

## Solutionset 4.

### Excercise 1

- 1a. To prove that  $|\lambda\rangle = \exp(-|\lambda|^2/2) \exp(\lambda a^\dagger)|0\rangle$  is a normalized coherent state we first show that  $a|\lambda\rangle = \lambda|\lambda\rangle$ :

$$\begin{aligned}
 a|\lambda\rangle &= \exp(-|\lambda|^2/2) a \exp(\lambda a^\dagger)|0\rangle \\
 &= \exp(-|\lambda|^2/2) a \sum_{n=0}^{\infty} \frac{(\lambda a^\dagger)^n}{n!} |0\rangle \\
 &= \exp(-|\lambda|^2/2) a \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle \\
 &= \exp(-|\lambda|^2/2) \sum_{n=1}^{\infty} \frac{\lambda^n}{\sqrt{(n-1)!}} |n-1\rangle \\
 &= \lambda \exp(-|\lambda|^2/2) \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle \\
 &= \lambda \exp(-|\lambda|^2/2) \sum_{n=0}^{\infty} \frac{(\lambda a^\dagger)^n}{n!} |0\rangle \\
 &= \lambda |\lambda\rangle
 \end{aligned}$$

Finally we check the normalization:

$$\begin{aligned}
 \langle \lambda | \lambda \rangle &= \exp(-|\lambda|^2) \sum_{m,n} \frac{\bar{\lambda}^m \lambda^n}{\sqrt{m!n!}} \langle m | n \rangle \\
 &= \exp(-|\lambda|^2) \sum_n \frac{(\bar{\lambda}\lambda)^n}{n!} \\
 &= \exp(-|\lambda|^2) \exp(|\lambda|^2) = 1
 \end{aligned}$$

- 1b. First we calculate the expectation values  $\langle x \rangle$  and  $\langle p \rangle$ :

$$\begin{aligned}
 \langle x \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle \lambda | a + a^\dagger | \lambda \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\lambda + \bar{\lambda}) \\
 \langle p \rangle &= -i\sqrt{\frac{\hbar m\omega}{2}} \langle \lambda | a - a^\dagger | \lambda \rangle = -i\sqrt{\frac{\hbar m\omega}{2}} (\lambda - \bar{\lambda})
 \end{aligned}$$

Now we calculate  $\langle x^2 \rangle$  and  $\langle p^2 \rangle$ :

$$\begin{aligned}\langle x^2 \rangle &= \frac{\hbar}{2m\omega} \langle \lambda | (a + a^\dagger)^2 | \lambda \rangle = \frac{\hbar}{2m\omega} \langle \lambda | (a^2 + 1 + 2a^\dagger a + (a^\dagger)^2) | \lambda \rangle \\ &= \frac{\hbar}{2m\omega} ((\lambda + \bar{\lambda})^2 + 1) \\ \langle p^2 \rangle &= -\frac{\hbar m\omega}{2} \langle \lambda | (a - a^\dagger)^2 | \lambda \rangle = -\frac{\hbar m\omega}{2} \langle \lambda | (a^2 - 1 - 2a^\dagger a + (a^\dagger)^2) | \lambda \rangle \\ &= -\frac{\hbar m\omega}{2} ((\lambda - \bar{\lambda})^2 - 1)\end{aligned}$$

Using  $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$  we directly obtain:

$$\begin{aligned}(\Delta x)^2 &= \frac{\hbar}{2m\omega} ((\lambda + \bar{\lambda})^2 + 1 - (\lambda + \bar{\lambda})^2) = \frac{\hbar}{2m\omega} \\ (\Delta p)^2 &= -\frac{\hbar m\omega}{2} ((\lambda - \bar{\lambda})^2 - 1 - (\lambda - \bar{\lambda})^2) = \frac{\hbar m\omega}{2}\end{aligned}$$

Therefore the uncertainty is minimal since  $(\Delta x)(\Delta p) = \frac{\hbar}{2}$ .

