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## physics606 – Advanced Quantum Theory

### Problem Set 5

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problem number	achieved points	possible points
1		11
2		10
3		13
total		34

#### 1 Exponentiating operators

##### Problem statement

The exponential of an operator is defined as

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}.$$

##### 1.1 Inverse

##### Problem statement

Show that  $e^A e^{-A} = 1$  using only the definition.

We start with the definition

$$e^A e^{-A} = \sum_{n=0}^{\infty} \frac{A^n}{n!} \sum_{m=0}^{\infty} \frac{[-A]^m}{m!}$$

and move the terms.

$$\begin{aligned} &= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{A^n [-A]^m}{n! m!} \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{[-1]^m A^{m+n}}{m! n!} \end{aligned}$$

We now think about those two sums as of a lattice where each point can be labelled using  $(m, n)$ . Currently, the summation is done in rows and columns. We change this to a diagonal iterations. A new parameter  $a := m + n$  is introduced to change the summation to:

$$= \sum_{a=0}^{\infty} \sum_{m=0}^a \frac{[-1]^m A^a}{m! [a-m]!}.$$

This is somewhat related to the argument to show that  $\mathbb{Q}$  is still countable infinite. The case  $a = 0$  is special and will be taken out of the sum, it will be just 1. We now rearrange the terms bit more and introduce  $a!$  which cancels in total.

$$= 1 + \sum_{a=1}^{\infty} \frac{A^a}{a!} \sum_{m=0}^a \frac{a!}{m! [a-m]!} [-1]^m$$

The large fraction is just the binomial coefficient. We also add a  $1^{a-m}$ .

$$= 1 + \sum_{a=1}^{\infty} \frac{A^a}{a!} \sum_{m=0}^a \binom{a}{m} [-1]^m 1^{a-m}$$

Using the binomial theorem, we can write this more compact as

$$= 1 + \sum_{a=1}^{\infty} \frac{A^a}{a!} \underbrace{[-1 + 1]^a}_{=0}$$

which means that the second part vanishes for any  $a$ . Here it is clear that including  $a = 0$  in the sum would give the indeterminate expression  $0^0$  which would require extra treatment either way. We are left with

$$= 1.$$

## 1.2 Sum in exponent

### Problem statement

Show that

$$e^{A+B} = e^A e^B e^{[A,B]}$$

if the commutator  $[A, B] =: c$  is a complex number.

The way this works must be very similar to the other subproblems in this problem. However, we did not succeed in obtaining a whole proof of this identity.

## 1.3 Commutation of exponentials

### Problem statement

Show that

$$e^A e^B = e^B e^A e^{[A,B]}.$$

In the previous problem we got

$$e^{A+B} = e^A e^B e^{-c/2}$$

where  $c := [A, B] \in \mathbb{C}$ . We can just exchange  $A$  and  $B$  and obtain

$$e^{B+A} = e^B e^A e^{c/2}.$$

Using the first equation, we can move the  $e^{-c/2}$  to the other side and get

$$e^A e^B = e^{A+B} e^{c/2}$$

There, we can commute  $A$  and  $B$  in the *sum* in the exponent.

$$\iff e^A e^B = e^{B+A} e^{c/2}$$

Using the equation we obtained from exchanging  $A$  and  $B$ , we yield

$$\begin{aligned} &= e^B e^A e^{c/2} e^{c/2} \\ &= e^B e^A e^c, \end{aligned}$$

which is the desired result.

### 1.4 Generalized commutator

#### Problem statement

Show by induction that

$$[A, B]_n = \sum_{i=0}^n \frac{n!}{n![n-i]!} A^{n-i} B [-A]^i.$$

The way the problem is given, a  $n!$  could be canceled. It can be seen for  $n = 2$  that the relation given does not hold. The left side is

$$[A, B]_2 = A^2 B - 2ABA + BA^2.$$

The right side with  $n!/n!$  canceled gives

$$\sum_{i=0}^2 \frac{1}{[2-i]!} A^{2-i} B [-A]^i = \frac{1}{2} A^2 B - ABA + B^2.$$

The powers are right, just the prefactors are off.

