delta^2}\right) \\ &= t \exp\left(-\frac{a^2}{2\Delta^2}\right) \end{aligned}$$

Our suppression has a factor 2, not 4 in it. Maybe one has to take two of them and distribute them equally to both electrons?

3.3

After applying the δ-distribution from the hints, the equation is

$$V_i j = \lambda \int \mathrm{d}^3 x \, |\phi(\boldsymbol{x} - \boldsymbol{R}_i)|^2 \left|\phi(\boldsymbol{x} - \boldsymbol{R}_j)\right|^2 .$$

Then the first part is quite easy, just put $i = j$.

$$V_i i = \lambda \int \mathrm{d}^3 x \, |\phi(\boldsymbol{x} - \boldsymbol{R}_i)|^4$$

Then insert ϕ ...

$$= \lambda \frac{1}{\Delta^6 \pi^3} \int \mathrm{d}^3 x \, \exp\left(-2 \frac{[\boldsymbol{x} - \boldsymbol{R}_i]^2}{\Delta^2}\right)$$

Apply yet another Gaussian integral ... well, you have to shift the integration variable before you do that, but we will not write that down.

$$= \lambda \frac{1}{\Delta^6 \pi^3} \left[\sqrt{\frac{\pi}{2}} \Delta\right]^3$$

Simplify ...

$$= \lambda \frac{1}{\sqrt{8} \Delta^3 \sqrt{\pi}^3}$$

Now one has to do the same exact thing as above and further above. So take two neighbors and compute the interaction for that as well.

$$\lambda \int \mathrm{d}^3 x \, |\phi(\boldsymbol{x} - \boldsymbol{R}_i)|^2 \, |\phi(\boldsymbol{x} - \boldsymbol{R}_i - a \hat{\boldsymbol{e}}_x)|^2 .$$

Just like above, there is an additional factor

$$\exp\left(-\frac{a^2}{\Delta^2}\right)$$

that arises here. Again, it has a factor 2 missing in the denominator. Probably just a different definition of suppression ...

3.4

In the limit $\Delta \ll a$, only the diagonal terms will contribute. That eliminates the sum over j directly. Then to get rid of the sum over s' it might be possible to use the anti-commutation properties of the fermionic creation and annihilation operators to obtain a $\delta_{ss'}$.

References

Schwabl, Franz (2005). *Quantenmechanik für Fortgeschrittene*. 4. Berlin: Springer. ISBN: 978-3-540-25904-6.