1c. We have already used the expansion in 1a.

$$\begin{aligned}|\lambda\rangle &= \exp(-|\lambda|^2/2) \exp(\lambda a^\dagger) |0\rangle \\ &= \exp(-|\lambda|^2/2) \sum_{n=0}^{\infty} \frac{(\lambda a^\dagger)^n}{n!} |0\rangle \\ &= \exp(-|\lambda|^2/2) \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle \\ &=: \sum_{n=0}^{\infty} f(n) |n\rangle\end{aligned}$$

Therefore we have  $|f(n)|^2 = \exp(-|\lambda|^2) \frac{|\lambda|^{2n}}{n!}$ .

1d. We apply the translation operator  $\exp(-ipl/\hbar)$  to the ground state:

$$\begin{aligned}e^{-ipl/\hbar} |0\rangle &= e^{l\sqrt{\frac{m\omega}{2\hbar}}(a - a^\dagger)} |0\rangle = e^{\lambda(a - a^\dagger)} |0\rangle \\ &= e^{\lambda a^\dagger} e^{-\lambda a} e^{-[\lambda a^\dagger, -\lambda a]/2} |0\rangle \\ &= e^{-\lambda^2/2} e^{\lambda a^\dagger} e^{-\lambda a} |0\rangle \\ &= e^{-\lambda^2/2} e^{\lambda a^\dagger} |0\rangle = |\lambda\rangle\end{aligned}$$

## Excercise 2

2a. Let's first try,

$$[c_k, c_l^\dagger]_{\pm} = \sum_{pq} [U_{kp} a_p, a_q^\dagger U_{ql}^\dagger]_{\pm} = \sum_{pq} U_{kp} U_{ql}^\dagger \delta_{pq} = \delta_{kl}$$

In case that the transformation is not unitary the last equality would not be true. It is of course a requirement that the statistics of the particles cannot be changed by unitary transformations on the single particle level. In fact, by construction  $U$  has to be unitary because the second quantization construction rests on single particle quantum mechanics.

2b. The Hamiltonian is written as,

$$\begin{aligned} \mathcal{H} &= \sum_p \sum_r \sum_k \sum_\ell c_k^\dagger U_{kp} h_{pr} U_{r\ell}^\dagger c_\ell \quad , \\ &= \sum_{k,\ell} \left( \sum_p \sum_r U_{kp} h_{pr} U_{r\ell}^\dagger \right) c_k^\dagger c_\ell \quad , \\ &= \sum_k \varepsilon_k c_k^\dagger c_k \quad . \end{aligned}$$

In the third line, the diagonal form is imposed and one recognizes the eigenvalue problem

$$\sum_p \sum_r U_{kp} h_{pr} U_{r\ell}^\dagger = \tilde{h}_{k\ell} = \delta_{k\ell} \varepsilon_k \quad .$$

the same problem as we would have to solve in first quantization.

2c. The number operator is

$$\begin{aligned} \hat{N} &= \sum_p a_p^\dagger a_p \\ &= \sum_{pkl} c_k^\dagger U_{kp} U_{pl}^\dagger c_l \\ &= \sum_k c_k^\dagger c_k \end{aligned}$$

2d. In the Heisenberg picture we find the equation of motion for the creation operator,

$$\begin{aligned} i \frac{da_q^\dagger}{dt} &= \sum_{pr} h_{pr} [a_q^\dagger, a_p^\dagger a_r] \\ &= - \sum_p h_{pq} a_p^\dagger \end{aligned}$$

To solve for this system look for new operators obeying,

$$i \frac{dc_k^\dagger}{dt} = -\varepsilon_k c_k^\dagger$$

such that  $c_k^\dagger = e^{i\epsilon_k t} c_k^\dagger(0)$ , while  $a_q^\dagger$  can be written as

$$a_q^\dagger = \sum_k e^{i\epsilon_k t} c_k^\dagger(0) U_{kq}$$

and this system is solved by ...

