Solutions to NS-202B Kwantummechanica 2016/17 Tentamen

(Dated: February 8, 2017)

I. 1. SEPARATIE VAN VARIABELEN (9 PT.)

A. Solution

(a) The time-dependent Schrøinger-equation for an spin-less electron in 3D space is

$$-\frac{\hbar^2\nabla^2\psi(\vec{x},t)}{2m}+V(\vec{x},t)\psi(\vec{x},t)=i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t}$$

Scoring:

- Full point if $V=V(\vec{x},t)$.
- No deduction of points if x not denoted as a vector.
- No deduction of points if $V=V(\vec{x})$.

(b) Intended answer: The equation is separable into a space and time dependent part if the potential is time-independent.
The separation constant is the energy eigenvalue, and the solutions of the separated equation are energy eigenstates. We plug the eigenstate expressed as the following

$$\psi(\vec{x},t)=c(t)\phi(\vec{x}) \tag{1}$$

into the Schrøinger-equation, obtaining,

$$\left(-\frac{\hbar^2\nabla^2\phi(\vec{x})}{2m}+V(\vec{x})\phi(\vec{x})\right)c(t)=i\hbar\frac{\partial c(t)}{\partial t}\phi(\vec{x}) \tag{2}$$

Dividing through by $c(t)\phi(\vec{x})$,

$$\left(-\frac{\hbar^2\nabla^2\phi(\vec{x})}{2m\phi(\vec{x})}+V(\vec{x})\right)=\frac{i\hbar}{c(t)}\frac{\partial c(t)}{\partial t} \tag{3}$$

Now the left side is a function of $\vec{x}$ alone, and the right side is a function of t alone. The only way this can possibly be true is both sides are in fact constant, which can be denoted as E. Then

$$\begin{aligned}\left(-\frac{\hbar^2\nabla^2\phi(\vec{x})}{2m\phi(\vec{x})}+V(\vec{x})\right) &= E\\ \frac{i\hbar}{c(t)}\frac{\partial c(t)}{\partial t} &= E\end{aligned} \tag{4}$$

Therefore the equation is separable as stated above.

Scoring: partial points for:

- 1.5 pt Condition of separability (time-independent potential)

– 0.5 pt Mentioning of Energy (eigenvalue) as the separation constant
– 1 pt The step 2 in the proof of separability, or the equivalent.

(c) The time-independent Schrødinger-equation is just

$$-\frac{\hbar^2\nabla^2\phi(\vec{x})}{2m} + V(\vec{x})\phi(\vec{x}) = E\phi(\vec{x}) \tag{5}$$

where E is the (energy) eigenvalue.

Scoring: Full points for the correct equation. No points if incorrect equation (still have t in somewhere, or wavefunction not explicitly function of x). Labels such as E_n may be attached. Wavefunction may be denoted by any Greek or non-Greek letter. No partial points.

(d) The condition where the equation can be separable once again in an radial part and an angular part is that the potential should be only radially dependent.

Scoring: Full points for mentioning of V only dependent on r, OR V independent of θ and ϕ. 1 point for a vague answer that goes in the right direction, or for saying " independent of phi" while forgetting theta v.v.. Mentioning the requirement that Psi is an eigenfunction of H is optional.

(e) The separation constant l and m are aizimuthal quantum number and magnetic quantum number separately.l is linked to the square of total angular momentum by,

$$\hat{L}^2\psi = l(l+1)\hbar^2\psi$$

, m is linked to the z-component measurement of the angular momentum, by

$$\hat{L}_z\psi = m\hbar\psi$$

Scoring:

– 1 pt: mention l as "azimuthal" or "total angular momentum", or even simply " angular momentum", or equation.
– 1 pt mention m as " magnetic" or "projection" or " z component of l" or equivalent, or equation.