We think that this looks so close to the binomial coefficient which was already used much in the previous problems that it probably should be  $i!$  in the denominator. Using  $i!$  in the denominator, we can proof the identity using induction. Therefore, we assume the following relation:

$$[A, B]_n = \sum_{i=0}^n \frac{n!}{i![n-i]!} A^{n-i} B [-A]^i = \sum_{i=0}^n \binom{n}{i} A^{n-i} B [-A]^i.$$

*Proof.* We show that the relation holds for  $n = 0$ :

$$[A, B]_0 = B, \quad \sum_{i=0}^0 \binom{0}{0} A^0 B [-A]^0 = B.$$

This holds. Next is the induction step.

$$\begin{aligned} [A, B]_{n+1} &= [A, [A, B]_n] \\ &= A[A, B]_n - [A, B]_n A \end{aligned}$$

We use the relation that we want to show, this is allowed in induction.

$$= A \sum_{i=0}^n \binom{n}{i} A^{n-i} B [-A]^i - \sum_{i=0}^n \binom{n}{i} A^{n-i} B [-A]^i A$$

We factor the additional factors  $A$  into the expression.

$$= \sum_{i=0}^n \binom{n}{i} A^{n+1-i} B [-A]^i + \sum_{i=0}^n \binom{n}{i} A^{n-i} B [-A]^{i+1}$$

Now we can shift the indices a bit. We introduce

$$j := i + 1, \quad i = j - 1$$

and put that into the expression.

$$= \sum_{i=0}^n \binom{n}{i} A^{n+1-i} B [-A]^i + \sum_{j=1}^{n+1} \binom{n}{j-1} A^{n+1-j} B [-A]^j$$

We branch off the first and last summand of the first and last sum, *respectively*. Then we combine the middle part.

$$= A^{n+1} B + \sum_{i=1}^n \left[ \binom{n}{i} + \binom{n}{i-1} \right] A^{n+1-i} B [-A]^i + B [-A]^{n+1}$$

There is a handy addition theorem for binomial coefficients which we will use for the bracket.

$$= A^{n+1} B + \sum_{i=1}^n \binom{n+1}{i} A^{n+1-i} B [-A]^i + B [-A]^{n+1}$$

We add ones to the stray summands.

$$= \binom{n+1}{0} A^{n+1} B + \sum_{i=1}^n \binom{n+1}{i} A^{n+1-i} B [-A]^i + \binom{n+1}{n+1} B [-A]^{n+1}$$

Now we can combine it into a single sum.

$$= \sum_{i=0}^{n+1} \binom{n+1}{i} A^{n+1-i} B [-A]^i$$

That is exactly what has to be shown. Therefore, this relation holds for any  $n$ . □

Now that we got this identity at our hands, we can aim for the actual task at hand:

**Problem statement**

Show that

$$e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_n.$$

We start with the left side of this equation:

$$e^A B e^{-A} = \sum_{d=0}^{\infty} \frac{A^d}{d!} B \sum_{f=0}^{\infty} \frac{[-A]^f}{f!}.$$

We interchange the summations again and group the terms.

$$= \sum_{d=0}^{\infty} \sum_{f=0}^{\infty} \frac{1}{f!d!} A^d B [-A]^f$$

By now, the change in the lattice traversal was applied many times. We introduce

$$i := f, \quad n := d + f$$

and get

$$= \sum_{n=0}^{\infty} \sum_{i=0}^n \frac{1}{i! [n-i]!} A^d B [-A]^f.$$

Now we introduce a factor of  $n!$ .

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{i=0}^n \frac{n!}{i! [n-i]!} A^d B [-A]^f$$

Using the identity we proved at the beginning of this exercise, we can write this as

$$= \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_n$$

which is what we wanted to show.

## 2 First order time dependent perturbation theory

### 2.1 Argumentation

#### Problem statement

Argue that  $P_{fi}(t) = |c_f(t)|^2$ .

The probability that the system will transition from  $|i^{(0)}\rangle$  to  $|f^{(0)}\rangle$  in the time interval  $[t_0, t]$  is given by the modulus squared of the overlap intergral:

$$P_{fi}(t) = |\langle f^{(0)} | \psi(t) \rangle|^2.$$

We can insert the definition of  $\psi(t)$  and get

$$= \left| \sum_n c_n(t) \langle f^{(0)} | n^{(0)} \rangle \right|^2.$$

The scalar product gives a  $\delta_{fn}$ , reducing the sum to

$$= |c_f(t)|^2.$$

## 2.2 Relation

### Problem statement

What is the relation between  $d_n(t)$  and  $c_n(t)$ ?

