Final exam for Kwantumfysica 1 - 2010-2011
Friday 28 January 2011, 9:00 - 12:00

READ THIS FIRST:

- Note that the lower half of this page lists some useful formulas and constants.
- Clearly write your name and study number on each answer sheet that you use.
- On the first answer sheet, write clearly the total number of answer sheets that you turn in.
- Note that this exam has 4 questions, it continues on the backside of the papers!
- Start each question (number 1, 2, 3, 4) on a new answer sheet.
- The exam is open book within limits. You are allowed to use the book by Liboff, the handout *Extra note on two-level systems and exchange degeneracy for identical particles*, and one A4 sheet with notes, but nothing more than this.
- If it says "make a rough estimate", there is no need to make a detailed calculation, and making a simple estimate is good enough. If it says "calculate" or "derive", you are supposed to present a full analytical calculation.
- If you get stuck on some part of a problem for a long time, it may be wise to skip it and try the next part of a problem first.
- If you are ready with the exam, please fill in the **course-evaluation question sheet**. You can keep working on the exam until 11:30, and fill it in shortly after 11:30 if you like.

Useful formulas and constants:

Electron mass	m_e	$= 9.1 \cdot 10^{-31}$ kg
Electron charge	$-e$	$= -1.6 \cdot 10^{-19}$ C
Planck's constant	h	$= 6.626 \cdot 10^{-34}$ Js $= 4.136 \cdot 10^{-15}$ eVs
Planck's reduced constant	$\hbar$	$= 1.055 \cdot 10^{-34}$ Js $= 6.582 \cdot 10^{-16}$ eVs

Fourier relation between x-representation and k-representation of a state

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \overline{\Psi}(k) e^{ikx}\, dk$$

$$\overline{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx}\, dx$$

Standard Fourier transform pairs:

$$\Psi(x) = \begin{cases} \frac{1}{\sqrt{2b}}, & |x| \le b \\ 0, & |x| > b \end{cases} \quad \overset{Fourier}{\leftrightarrow} \quad \overline{\Psi}(k) = \sqrt{\frac{b}{\pi}} \frac{\sin kb}{kb}$$

$$\Psi(x) = \sqrt{\frac{b}{\pi}} \frac{\sin bx}{bx} \quad \overset{Fourier}{\leftrightarrow} \quad \overline{\Psi}(k) = \begin{cases} \frac{1}{\sqrt{2b}}, & |k| \le b \\ 0, & |k| > b \end{cases}$$

Standard integrals:

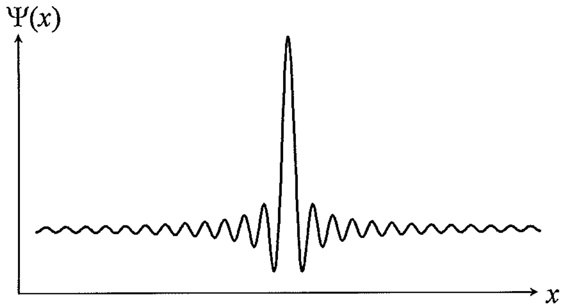
$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} dx = \tfrac{1}{2}\sqrt{\pi}$$

Problem 1

Consider an electron, that behaves as a one-dimensional quantum particle with position x. At some time t_0 the electron is in the following normalized state (see also figure), where the constant $a = 10^9$ m^{-1}.

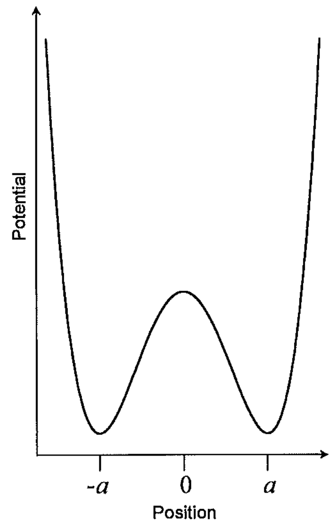
$$\Psi(x) = \sqrt{\frac{a}{\pi}}\,\frac{\sin(ax)}{ax}$$



One is going to measure the velocity of this electron at this time t_0. Calculate the probability for getting a result between +80 km/s and +120 km/s.