II. 2. TWEE NEUTRONEN (9 PT.)

A. Solution

(a) Inside the well, We have the time-independent Schrøinger-equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(\vec{x})}{\partial x^2} = \epsilon\phi(\vec{x})$$

whose solution are given by

$$\phi(x) = A\sin kx + B\cos kx$$

where k is defined by,

$$k \equiv \frac{\sqrt{2m\epsilon}}{\hbar}$$

The constants inside the solution are determined by the boundary condition,

$$\phi(-a) = \phi(a) = 0$$

, which gives us

$$A \sin ka + B \cos ka = 0$$

and

$$-A \sin ka + B \cos ka = 0$$

This separates (add/subtract the equations) into

$$A \sin ka = 0$$

and

$$B \cos ka = 0$$

So that either $A = 0$ and $\cos ka = 0$ or $B = 0$ and $\sin ka = 0$. The lowest energy eigenvalue is for the symmetric wavefunction

$$B \cos kx$$

with $k = \pi/2a$ and energy eigenvalue:

$$E_0 = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 \hbar^2}{8ma^2}$$

To find A, we have the normalized condition,

$$\int_{-a}^{a} |A|^2 \cos^2(kx) dx = 1$$

so $|A| = \sqrt{\frac{1}{a}}$, therefore we get the normalized ground state at $n = 1$, which is

$$\psi_0(x) = \sqrt{\frac{1}{a}} \cos(\frac{\pi}{2a} x)$$

Scoring: 2 points for fully correct answer (even if no calculation). 1.5 points if calculation is given and the answer is wrong due to one or more simple arithmetic errors (factors 2 etc.).

Scoring exceptions:

- Full points if accidentally taking the wrong boundary condition (psi=0 at x=0) is followed by a correct calculation leading to the wavefunction $\sqrt{\frac{1}{a}} \sin(\frac{\pi}{a} x)$ and energy $\frac{\pi^2 \hbar^2}{2ma^2}$.
- 1.5 points if wrong boundary condition followed by calculation with arithmetic errors.
- No points if simply stating wrong answer without motivation or calculation.

(b) The normalized first-excited state must have exactly one node, same boundary conditions as above.

$$\psi_1(x) = \sqrt{\frac{1}{a}}\sin(\frac{\pi}{a}x)$$

and the energy of first excited state is

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

Scoring rules:

- 2 points if fully correct
- 2 points for an incorrect answer but consistent with (a). ($\frac{2\pi^2\hbar^2}{ma^2}$, $\sin 2\pi x/a$)
- 1.5 points for an answer that contains arithmetic errors but otherwise consistent with (a)
- No points for a wrong answer inconsistent with (a) without calculation.

(c) Since the neutrons are Fermions, the total wavefunction needs to be anti-symmetrical, thus the spin singlet is given as below,

$$\Psi_{S=0}(x_1, x_2) = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\psi_0(x_1)\psi_0(x_2) \tag{6}$$

where x_1, x_2 denotes the spatial coordinates of these two neutrons. And the ground state energy is

$$E_{S=0} = 2E_0$$

There's no degeneracy in this spin singlet.

Scoring:

- 2 points if fully correct
- 1 point if accidentally ANTIsymmetrized the spatial part.
- 1.5 point if wrong or non-understandable wavefuntion but correct spin part and energy.
- 1.5 point if mention Pauli principle allows both in the ground state and correct energy (with no or wrong wavefunction given)
- 0.5 point if only the degeneracy question correct.

(d) For the spin triplet, we have three choices for the spin part of the total wavefunctions,

$$\begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases} \tag{7}$$

and one choice for the spatial part

$$\psi_0(x_0)\psi_1(x_2) - \psi_0(x_2)\psi_1(x_1)$$

Thus the spin triplet states can be expressed as the following

$$(\psi_0(x_0)\psi_1(x_2) - \psi_0(x_2)\psi_1(x_1)) \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases} \tag{8}$$

and has a degeneracy of 3.
The energy is

$$E_{S=1} = E_0 + E_1$$

Scoring:

- 2 points if fully correct
- 1 point if accidentally symmetrized the spatial part (if consistent with (c)).
- 1.5 point if wrong or non-understandable wavefuntion but correct spin part and energy.
- 1.5 point if mention Pauli principle one in the ground state one in the excited state and correct energy (with no or wrong wavefunction given)
- 1.5 point if correct spatial part but wrong spin part.
- 0.5 point if only the degeneracy question correct.

(e) Since the neutrons are Fermions, the total wavefunction needs to be anti-symmetrical, then for the spin triplet, whose spin part of wavefunction is symmetrical, the spatial part of wavefunction has to be anti-symmetrical so that one of the neutrons has to be excited. While for the case of singlet state, the spatial part of wavefunction is just symmetrical, thus making both neutrons stay in their ground state possible. That's why the singlet state is the ground state. **Scoring:**

- 1 point if invoking the results of (c) and (d), e.g. " we calculate a lower energy in c"
- 1 point if a reasoning using Pauli principle.
- No points if mentioning interactions are the cause (we were explicitly excluding those!).