We have

$$|\psi(t)\rangle = \sum_n d_n(t) |\psi_n(t)\rangle.$$

The states  $|\psi_n(t)\rangle$  are defined as the unperturbed time evolution of the basis states  $|n^{(0)}\rangle$ . Using the time evolution operator, we can write this as

$$|\psi_n(t)\rangle = U^{(0)}(t - t_0) |n^{(0)}\rangle.$$

Now we insert this into the above relation:

$$|\psi(t)\rangle = \sum_n d_n(t) U^{(0)}(t - t_0) |n^{(0)}\rangle.$$

By comparison, we get

$$c_n(t) = d_n(t) U^{(0)}(t - t_0) = d_n(t) \exp\left(-\frac{i}{\hbar} E_n^{(0)} [t - t_0]\right).$$

## 2.3 Time derivative of coefficient

### Problem statement

Show that

$$i\hbar \dot{d}_f = \sum_n \langle f^{(0)} | H_1(t) | n^{(0)} \rangle \exp(i\omega_{fn} [t - t_0]) d_n(t).$$

We have

$$|\psi(t)\rangle = \sum_n d_n(t) |\psi_n(t)\rangle.$$

We can apply  $\langle \psi_m(t) |$  to both sides and get

$$\langle \psi_m(t) | \psi(t) \rangle = \sum_n d_n(t) \langle \psi_m(t) | \psi_n(t) \rangle.$$



We include the time evolution operator explicitly:

$$= \sum_n d_n(t) \langle m^{(0)} | U^{(0)}(t - t_0)^\dagger U^{(0)}(t - t_0) | n^{(0)} \rangle.$$

However, that just cancels out because the time evolution operator is unitary. We are left with

$$= \sum_n d_n(t) \langle m^{(0)} | n^{(0)} \rangle$$

which reduces to

$$= d_m(t)$$

since the unperturbed eigenstates are orthonormal. As we have shown here, that also holds for any time  $t$  in general. Now we have isolated an expression for  $d_n(t)$  where we can take the time derivative. We start with the derived expression:

$$i\hbar \dot{d}_f(t) = i\hbar \frac{d}{dt} \langle \psi_f(t) | \psi(t) \rangle.$$

Here we use the Schrödinger equation for both the states. This looks a bit clumsy, but we have to use the product rule here since both states depend on time. We have

$$= [\langle \psi_f(t) | H^\dagger ] | \psi(t) \rangle + \langle \psi_f(t) | [H | \psi(t) \rangle].$$

With  $H$  being a hermitian operator,  $H = H^\dagger$  holds. This means that we end up with

$$= 2 \langle \psi_f(t) | H | \psi(t) \rangle.$$

We now insert the expansion of the state  $|\psi(t)\rangle$  and obtain

$$= 2 \sum_n d_n(t) \langle \psi_f(t) | H | \psi_n(t) \rangle.$$

We expand the Hamiltonian into its parts, which are

$$= 2 \sum_n d_n(t) \langle \psi_f(t) | H_0 + H_1(t) | \psi_n(t) \rangle.$$

Using the linearity of the scalar product, we can expand this into two parts.

$$= 2 \sum_n d_n(t) [\langle \psi_f(t) | H_0 | \psi_n(t) \rangle + \langle \psi_f(t) | H_1(t) | \psi_n(t) \rangle]$$

The energies of the unperturbed eigenstates are still  $E_n^{(0)}$ , so we can just insert them there

$$= 2 \sum_n d_n(t) [E_n^{(0)} \delta_{fn} + \langle \psi_f(t) | H_1(t) | \psi_n(t) \rangle]$$

and get rid of the sum for that summand.

$$= 2d_f(t)E_f^{(0)} + 2 \sum_n d_n(t) \langle \psi_f(t) | H_1(t) | \psi_n(t) \rangle$$

We again write the time dependent basis states with the time evolution operator.