2e. It follows straightforwardly from the equation of motion,

$$\begin{aligned} i \frac{da_l^\dagger}{dt} &= [a_l^\dagger, (1/2) \sum_{pqrs} V_{pqrs} a_p^\dagger a_q^\dagger a_s a_r]_{\pm} \\ &= (1/2) \sum_{r,p,q} (V_{pqr l} \pm V_{pql r}) a^\dagger a_{qa_r} \end{aligned}$$

Next to changing its own quantum number, the particle  $l$  now causes another fermion to change its quantum number: the particle ‘scatters against a particle hole pair’. These are yet other states in  $N$  particle Hilbert space and the problem cannot possibly be diagonalized by a single particle transformation. For instance considering the equation of motion of the state on the r.h.s. one will find that these couple to states like  $a^\dagger a^\dagger a^\dagger a a$  and so on.

The operator  $a_p^\dagger a_q^\dagger a_r$  has of course also a time evolution of its own, connecting it via the interaction term with operators composed of five fermion operators, and so on. In this way one has to explore the full  $N$  particle Hilbert space in order to establish the time evolution of even the simplest object, the single particle. I already announced that an exact solution is per default not possible.

### Exercise 3

- 3a. Including spin, the single particle basis is chosen to be the unhybridized site basis  $\{|i\sigma\rangle\}, i = 1, 2; \sigma = \uparrow, \downarrow$ . We define the two particle states as Slater determinants ( $\{i, i'\} \in \{1, 2\}$ )

$$|j\rangle_2 \equiv |i\sigma i'\sigma'\rangle \equiv \frac{1}{\sqrt{2}} (|i(1)\rangle |\sigma(1)\rangle |i'(2)\rangle |\sigma'(2)\rangle - |i(2)\rangle |\sigma(2)\rangle |i'(1)\rangle |\sigma'(1)\rangle) \quad (1)$$

The complete *two* particle basis is,

$$\begin{aligned} |1\rangle_2 &= |1\uparrow 2\downarrow\rangle, & |2\rangle_2 &= |2\uparrow 1\downarrow\rangle, & |3\rangle_2 &= |1\uparrow 1\downarrow\rangle \\ |4\rangle_2 &= |2\uparrow 2\downarrow\rangle, & |5\rangle_2 &= |1\uparrow 2\uparrow\rangle, & |6\rangle_2 &= |1\downarrow 2\downarrow\rangle \end{aligned} \quad (2)$$

The two particle Hilbert space is 6-dimensional. The two particle Hamiltonian has the structure  $H = \sum_{k=1,2} |i\sigma(k)\rangle h_{ij} \langle j\sigma(k)|$ , i.e. a copy for both particle  $k = 1$  and  $k = 2$ . Sandwiching this Hamiltonian between the two particle states and taking innerproducts in the Hilbert space of particle 1 and 2 separately one finds that the Hamiltonian becomes in two particle Hilbert space,

$$\begin{aligned} \mathcal{H} &= 2\varepsilon \sum_{j=1}^6 |j\rangle_2 \langle j|_2 - \\ &t ( |1\rangle_2 \langle 3|_2 + |1\rangle_2 \langle 4|_2 + |2\rangle_2 \langle 3|_2 + |2\rangle_2 \langle 4|_2 + h.c.) \end{aligned} \quad (3)$$

*h.c.* means hermitian conjugate. The Hamiltonian is diagonalized by,

$$\begin{aligned} |a\rangle_2 &= \frac{1}{2} (-|1\rangle_2 - |2\rangle_2 + |3\rangle_2 + |4\rangle_2) \\ |b\rangle_2 &= \frac{1}{2} (|1\rangle_2 + |2\rangle_2 + |3\rangle_2 + |4\rangle_2) \\ |c\rangle_2 &= \frac{1}{\sqrt{2}} (|1\rangle_2 - |2\rangle_2) \\ |d\rangle_2 &= \frac{1}{\sqrt{2}} (|3\rangle_2 - |4\rangle_2) \end{aligned} \quad (4)$$

and the diagonalized Hamiltonian becomes,

$$\begin{aligned} \mathcal{H} &= 2\varepsilon (|5\rangle_2 \langle 5|_2 + |6\rangle_2 \langle 6|_2 + |c\rangle_2 \langle c|_2 + |d\rangle_2 \langle d|_2) + \\ &|a\rangle_2 (2\varepsilon + 2t) \langle a|_2 + |b\rangle_2 (2\varepsilon - 2t) \langle b|_2 \end{aligned} \quad (5)$$