Problem 2

Consider a one-dimensional quantum particle in a double-well potential (see figure).



We will assume that only the low-energy dynamics of this system is relevant. In that case, it can be described as an effective two-state system. The system then has two position eigenstates, which belong to the operator (observable) $\hat{A}$ for the position of the particle in this double-well system,

$$\hat{A} \leftrightarrow \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}, \quad |\varphi_L\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\varphi_R\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

One of these states, denoted as $|\varphi_L\rangle$, corresponds to the particle being localized at $-a$ (in the left well), and has the position eigenvalue $-a$. The other position eigenstate, denoted as $|\varphi_R\rangle$ with eigenvalue $+a$ corresponds to the particle being localized in the right well. We also introduced a matrix and vector notation for representing the operators and states of this system, using the basis spanned by $|\varphi_L\rangle$ and $|\varphi_R\rangle$.

The particle can go from the left well to the right well by tunneling through the barrier. Using the same matrix notation as before (in the same basis spanned by $|\varphi_L\rangle$

and $|\varphi_R\rangle$), the Hamiltonian for the particle is (here T is a real and negative number, and E_0 is a real positive number)

$$\hat{H} \leftrightarrow \begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}.$$

a) Calculate whether $\hat{A}$ and $\hat{H}$ commute.

b) Proof (or better, derive) that the energy eigenstates of this system are

$$|\varphi_g\rangle \leftrightarrow \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad \text{with eigenvalue } E_g$$

$$|\varphi_e\rangle \leftrightarrow \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} \quad \text{with eigenvalue } E_e$$

and give the values of E_g and E_e in terms of E_0 and T. Confirm that $|\varphi_g\rangle$ is the ground state.

c) Calculate for the following four states $|\Psi\rangle$ the probability that a measurement with observable $\hat{A}$ gives as result $-a$.

c-i) $|\Psi\rangle = |\varphi_g\rangle$

c-ii) $|\Psi\rangle = |\varphi_e\rangle$

c-iii) $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_g\rangle + |\varphi_e\rangle \right)$

c-iv) $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_g\rangle - |\varphi_e\rangle \right)$

d) Calculate the value of the four quantities

$$\langle \varphi_g|\hat{A}|\varphi_g\rangle,\ \langle \varphi_e|\hat{A}|\varphi_e\rangle,\ \langle \varphi_g|\hat{A}|\varphi_e\rangle \text{ and } \langle \varphi_e|\hat{A}|\varphi_g\rangle.$$

Describe in words what these quantities represent.

e) The outcome of a measurement of $\hat{A}$ (which ended at time $t = 0$) is that the particle is in the left well. The measurement is then stopped, and the quantum system evolves again on itself. Calculate how $\langle \hat{A} \rangle$ now depends on time for $t > 0$. Describe in words what the calculation represents.

Problem 3

Consider again the type of system of **Problem 2**. Now, however, consider that you have two identical versions of it at two different locations (two double-well potentials, each with one particle in it). One of the systems is at place P1, and the other at place P2, and the distance between these two places is much larger than the size of the double-well potential.

a) At both places, you will do a measurement with observable $\hat{A}$. What is the probability that you will get the outcome $-a$ for both systems, if the states of the systems at the moment just before the measurement are as follows?

a-i) the system at P1 is in the state $|\varphi_g\rangle$ and the system at P2 is in the state $|\varphi_e\rangle$.

a-ii) the system at P1 is in the state $|\varphi_e\rangle$ and the system at P2 is in the state $|\varphi_g\rangle$.

Now consider that you have again only a single double-well potential (exactly the same as before), but that this double-well potential contains two identical particles (the same type of particle as before). To describe this system, we need to label the particles from now on. We will use the indices 1 and 2 to label the particles, and the index T refers to the total system. These two particle do not interact. This means that the Hamiltonian of the total system is now

$$\hat{H}_T = \hat{H}_1 + \hat{H}_2 \ ,$$

where $\hat{H}_1$ and $\hat{H}_2$ the operators $\hat{H}$ for each particle (now in the Hilbert space with states of the two-particle system).