III. 3. DE GESTOORDE HARMONISCHE OSCILLATOR (13 PT.)

A. Solution

(a) We have the Hamiltonian written as

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

And with $y = x\sqrt{\frac{m\omega}{\hbar}}$, we have

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial y}\frac{\partial y}{\partial x} \tag{9}$$

$$\frac{\partial^2}{\partial x^2} = \frac{\partial^2}{\partial y^2}(\frac{\partial y}{\partial x})^2 \tag{10}$$

$$\tag{11}$$

Plug the relations above into the Hamiltonian, we immediately get

$$\hat{H} = \hbar\omega\big(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2\big) \tag{12}$$

Scoring:

- The point is given for the step where the differential operators are transformed, i.e. $\partial_x = \sqrt{\frac{m\omega}{\hbar}}\partial_y$ or the equivalent.

(b) With the ladder operator,

$$\hat{a} = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right),\ \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right). \tag{13}$$

the Hamiltonian becomes

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) \tag{14}$$

With the Schrøinger-equation, we have,

$$\hat{H}|n\rangle = E_n|n\rangle$$

For the LHS,

$$\begin{aligned}
\hat{H}|n\rangle &= \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})|n\rangle && (15)\\
&= \hbar\omega(\hat{a}^\dagger\sqrt{n}|n-1\rangle + \frac{1}{2}|n\rangle) && (16)\\
&= \hbar\omega(n|n\rangle + \frac{1}{2}|n\rangle) && (17)\\
&= \hbar\omega(n + \frac{1}{2})|n\rangle && (18)\\
&= RHS \equiv E_n|n\rangle && (19)
\end{aligned}$$

where $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ are applied.
Therefore we have the eigenvalues for the undisturbed Hamiltonian as below,

$$E_n = \hbar\omega(n + \frac{1}{2})$$

Scoring:

- 1 point for writing the Schrodinger equation in form 14 or the equivalent steps. (no point if n+1 instead of n+1/2).
- 1 point for showing $a^\dagger a = n$, or the equivalent.

(c) Adding the perturbation, we have the Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + (\frac{1}{2}m\omega^2 + \lambda\alpha)x^2$$

Changing the variable by $\omega' = \sqrt{\omega^2 + \lambda\frac{2\alpha}{m}}$, we have the

$$\hat{H}' = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega'^2x^2$$

which we recognize as just the harmonic oscillator with frequency ω'. **Scoring:**

– 1 point for the step showing that we now have the exact same equation with frequency ω'.

(d) Using

$$(1+x)^b \approx 1 + bx + \frac{b(b-1)}{2}x^2 + \mathcal{O}(x^3)$$

In the case where λ is small, we have,

$$\omega' = \sqrt{\omega^2 + \lambda\frac{2\alpha}{m}} \tag{20}$$

$$= \omega + \lambda\frac{\alpha}{m\omega} - \lambda^2\frac{\alpha^2}{2m^2\omega^3} + \mathcal{O}(\lambda^3) \tag{21}$$

Therefore the Taylor expansion(until 2nd order)of the exact energy of the ground state is

$$E_0(\lambda) = \frac{\hbar}{2}\left(\omega + \lambda\frac{\alpha}{m\omega} - \lambda^2\frac{\alpha^2}{2m^2\omega^3} + \mathcal{O}(\lambda^3)\right)$$

The 2nd order contribution is just $-\frac{\lambda^2\hbar\alpha^2}{4m^2\omega^3}$.

Scoring:

– Needs to be fully correct to gain 1 point.

(e) The units of α is

$$[\alpha] = [m\omega^2] = kg \cdot s^{-2}$$

Scoring:

– Needs to be fully correct to gain 1 point. Jm^{-2} is acceptable.