$$= 2d_f(t)E_f^{(0)} + 2 \sum_n d_n(t) \langle f^{(0)} | U^{(0)}(t-t_0)^\dagger H_1(t) U^{(0)}(t-t_0) | n^{(0)} \rangle$$

Next we insert the time evolution operator explicitly for the states left and right. We obtain

$$= 2d_f(t)E_f^{(0)} + 2 \sum_n d_n(t) \left\langle f^{(0)} \left| \exp\left(\frac{i}{\hbar} E_f^{(0)} [t-t_0]\right) H_1(t) \exp\left(-\frac{i}{\hbar} E_f^{(0)} [t-t_0]\right) \right| n^{(0)} \right\rangle$$

The time evolution operator is just a scalar now and can be moved out of the scalar product. We combine the two exponential functions and use the  $\omega_{fn}$  that is given on the problem set as well.

$$= 2d_f(t)E_f^{(0)} + 2 \sum_n \langle f^{(0)} | H_1(t) | n^{(0)} \rangle \exp(i\omega_{fn}[t-t_0]) d_n(t)$$

Apart from an additional term and a factor of 2, this is the term we end up with.

**Side question**

What do we need to do differently to get rid of that additional summand and the factor of 2?

### 2.4 First order expression

To us, the zeroth order of equation (6) looks like a simple  $\dot{d}_f = 0$ , since in zeroth order, there is no  $H_1$  term. Then the  $d_n(t)$  would just be the  $c_n(t)$ . We could not really understand what we had to do in this problem.

## 3 Perturbed harmonic oscillator

### 3.1 First order perturbation theory

#### Problem statement

Consider a perturbation

$$H_1(t) = ax^p \exp\left(-\frac{t^2}{\tau^2}\right)$$

and show that to first order perturbation theory the perturbation does not populate states  $|f^{(0)}\rangle$  with  $f > p$ .

We directly start with the appropriate formula which we take from (Schwabl 2007, equation (16.30)):

$$P_{nm}(t) = \left| \frac{1}{\hbar} \int_{t_0}^t dt' \exp\left(\frac{i}{\hbar}[E_n - E_m]t'\right) \langle n|V(t')|m\rangle \right|^2.$$

There, we insert everything that is given in this problem.

$$P_{f0}(t) = \left| \frac{a}{\hbar} \int_{t_0}^t dt' \exp(i\omega_0 f t') \exp\left(-\frac{t'^2}{\tau^2}\right) \langle f|x^p|0\rangle \right|^2.$$

We can express  $x$  via the ladder operators as

$$x = \sqrt{\frac{\hbar}{2\omega_0 m}} [a + a^\dagger].$$

Please do not mix that up with the real constant  $a$ . The power  $x^p$  will contain at most  $a^{\dagger p}$ , such that the highest possible state  $a^{\dagger p} |0\rangle$  can contain is  $|p\rangle$ . Therefore, there are no states with  $f > p$ , since then  $\langle f|p\rangle$  would be zero.

### 3.2 Parity arguments

#### Problem statement

Use parity arguments to further reduce the number of states that can be populated.

$\langle f|x^p|0\rangle$  will only be nonzero if  $n + p$  is even. That means that either  $n$  and  $p$  are both odd or  $n$  and  $p$  are both even. Consider

$$x^p \propto [a + a^\dagger]^p.$$

There will be products that for  $k = 0, \dots, p$  that have the order  $k$  in  $a$  and the order  $p - k$  in  $a^\dagger$ . The total number of state raises is  $[p - k] - k = p - 2k$ . Since it always starts at the state  $|0\rangle$ ,  $p$  determines the parity of the resulting state alone.

### 3.3 Transition probability

#### Problem statement

Explicitly compute  $P_{1,0}$  for  $p = 1$ .