b) Assume that this total system (combined system with two particles) is prepared in a state with total energy $E_T = E_g + E_e$. Show that the following three states are all an eigenstate of $\hat{H}_T$ with energy $E_T = E_g + E_e$.

b-i) $\left|\Psi_T\right\rangle_{C\alpha} = \left|\varphi_{g1}\right\rangle\left|\varphi_{e2}\right\rangle$

b-ii) $\left|\Psi_T\right\rangle_{C\beta} = \left|\varphi_{e1}\right\rangle\left|\varphi_{g2}\right\rangle$

b-iii) $\left|\Psi_T\right\rangle_{\alpha\beta} = \alpha\left|\Psi_T\right\rangle_{C\alpha} + \beta\left|\Psi_T\right\rangle_{C\beta}$ (see definitions in b-i) and b-ii))

c) It can be shown that in the case of identical particles, the only states $\left|\Psi_T\right\rangle_{\alpha\beta}$ (see definition in **b)**) that occur in nature are for $\alpha = +\frac{1}{\sqrt{2}}$ and $\beta = \pm\frac{1}{\sqrt{2}}$,

$$\left|\Psi_T\right\rangle_S = \tfrac{1}{\sqrt{2}}\left|\varphi_{g1}\right\rangle\left|\varphi_{e2}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\varphi_{e1}\right\rangle\left|\varphi_{g2}\right\rangle$$
$$\left|\Psi_T\right\rangle_{AS} = \tfrac{1}{\sqrt{2}}\left|\varphi_{g1}\right\rangle\left|\varphi_{e2}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\varphi_{e1}\right\rangle\left|\varphi_{g2}\right\rangle .$$

Show that $\left|\Psi_T\right\rangle_S$ is symmetric and that $\left|\Psi_T\right\rangle_{AS}$ is anti-symmetric with respect to exchanging the two particles in the system.

d) We do a measurement to determine for both particles whether they are in the right well or in the left well (measurement in the sense of observable $\hat{A}$). Calculate for the following two states the probability that you will get the outcome $-a$ for both particles.

d-i) $\left|\Psi_T\right\rangle_S$ (see definition in **c)**).

d-ii) $\left|\Psi_T\right\rangle_{AS}$ (see definition in **c)**).

Problem 4

Consider a one-dimensional system, with a single particle with mass $m = 10^{-20}$ kg at position x in the potential

$$V(x) = \tfrac{1}{2}\left(m\omega_0^2\right)x^2 .$$

Given the mass m, the constant ω_0 defines how steep the potential is. This system concerns a particle that is bound in a static potential, so it must have a discrete set of energy eigenstates $\chi_n(x)$ (or in Dirac notation, $|\chi_n\rangle$), where n is an index $n = 0,1,2,3 \ldots$ for labeling these states.

a) Write down the Hamiltonian H of this system in x-representation. Write it out in an expression that uses the constants m and ω_0 where possible.

Assume that it is known that the ground state (lowest energy eigenstate) of this system is of the form

$$\Psi(x) = Ae^{-bx^2} ,$$

(in Dirac notation denoted as $|\Psi\rangle$) but that the values of A and b (real constants) are not known, and also the eigenvalue that belongs to this eigenstate is not known.

b) Draw a graph of $\Psi(x)$. For which value of A (in terms of constants b and others that you may need) is this state normalized?

In order to find the values for A and b for which the state $\Psi(x)$ represents the true ground state $\chi_0(x)$, you must use in this problem the *variational method.* For this case, this implies that $\langle \hat{H} \rangle$ is minimum with respect to the variation of the parameter b.

c) Say that the real (but still unknown to us) ground state energy of the system is E_0, with the corresponding eigenstate $|\chi_0\rangle$. Use Dirac notation to proof that for any state $|\Psi\rangle$ that we may consider, it will always obey $\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0$.

Hint: Use that any trial state $|\Psi\rangle$ can always be written as a superposition of all the real energy eigenstates $|\chi_n\rangle$.

d) The results of **c)** shows that equality $\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = E_0$ holds only for the case $|\Psi\rangle = |\chi_0\rangle$.