(f) The perturbation term $\hat{H}_1 = \lambda\alpha x^2$ can be rewritten as

$$\hat{H}_1 = \lambda\alpha(y\sqrt{\frac{\hbar}{m\omega}})^2 \tag{22}$$

$$= \frac{\lambda\alpha\hbar}{m\omega}y^2 \tag{23}$$

$$= \frac{\lambda\alpha\hbar}{m\omega}(\frac{\hat{a}+\hat{a}^\dagger}{\sqrt{2}})^2 \tag{24}$$

$$= \frac{\lambda\alpha\hbar}{2m\omega}(\hat{a}+\hat{a}^\dagger)^2 \tag{25}$$

$$= \frac{\lambda\alpha\hbar}{2m\omega}(\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger) \tag{26}$$

$$= \frac{\lambda\alpha\hbar}{2m\omega}(\hat{a}\hat{a} + \hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \tag{27}$$

$$= \frac{\lambda\alpha\hbar}{2m\omega}(\hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a} + 2\hat{a}^\dagger\hat{a} + 1) \tag{28}$$

where in the last step we used the relation for bosonic operator.

$$[\hat{a}, \hat{a}^\dagger] = 1$$

There, with the help of undisturbed ladder operators, the perturbation term can be expressed as,

$$\hat{H}_1 = \lambda g(\hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a} + 2\hat{a}^\dagger\hat{a} + 1) \tag{29}$$

where

$$g = \frac{\alpha\hbar}{2m\omega} \tag{30}$$

Scoring:

- Also acceptable to work backwards from the answer.
- 1.5 point for the operator part
- 0.5 point for prefactor.

(g) **Algebraic solution:**

$$E_0^{(1)}(\lambda) = \langle 0|\hat{H}_1|0\rangle$$

$$= \lambda g\langle 0|\hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a} + 2\hat{a}^\dagger\hat{a} + 1|0\rangle$$

The two middle terms terms with a on the right are zero, as $a|0\rangle = 0$. The term with twice $a^\dagger$ is $\sqrt{2}|2\rangle$, which is orthogonal to $|0\rangle$ so also contributes zero. The only term left is the 1, so we find

$$E_0^{(1)}(\lambda) = \lambda g$$

Integral solution: First we have the ground state wave function for $\hat{H}_0$,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$$

The first-order perturbation of the energy of the ground state can be calculated as

$$\begin{aligned} E_0^{(1)}(\lambda) &= \langle\psi_0(x)|\hat{H}_1|\psi_0(x)\rangle && (31)\\ &= \lambda\alpha\langle\psi_0(x)|x^2|\psi_0(x)\rangle && (32)\\ &= \lambda\alpha\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega x^2}{\hbar}} && (33)\\ &= \frac{\hbar\lambda\alpha}{2m\omega} = \lambda g && (34) \end{aligned}$$

Scoring:

- 1 point for use of the formula for first-order perturbation (in bra-ket or integral form)
- 1 point for the correct calculation
- 0.5 point for a sensible calculation with incorrect result (factors 2 etc).

(h) We are going to calculate the contribution from second order perturbation to the eigen energy using an algebraic way. Since

$$\hat{H}_1 = \frac{\lambda\alpha\hbar}{2m\omega}(\hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a} + 2\hat{a}^\dagger\hat{a} + 1)$$

we have

$$E_0^{(2)} = \sum_{m\neq 0} \frac{|\langle\psi_m^{(0)}|\hat{H}_1|\psi_0^{(0)}\rangle|^2}{E_0^{(0)} - E_m^{(0)}} \tag{35}$$

$$= \left(\frac{\lambda\alpha\hbar}{2m\omega}\right)^2 \sum_{m\neq 0} \frac{|\langle m|(\hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a} + 2\hat{a}^\dagger\hat{a} + 1)|0\rangle|^2}{-m\hbar\omega} \tag{36}$$

$$\tag{37}$$

We calculate

$$(\hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a} + 2\hat{a}^\dagger\hat{a} + 1)|0\rangle$$

$$= (\hat{a}^\dagger\hat{a}^\dagger + 1)|0\rangle$$

$$= |0\rangle + \sqrt{2}|2\rangle$$

So that the only nonzero term in the sum is for $m = 2$, and the value is

$$E_0^{(2)} = \left(\frac{\lambda\alpha\hbar}{2m\omega}\right)^2 \frac{2}{-2\hbar\omega} \tag{38}$$

$$= -\frac{\lambda^2\hbar\alpha^2}{4m^2\omega^3} \tag{39}$$

Scoring:

- 2 points for the fully correct answer. Also give full points for small mistakes (e.g. factors 2 or confusing m and mass).
- 1 point for correctly using the formula even if the further calculation is missing or wrong.

(i) We get the contribution from second order perturbation to the eigen energy using perturbation theory as the same value as the one got from Taylor expansion.

Scoring:

- Depending on what the student found, any reasonable attempt at comparing the values (the same, different) with a reasonable conclusion is awarded the point.