Hence, we find four non-bonding two particle states ( $|5\rangle_2, |6\rangle_2, |c\rangle_2, |d\rangle_2$ ), one bonding state ( $|a\rangle_2$ ), yielding twice as much kinetic energy as the single-particle bonding state, and one antibonding state ( $|b\rangle_2$ ).

- 3b. Of course, we could have saved the effort of diagonalizing in the ‘big’ two particle Hilbert space: this is a non-interacting problem, and in this case we can profit fully from the solution of the one particle problem. Spanning the two-particle Hilbert space using the one particle eigenstates  $|\pm\sigma\rangle$  instead, the problem is directly solved. According to the Pauli principle we can put two electrons with opposite spin in the ‘bonding molecular orbital’  $|+\rangle$  and this

state has energy  $2(\epsilon - t)$ , two electrons in the ‘antibonding’  $|-\rangle$  state ( $2(\epsilon + t)$ ) one in the bonding and one in the antibonding state ( $2\epsilon$ ) but now with spins antiparallel or parallel. Writing out the two particle states in the ‘atomic’ single particle basis on 3a one finds the following correspondence,

$$\begin{aligned}
|-\uparrow -\downarrow\rangle &= |a\rangle_2 \\
|+\uparrow +\downarrow\rangle &= |b\rangle_2 \\
|-\uparrow +\downarrow\rangle &= \frac{1}{\sqrt{2}}(|c\rangle_2 + |d\rangle_2) \\
|+\uparrow -\downarrow\rangle &= \frac{1}{\sqrt{2}}(-|c\rangle_2 + |d\rangle_2) \\
|+\uparrow -\uparrow\rangle &= -|5\rangle_2 \\
|+\downarrow -\downarrow\rangle &= -|6\rangle_2
\end{aligned} \tag{6}$$

This makes clear where the hidden simplicity in part (3a) was coming from. Notice that spin symmetry is playing an important role. The states  $|5\rangle_2, |6\rangle_2$  and  $|c\rangle_2$  form a spin triplet which is of course non-bonding (occupancy of both  $|+\rangle$  and  $|-\rangle$ ), and the remaining 3 states are a bonding, non-bonding and antibonding spin singlet

3c. The Hamiltonian is according to standard procedure,

$$H = \sum_{i\sigma} \epsilon c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\sigma} \left( c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma} \right) \tag{7}$$

where  $c_{i\sigma}^\dagger$  creates a fermion on atom  $i$  with spin  $\sigma$ . This is diagonalized by,

$$\begin{aligned}
a_{+\sigma}^\dagger &= \frac{1}{\sqrt{2}}(c_{1\sigma}^\dagger + c_{2\sigma}^\dagger) \\
a_{-\sigma}^\dagger &= \frac{1}{\sqrt{2}}(c_{1\sigma}^\dagger - c_{2\sigma}^\dagger)
\end{aligned} \tag{8}$$

such that

$$H = \sum_{\sigma} \left( (\epsilon - t) a_{+\sigma}^\dagger a_{+\sigma} + (\epsilon + t) a_{-\sigma}^\dagger a_{-\sigma} \right) \tag{9}$$

as is easily checked by inserting the transformed operators in the diagonal Hamiltonian. The two particle states are now,