Here $\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ has a minimum value, so $|\chi_0\rangle$ and E_0 can be found by a procedure that minimizes the expression with respect to b. Obviously, this must be carried out in the x-representation. Use this approach to derive the values of b, A and E_0 in terms of m and ω_0.

e) Calculate for the ground state that you found in **d)**, the expectation value for kinetic energy and the expectation value for potential energy. Explain the result of qualitatively in terms of the Heisenberg uncertainty relation.

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Uitwerking Final Exam
Kwantumfysica 1 — 28 JAN 2011

Problem 1

The quantum state is given as a function of position, but we need to know the state in relation to velocity.

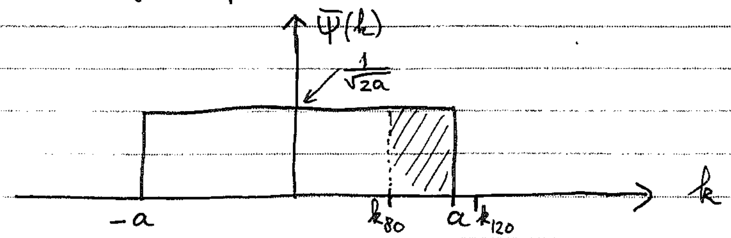
Velocity is proportional to momentum and k-number

$$v = \frac{p}{m} = \frac{\hbar k}{m}$$

We must therefore evaluate this state using the Fourier transform $\bar{\Psi}(k)$ of the state $\Psi(x)$

$$\bar{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x)\, e^{-ikx}\, dx = \begin{cases} \frac{1}{\sqrt{2a}}, & |k| \leq a \\ 0, & |k| > a \end{cases},$$

where we used the standard Fourier transform on p. 1 of the problem set.



The probability for a measurement result between +80 km/s and 120 km/s is now

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$$P = \int_{k_{80}}^{k_{120}} \bar{\Psi}(k)^* \, \bar{\Psi}(k)\, dk, \quad \text{where}$$

$$k_{80} = \frac{v_{80}\, m_e}{\hbar} \quad \text{for} \quad v_{80} = 80 \text{ km/s} \quad \text{and}$$

$$k_{120} = \frac{v_{120}\, m_e}{\hbar} \quad \text{for} \quad v_{120} = 120 \text{ km/s}.$$

To evaluate this integral, we need to compare k_{80} and k_{120} to a (also sketched in figure, not to scale)

$$\left.\begin{aligned} a &= 10^9 \text{ m}^{-1} \\ k_{80} &= \frac{80 \cdot 10^3 \cdot 9.1 \cdot 10^{-31}}{1.055 \cdot 10^{-34}} = 0.690 \cdot 10^9 \text{ m}^{-1} \\ k_{120} &= \frac{120 \cdot 10^3 \cdot 9.1 \cdot 10^{-31}}{1.055 \cdot 10^{-34}} = 1.035 \cdot 10^9 \text{ m}^{-1} \end{aligned}\right\} k_{80} < a < k_{120} \Rightarrow$$

$$P = \int_{k_{80}}^{a} \left(\frac{1}{\sqrt{2a}}\right)^2 dk = \frac{1}{2a}(a - k_{80})$$

$$= \frac{1}{2}\left(\frac{1 - 0.69}{1}\right) = 0.155$$

So, probability is $\underline{15.5\ \%}$

Problem 2

a) $\hat{H}$ and $\hat{A}$ commute when $[\hat{H},\hat{A}] = \hat{H}\hat{A} - \hat{A}\hat{H} = 0 \Rightarrow$

$$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix} - \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix} = \begin{pmatrix} -aE_0 & aT \\ -aT & aE_0 \end{pmatrix} - \begin{pmatrix} -aE_0 & -aT \\ aT & aE_0 \end{pmatrix} = \begin{pmatrix} 0 & +2aT \\ -2aT & 0 \end{pmatrix}$$

$\neq \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \Rightarrow \hat{H}$ and $\hat{A}$ do <u>not</u> commute

(We give here full derivation, but only proof, given the eigenstates was sufficient)

b) We need to solve the eigen value problem

$$\hat{H}|\varphi_i\rangle = E_i|\varphi_i\rangle \Rightarrow \begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E_i\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \Rightarrow$$