IV. 4. WATERSTOFATOOM (3 PT.)

A. Solution

(a) Since the electron feels an highly symmetrical potential field, the expectation value of $\vec{x}$ will just vanish for any eigenstate, which can be seem from

$$|\psi_{n,l,m}(x)|^2 = |\psi_{n,l,m}(-x)|^2 \tag{40}$$

The electric dipole moment is odd in x, therefore the integral of its expectation value $\boldsymbol{p} = -e\boldsymbol{x}$ for an atom in the ground state and for the state $|n, l, m\rangle = |2, 1, 1\rangle$ are both zero.

Alternative answer: Write the integrals and show the integrand is odd.

Scoring:

– Any mention the fact that the dipole moment is odd while psi-squared is even is worth the point

(b) We have

$$\psi_{100}(\vec{x}) = \psi_{100}(-\vec{x}) \tag{41}$$
$$\psi_{211}(\vec{x}) = -\psi_{211}(-\vec{x}) \tag{42}$$

Then probability density function corresponding to state $(|2, 1, 1\rangle) + |1, 0, 0\rangle)/\sqrt{2}$ can be written as

$$PDF \equiv |(|2, 1, 1\rangle) + |1, 0, 0\rangle)/\sqrt{2}|^2 \tag{43}$$
$$= (\psi_{100}(\vec{x}) + \psi_{211}(\vec{x}))^2/2 \tag{44}$$
$$= (\psi_{100}(-\vec{x}) - \psi_{211}(\vec{-x}))^2/2 \tag{45}$$

therefore we have,

$$\langle\vec{x}\rangle = \iiint \vec{x}(\psi_{100}(\vec{x}) + \psi_{211}(\vec{x}))^2/2\, d\vec{x} \tag{46}$$
$$= \iiint \vec{x}(\psi_{100}(\vec{-x}) - \psi_{211}(\vec{-x}))^2/2\, d\vec{x} \tag{47}$$
$$\langle\vec{x}\rangle = -\langle -\vec{x}\rangle \tag{48}$$
$$= -\iiint -\vec{x}(\psi_{100}(-\vec{x}) + \psi_{211}(-\vec{x}))^2/2\, d(-\vec{x}) \tag{49}$$
$$= -\iiint \vec{x}(\psi_{100}(-\vec{x}) + \psi_{211}(-\vec{x}))^2/2\, d\vec{x} \tag{50}$$

Plus the two equations above together for both sides, we have,

$$\langle\vec{x}\rangle = \iiint \vec{x}\psi_{100}(\vec{x})\psi_{211}(\vec{x})\, d\vec{x} \tag{51}$$

From the right side of the equation above, whose integrand is an even symmetrical function, we find that $\langle\vec{x}\rangle \neq 0$, thus we get a nonzero electrical dipole moment for this superposition state.

Alternative:

$$\langle\mathbf{x}\rangle = \frac{1}{2}(\langle 2, 1, 1| + \langle < 1, 0, 0|)\mathbf{x}(|2, 1, 1\rangle + |1, 0, 0\rangle)$$

We see 4 terms. 2 of them are zero (we just found) as they are odd (odd x odd x odd, or even x even x odd). The other 2 are even (odd x odd x even), so it is plausible that they are not zero.

Scoring:

– Any mention of these even (symmetric) terms is worth the point

– One could also reason that the function is not an eigenfunction therefore the expectation value could be nonzero.(full points)

(c) The probability can be calculated as

$$Prob. = \int\int\int_0^{r_p} |\psi_{100}(r)|^2 d^3\,\vec{r} \tag{52}$$

$$= \int\int\int_0^{r_p} |\frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}|^2 d^3\,\vec{r} \tag{53}$$

$$\tag{54}$$

We can solve the integral with the help of the formularium, or we can realize that the exponent is very small over the entire nucleus so that the wavefunction is constant to very good approximation (much better than 1 %). So the value of the integral is just the wavefunction-squared (which is $1/(\pi a_0^3)$) times the volume of the nucleus (which is $\frac{4}{3}\pi r_n^3$), to yield

$$P = \frac{4}{3}\frac{r_n^3}{a_0^3} = 1.3 \times 10^{-15}$$

Since $\frac{r_p}{a_0}$ is very tiny, it's not necessary to calculate an integral here. However it is correct to do so.

Scoring:

– Any answer in the 10^{-15} range is awarded 1 pt.

DONE.