$$\begin{aligned}
|-\uparrow -\downarrow\rangle &= a_{-\uparrow}^\dagger a_{-\downarrow}^\dagger |0\rangle \\
|+\uparrow +\downarrow\rangle &= a_{+\uparrow}^\dagger a_{+\downarrow}^\dagger |0\rangle \\
|-\uparrow +\downarrow\rangle &= a_{-\uparrow}^\dagger a_{+\downarrow}^\dagger |0\rangle \\
|+\uparrow -\downarrow\rangle &= a_{+\uparrow}^\dagger a_{-\downarrow}^\dagger |0\rangle \\
|+\uparrow -\uparrow\rangle &= a_{+\uparrow}^\dagger a_{-\uparrow}^\dagger |0\rangle \\
|+\downarrow -\downarrow\rangle &= a_{+\downarrow}^\dagger a_{-\downarrow}^\dagger |0\rangle
\end{aligned} \tag{10}$$

by just expressing the  $a^\dagger$ 's as linear combinations of the  $c^\dagger$ 's one immediately recovers the way it looks like in the atomic basis, for instance,

$$\begin{aligned}
 |+\uparrow+\downarrow\rangle &= a_{-\uparrow}^\dagger a_{-\downarrow}^\dagger |0\rangle \\
 &= \frac{1}{2}(c_{1\uparrow}^\dagger + c_{2\uparrow}^\dagger)(c_{1\downarrow}^\dagger + c_{2\downarrow}^\dagger) \\
 &= \frac{1}{2}(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger + c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger + c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger)|0\rangle
 \end{aligned} \tag{11}$$

and of course  $|1\rangle_2 = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$ , etcetera. It is also interesting to consider a triplet,

$$\begin{aligned}
 |+\uparrow-\uparrow\rangle &= \frac{1}{2}(c_{1\uparrow}^\dagger + c_{2\uparrow}^\dagger)(c_{1\uparrow}^\dagger - c_{2\uparrow}^\dagger) \\
 &= \frac{1}{\sqrt{2}}(-c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger + c_{2\uparrow}^\dagger c_{1\uparrow}^\dagger)|0\rangle
 \end{aligned}$$

where the anticommutation relation takes care that the states violating the Pauli principle are automatically removed. Be aware that one has to adjust the normalization.

## Excercise 4

- 4a. This ‘Hubbard’ interaction is just expressing that the states where two electrons are on the same atom ( $a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger |0\rangle$ ,  $i = 1, 2$ ) are penalized by an energy  $U$  as compared to the states where electrons are on different atoms ( $c_{1\sigma}^\dagger c_{2\sigma'}^\dagger |0\rangle$ ). because  $n_{i\uparrow} n_{i\downarrow} = 1$  for the former and 0 for the latter (just read ‘we’ve to count with  $n_i$  at the same time both an up- and down electron on that particular atom’).  $n_{i\uparrow} n_{i\uparrow}$  does not make sense because the Pauli principle forbids anyhow that two electrons are in exactly the same state (up on atom  $i$ ) and the fermion anti-commutation relations take care of this automatically.
- 4b. One can construct the two particle Hamiltonian in the ‘molecular orbital basis’ of exc. 3b, but one will find that  $U$  now appears in inconvenient, off-diagonal places in the Hamiltonian. This is not wrong, but it is more convenient and conceptually more transparent to use the ‘clumsy’ basis of exc. 3a: the bottomline is that the interactions  $\sim U$  are active in real space, the electrons have to be on the same atom. The states  $|3\rangle_2$  and  $|4\rangle_2$  have now a (diagonal) energy  $2\epsilon + U$  instead of  $2\epsilon$  while anything else in the starting Hamiltonian of exc. 3a is the same. One infers immediately that the triplets  $|5\rangle_2$  and  $|6\rangle_2$  are not affected (every electron is localized on its own atom by the Pauli principle) and the same is true for the  $M_s = 0$  triplet  $|c\rangle_2$ . The non-bonding singlet  $|d\rangle_2$  is now at  $2\epsilon + U$  and we are left with the following states,

$$\begin{aligned} |A\rangle_2 &= \frac{1}{\sqrt{2}}(|1\rangle_2 + |2\rangle_2) \\ |B\rangle_2 &= \frac{1}{\sqrt{2}}(|3\rangle_2 + |4\rangle_2) \end{aligned} \quad (12)$$

with Hamiltonian

$$H_{AB} = 2\epsilon |A\rangle_2 \langle A| + (2\epsilon + U) |B\rangle_2 \langle B| - 2t(|A\rangle_2 \langle B| + |B\rangle_2 \langle A|) \quad (13)$$