For eigen values Solve $\begin{vmatrix} E_0 - E_i & T \\ T & E_0 - E_i \end{vmatrix} = 0 \Rightarrow$

$$(E_0 - E_i)^2 - T^2 = 0 \Rightarrow E_i^2 - 2E_0E_i + E_0^2 - T^2 = 0 \Rightarrow$$

$$E_i = \frac{2E_0 \pm \sqrt{4E_0^2 - 4(E_0^2 - T^2)}}{2} = E_0 \pm T$$

The eigen states that belong to these two eigen values:

$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = (E_0 + T)\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ solving for c_1 and c_2 gives $c_1 = c_2 \Rightarrow$ <u>normalized</u> eigenstate is

$e^{i\varphi}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$ is eigen state for eigenvalue $E_0 + T$

where we can choose the global phase $\varphi = 0 \Rightarrow \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

Similar for the eigenvalue: $E_0 - T$

$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = (E_0 - T)\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$; Solve again for c_1 and $c_2 \Rightarrow$ (let's fully write it out this time)

$$\begin{cases} E_0c_1 + Tc_2 - E_0c_1 + Tc_1 = 0 \\ Tc_1 + E_0c_2 - E_0c_2 + Tc_2 = 0 \end{cases} \Rightarrow \begin{cases} T(c_1 + c_2) = 0 \\ T(c_1 + c_2) = 0 \end{cases} \Rightarrow$$

$c_1 = -c_2 \Rightarrow$ For normalized state and global phase that makes c_1 real and positive this gives $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$

$T < 0$, therefore $(E_0 + T) < (E_0 - T) \Rightarrow$

ground state is $|\varphi_g\rangle$ with $E_g = E_0 + T$

excited state is $|\varphi_e\rangle$ with $E_e = E_0 - T$

c) The state that we need to calculate the probability for is $|\varphi_L\rangle$

c-i) $P = |\langle\varphi_L|\varphi_g\rangle|^2 = |\langle\varphi_L|(\frac{1}{\sqrt{2}}|\varphi_L\rangle + \frac{1}{\sqrt{2}}|\varphi_R\rangle)|^2$

$= |\frac{1}{\sqrt{2}} + 0|^2 = \frac{1}{2}$ OR in matrix notation

$$P = \left|(1\ 0)\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}\right|^2 = \frac{1}{2}$$

c-ii) $P = \left| (1\ 0) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \right|^2 = \frac{1}{2}$

c-iii) $P = \left| (1\ 0) \cdot \left(\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \right) \frac{1}{\sqrt{2}} \right|^2 = \left| (1\ 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 = 1$

c-iv) $P = \left| \langle \varphi_L | \left(\frac{1}{\sqrt{2}} |\varphi_g\rangle - \frac{1}{\sqrt{2}} |\varphi_e\rangle \right) \right|^2 = \left| \langle \varphi_L | \varphi_R \rangle \right|^2 = 0$

d) $\langle \varphi_g | \hat{A} | \varphi_g \rangle = \left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}} \right) \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = 0 \Rightarrow$ expectation value for position is zero for system in state $|\varphi_g\rangle$

$\langle \varphi_e | \hat{A} | \varphi_e \rangle = \left(\frac{1}{\sqrt{2}}\ -\frac{1}{\sqrt{2}} \right) \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = 0$ " " " $|\varphi_e\rangle$

$\langle \varphi_g | \hat{A} | \varphi_e \rangle = \left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}} \right) \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = -a$

$\langle \varphi_e | \hat{A} | \varphi_g \rangle = \left(\frac{1}{\sqrt{2}}\ -\frac{1}{\sqrt{2}} \right) \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = -a$

When the system is in a superposition of $|\varphi_g\rangle$ and $|\varphi_e\rangle$ the expectation value for position can be different from zero.

e) The state at $t=0$ is denoted as $|\psi_0\rangle = |\varphi_L\rangle = \frac{1}{\sqrt{2}}(|\varphi_g\rangle + |\varphi_e\rangle)$ since the measurement result was "left" $= -a$.