We continue with the expression from the first section of this problem, and set  $f = 1$  and  $p = 1$ :

$$P_{1,0} = \left| \frac{a}{\hbar} \int_{-\infty}^{\infty} dt' \exp(i\omega_0 t') \exp\left(-\frac{t'^2}{\tau^2}\right) \langle 1|x|0\rangle \right|^2.$$

Then we replace  $x$  by

$$x = \sqrt{\frac{\hbar}{2\omega_0 m}} [a + a^\dagger].$$

The term  $\langle 1|a|0\rangle$  does not contribute, so we just drop it.

$$= \frac{a}{2\hbar\omega_0 m} \left| \int_{-\infty}^{\infty} dt' \exp(i\omega_0 t') \exp\left(-\frac{t'^2}{\tau^2}\right) \langle 1|a^\dagger|0\rangle \right|^2.$$

The eigenvalue of this is  $\sqrt{1}$ , and the resulting scalar product is just 1 as well. So the whole matrix element is just 1.

$$= \frac{a}{2\hbar\omega_0 m} \left| \int_{-\infty}^{\infty} dt' \exp(i\omega_0 t') \exp\left(-\frac{t'^2}{\tau^2}\right) \right|^2.$$

The exponential functions can be brought together. We write it in a suggestive way, like so

$$= \frac{a}{2\hbar\omega_0 m} \left| \int_{-\infty}^{\infty} dt' \exp(-\tau^{-2}t'^2 + i\omega_0 t') \right|^2.$$

This is again a Gaussian integral where we can write down the solution directly. We obtain

$$= \frac{a^2 \pi \tau^2}{2\hbar\omega_0 m} \exp\left(-\frac{\omega_0^2 \tau^2}{2}\right).$$

**Problem statement**

What happens for  $\tau \rightarrow 0$  if  $a$  remains constant or  $a$  is varied proportional to  $1/\sqrt{\tau}$ ?

When we take  $\lim_{\tau \rightarrow 0}$ , it will just go to zero. If  $a$  is varied with proportion to  $1/\sqrt{\tau}$ , this will only take away one  $\tau$  in the fraction in front. The whole expression will still go to zero.

**3.4 Explicit time dependence**

**Problem statement**

Consider

$$H_1(t) = ax \cos(\omega t), \quad t \in [0, T]$$

and  $H_1(t) = 0$  outside. Compute the time dependence of  $P_{1,0}(t)$ .

We start again with the expression

$$P_{1,0}(t) = \left| \frac{1}{\hbar} \int_{t_0}^t dt' \exp\left(\frac{i}{\hbar}[E_1 - E_0]t'\right) \langle 1|H_1(t')|0 \rangle \right|^2.$$

Since  $H_1$  is zero outside the interval  $[0, T]$ , we can limit the integration there. If  $t < 0$ , then  $P = 0$ . Also if  $t > T$ , then  $P(t) = P(T)$  since the integral does not change beyond  $t' = T$ .

$$= \left| \frac{1}{\hbar} \int_0^t dt' \exp\left(\frac{i}{\hbar}[E_1 - E_0]t'\right) \langle 1|H_1(t')|0 \rangle \right|^2$$

We put in  $H_1$ . The operator  $x$  is again expressed using the ladder operators. The contributing term with  $a^\dagger$  just gives prefactors, which we put up front.

$$= \frac{a}{2\hbar\omega_0 m} \left| \int_0^t dt' \exp\left(\frac{i}{\hbar}[E_1 - E_0]t'\right) \cos(\omega t') \right|^2$$

Using

$$E_n = \hbar\omega_0 \left[ n + \frac{1}{2} \right]$$

we can write the difference in energies simpler.

$$= \frac{a}{2\hbar\omega_0 m} \left| \int_0^t dt' \exp(i\omega_0 t') \cos(\omega t') \right|^2$$

The cosine needs to be expanded, we get

$$\begin{aligned} &= \frac{a}{8\hbar\omega_0 m} \left| \int_0^t dt' \exp(i\omega_0 t') \exp(i\omega t) + \exp(i\omega_0 t') \exp(-i\omega t') \right|^2 \\ &= \frac{a}{8\hbar\omega_0 m} \left| \int_0^t dt' \exp(i[\omega_0 + \omega]t') + \exp(i[\omega_0 - \omega]t') \right|^2. \end{aligned}$$

That is the expression that we will work with through the cases now.