In the non interacting case the ‘singly’ (A) and ‘doubly occupied’ (B) states were degenerate but this degeneracy is lifted by the interaction  $U$ . One readily infers the energy eigenvalues,

$$\omega_{\pm} = \frac{1}{2} \left( 1 \pm \sqrt{1 + 16 \frac{t^2}{U^2}} \right) \quad (14)$$

The ground state has an energy  $\omega$ . For  $U = 0$  one recovers a ‘covalency’ or ‘hybridization’ energy  $-2t$  expressing that an electron can use the ‘room’ in the molecule to lower their kinetic energy, unhindered by the other electron. When  $U$  is large compared to  $t$  one can expand the expression for  $\omega_-$  and it follows immediately that  $\omega \simeq 2\epsilon + 4t^2/U$ , a number small compared to  $t$ : the molecule is much less stable. How can that be? By inspecting  $H_{AB}$  one immediately infers that in order for the electrons to delocalize they have to tunnel from two particle state  $|A\rangle_2$  to  $|B\rangle_2$  and the  $|B\rangle_2$  corresponds with a state where two electrons are on the same atom – starting out with one electron on every atom it has to be that when one of the electrons hops it ends up on an atom where the other electron was already present!

- 4c One can do this in a fanciful way employing an operator unitary transformation and the Baker-Hausdorff lemma to formulate the perturbation expansion, finding the spin Hamiltonian explicitly up to second order. Anyone who has rediscovered this by either using Google



Scholar or by reinventing the wheel can count n lots of bonus points. However, it suffices to use the conceptual side of perturbation theory to get at the right answer. For  $U \gg t$  the ground state wave function with energy  $\omega$  becomes to first order in  $t/U$ ,

$$|-\rangle_2 = |1(1)\rangle |2(2)\rangle + \frac{1}{\sqrt{2}}(|\uparrow(1)\rangle |\downarrow(2)\rangle - |\downarrow(1)\rangle |\uparrow(2)\rangle) + \frac{2t}{U}|B\rangle_2 \quad (15)$$

where we have written  $|A\rangle_2$  explicitly as a tensor product state to make clear that it is a spin singlet. All other states are at high energy  $\sim U$  except for the triplets which are all at energy  $2\epsilon$ . Imagine that you're an intellect living in a world where the largest particle collider can only probe energies  $\ll U$ . All you know is that there is a difference in energy between spin singlets and spin triplets made out of two electrons. You can't actually see that electrons also carry electrical charge because for that purpose you have to bring them together on one atom (you get  $H^+$  and  $H^-$  instead of neutral  $H_2$ ) and your accelerator is too cheap for that. Since you only know about spins you can for every purpose in your low energy universe use as well the Hamiltonian

$$H = 2\epsilon\hat{1} + \frac{4t^2}{U} \left( \vec{S}_1 \cdot \vec{S}_2 - \frac{1}{4}\hat{1} \right) \quad (16)$$

where  $\hat{1} = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|$  and  $S^z = (1/2)(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)$ , etcetera. This works as well in arrays of atoms and it is actually so that nearly salts formed with transition- or rare earth metals are insulating because of the Hubbard  $U$  (these are called 'Mott-insulators') and these are usually characterized by spin systems with antiferromagnetic interactions of the type just explained. This 'superexchange mechanism' was invented by P.W Anderson in the early 1950's and it took a surprisingly long time to get generally accepted.