For investigating time evolution of $\langle \hat{A} \rangle$, describe the state of the system as a superposition of energy eigen states:

$$\langle \hat{A}(t) \rangle = \langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \psi_0 | \hat{U}^\dagger \hat{A} \hat{U} | \psi_0 \rangle$$

with $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t} \Rightarrow$

$$\langle \hat{A}(t) \rangle = \frac{1}{2} \left(\langle \varphi_g | + \langle \varphi_e | \right) \hat{U}^\dagger \hat{A} \hat{U} \left(|\varphi_g\rangle + |\varphi_e\rangle \right)$$

$$= \frac{1}{2} \left(e^{+i\omega_g t} \langle \varphi_g | + e^{+i\omega_e t} \langle \varphi_e | \right) \hat{A} \left(e^{-i\omega_g t} |\varphi_g\rangle + e^{-i\omega_e t} |\varphi_e\rangle \right)$$

(where $\omega_g = E_g/\hbar$ and $\omega_e = E_e/\hbar$)

$$= \frac{1}{2} \left(\langle \varphi_g | \hat{A} | \varphi_g \rangle + \langle \varphi_e | \hat{A} | \varphi_e \rangle + e^{+i(\omega_g - \omega_e)t} \langle \varphi_g | \hat{A} | \varphi_e \rangle + e^{+i(\omega_e - \omega_g)t} \langle \varphi_e | \hat{A} | \varphi_g \rangle \right)$$

$$= \frac{1}{2} \left(0 + 0 + e^{-i(\omega_e - \omega_g)t}(-a) + e^{+i(\omega_e - \omega_g)t}(-a) \right)$$

$$= -\frac{1}{2} a \, 2 \cos\left((\omega_e - \omega_g) t \right)$$

$$= -a \cos\left((\omega_e - \omega_g) t \right) = -a \cos\left(\frac{2|T|}{\hbar} \cdot t \right)$$

The system oscillates between the two wells, and (as it should be) the dynamics starts at position $-a$ for $t=0$. The amplitude is a, so the particle goes from $-a$ to $+a$ and back and so forth.

The angular frequency is set by the strength of the tunnel coupling $|T|$, and equal to $\frac{2|T|}{\hbar}$.

Problem 3

a) a-i) With the result of problem 2c (or calculate directly, see problem 3d)

$P_{L1} = \frac{1}{2}$, $P_{L2} = \frac{1}{2}$, so both particles in left well has probability $P_{LL} = P_{L1} \cdot P_{L2} = \frac{1}{4}$

a-ii) As for a-i), $P_{L1} = \frac{1}{2}$, $P_{L2} = \frac{1}{2}$, so $P_{LL} = \frac{1}{4}$

b) b-i) Need to proof $\hat{H}|\psi_T\rangle_{c\alpha} = (E_g + E_e)|\psi_T\rangle_{c\alpha} \Rightarrow$

$$\hat{H}|\psi_T\rangle_{c\alpha} = \hat{H}|\varphi_{g1}\rangle|\varphi_{e2}\rangle = (\hat{H}_1 + \hat{H}_2)|\varphi_{g1}\rangle|\varphi_{e2}\rangle$$

$$= (E_g|\varphi_{g1}\rangle)|\varphi_{e2}\rangle + |\varphi_{g1}\rangle(E_e|\varphi_{e2}\rangle)$$

$$= (E_g + E_e)|\varphi_{g1}\rangle|\varphi_{e2}\rangle = (E_g + E_e)|\psi_T\rangle_{c\alpha} \quad \text{q.e.d.}$$

b-ii) As for b-i), need to proof $\hat{H}|\psi_T\rangle_{c\beta} = (E_g + E_e)|\psi_T\rangle_{c\beta} \Rightarrow$

$$\hat{H}|\psi_T\rangle_{c\beta} = (\hat{H}_1 + \hat{H}_2)|\varphi_{e1}\rangle|\varphi_{g2}\rangle = E_e|\varphi_{e1}\rangle|\varphi_{g2}\rangle + |\varphi_{e1}\rangle E_g|\varphi_{g2}\rangle = (E_g + E_e)|\psi_T\rangle_{c\beta}$$

b-iii) Need to proof $\hat{H}|\psi_T\rangle_{\alpha\beta} = (E_g + E_e)|\psi_T\rangle_{\alpha\beta} \Rightarrow$