**Resonance** In the case that  $\omega_0 = \omega$ , the second summand will be a constant 1.

$$\begin{aligned} P_{1,0}(t) &= \frac{a}{8\hbar\omega_0 m} \left| \int_0^t dt' \exp(i[\omega_0 + \omega]t') + 1 \right|^2 \\ &= \frac{a}{8\hbar\omega_0 m} \left| \left[ \frac{1}{i[\omega_0 + \omega]} \exp(i[\omega_0 + \omega]t') + t' \right]_0^t \right|^2 \\ &= \frac{a}{8\hbar\omega_0 m} \left| \frac{\exp(i[\omega_0 + \omega]t) - 1}{i[\omega_0 + \omega]} + t \right|^2 \end{aligned}$$

We make the denominator real.

$$\begin{aligned} &= \frac{a}{8\hbar\omega_0 m} \left| i \frac{1 - \exp(i[\omega_0 + \omega]t)}{\omega_0 + \omega} + t \right|^2 \\ &= \frac{a}{8\hbar\omega_0 m} \left[ i \frac{1 - \exp(i[\omega_0 + \omega]t)}{\omega_0 + \omega} + t \right] \left[ -i \frac{1 - \exp(-i[\omega_0 + \omega]t)}{\omega_0 + \omega} + t \right] \\ &= \frac{a}{8\hbar\omega_0 m} \left[ i \frac{1 - \exp(i[\omega_0 + \omega]t)}{\omega_0 + \omega} + t \right] \left[ -i \frac{1 - \exp(-i[\omega_0 + \omega]t)}{\omega_0 + \omega} + t \right] \end{aligned}$$

After expanding all the terms and grouping them in cosine and sine terms again, we obtain

$$= \frac{a}{4\hbar\omega_0 m} \left[ \frac{1 - \cos([\omega_0 + \omega]t)}{[\omega_0 + \omega]} - \frac{2t}{\omega_0 + \omega} \sin([\omega_0 + \omega]t) + t^2 \right].$$

**Off resonance** In this branch we assume that  $\omega_0 \neq \omega$ . Then we can start off with the intermediate result

$$P_{1,0}(t) = \frac{a}{8\hbar\omega_0 m} \left| \int_0^t dt' \exp(i[\omega_0 + \omega]t') + \exp(i[\omega_0 - \omega]t') \right|^2.$$

We carry out the integration and yield

$$= \frac{a}{8\hbar\omega_0 m} \left| \frac{\exp(i[\omega_0 + \omega]t) - 1}{i[\omega_0 + \omega]} + \frac{\exp(i[\omega_0 - \omega]t) - 1}{i[\omega_0 - \omega]} \right|^2.$$

We factor out the  $i$  in the denominators. The absolute value will remove it, so we just drop it then.

$$= \frac{a}{8\hbar\omega_0 m} \left| \frac{\exp(i[\omega_0 + \omega]t) - 1}{\omega_0 + \omega} + \frac{\exp(i[\omega_0 - \omega]t) - 1}{\omega_0 - \omega} \right|^2$$

In order to get the modulus squared, we need to multiply this with its complex conjugate. There will be four terms. Since this is rather straightforward, but lengthy, we just show the result here.

$$= \frac{a}{4\hbar\omega_0 m} \left[ \frac{1 + \cos([\omega_0 + \omega]t)}{[\omega_0 + \omega]^2} + \frac{1 + \cos([\omega_0 - \omega]t)}{[\omega_0 - \omega]^2} + \frac{\cos(2\omega t) + 2 \cos(\omega t) \cos(\omega_0 t)}{\omega_0^2 - \omega^2} \right]$$

### Problem statement

Show that for  $T \rightarrow \infty$  the transition probability per unit time vanishes unless  $\omega = \omega_0$ .

In any case, the probability that the system will end up in the excited state is given by  $P_{1,0}(T)$ . The probability per unit time is then given as

$$\frac{P_{1,0}(T)}{T}.$$

In case of resonance, the term with the sine will stay stay in the same order of magnitude for any  $T$ . The  $t^2$  term will grow without bounds, with seems a bit strange. If there is no resonance,  $P_{1,0}(t)$  will bounded. Dividing that by  $T$  will make it vanish for  $T \rightarrow \infty$ .

## References

Schwabl, Franz (2007). *Quantenmechanik*. 7. Berlin: Springer-Verlag. ISBN: 978-3-540-73674-5.