$$\hat{H}|\psi_T\rangle_{\alpha\beta} = (\hat{H}_1 + \hat{H}_2)(\alpha|\varphi_{g1}\rangle|\varphi_{e2}\rangle + \beta|\varphi_{e1}\rangle|\varphi_{g2}\rangle)$$

$$= \alpha((E_g + E_e)|\varphi_{g1}\rangle|\varphi_{e2}\rangle) + \beta((E_g + E_e)|\varphi_{e1}\rangle|\varphi_{g2}\rangle)$$

$$= (E_g + E_e)(\alpha|\psi_T\rangle_{c\alpha} + \beta|\psi_T\rangle_{c\beta}) = (E_g + E_e)|\psi_T\rangle_{\alpha\beta} \quad \underline{\text{q.e.d.}}$$

c) Exchanging particles means putting all cases of particle 1 in state (or orbital) $|\varphi_{g1}\rangle$ into $|\varphi_{e2}\rangle$ (so it becomes $|\varphi_{e1}\rangle$) and $|\varphi_{e1}\rangle$ into $|\varphi_{g2}\rangle$, and vice versa for particle 2

$$|\psi_T\rangle_S = \frac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle + \frac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle \xleftrightarrow{\text{exchange}}$$

$$\frac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle + \frac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle =$$

$$\frac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle + \frac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle = +|\psi_T\rangle_S$$

So $|\psi_T\rangle_S$ is symmetric under exchange of particles

$$|\psi_T\rangle_{AS} = \frac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle - \frac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle \xleftrightarrow{\text{exchange}}$$

$$\frac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle - \frac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle =$$

$$-\frac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle + \frac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle = -|\psi_T\rangle_{AS}$$

So $|\psi_T\rangle_{AS}$ is anti-symmetric under exchange of two identical particles.

d) We need to minimize $\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$ under variation of b.

Note that $\langle\psi|\psi\rangle$ always equals 1 if we always use $A=\left(\frac{2b}{\pi}\right)^{1/4}$ (from question b)), so we only need to minimize $\langle\psi|\hat{H}|\psi\rangle$ in that case, that is solve $\frac{d(\langle\psi|\hat{H}|\psi\rangle)}{db}=0$.

$$\langle\psi|\hat{H}|\psi\rangle = \langle\psi|\hat{T}|\psi\rangle + \langle\psi|\hat{V}|\psi\rangle .$$

$$\langle\psi|\hat{V}|\psi\rangle = \sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\left(\tfrac{1}{2}m\omega_0^2x^2\right)e^{-bx^2}\,dx$$

$$= \sqrt{\frac{2b}{\pi}}\,\frac{\frac{1}{2}m\omega_0^2}{2b}\int_{-\infty}^{\infty} 2bx^2\, e^{-2bx^2}\frac{1}{\sqrt{2b}}\,d(\sqrt{2b}x)$$

$$= \sqrt{\frac{2b}{\pi}}\,\frac{\frac{1}{2}m\omega_0^2}{2b}\,\frac{1}{\sqrt{2b}}\cdot\frac{1}{2}\sqrt{\pi} = \frac{m\omega_0^2}{8b}$$

$$\langle\psi|\hat{T}|\psi\rangle = \sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)e^{-bx^2}\,dx$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\left(-2be^{-bx^2}+4b^2x^2e^{-bx^2}\right)dx$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} -2be^{-2bx^2} + 4b^2x^2e^{-2bx^2}\,dx$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\left(-2b\int_{-\infty}^{\infty} e^{-2bx^2}\frac{1}{\sqrt{2b}}\,d(\sqrt{2b}x) + 2b\int_{-\infty}^{\infty}(\sqrt{2b}x)^2e^{-(\sqrt{2b}x)^2}\frac{1}{\sqrt{2b}}\,d(\sqrt{2b}x)\right)$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\left(\frac{-2b\sqrt{\pi}}{\sqrt{2b}} + \frac{2b\,\frac{1}{2}\sqrt{\pi}}{\sqrt{2b}}\right) = \frac{\hbar^2 b}{2m}$$

$$\Rightarrow \langle\psi|\hat{H}|\psi\rangle = \frac{m\omega_0^2}{8b} + \frac{\hbar^2 b}{2m} \Rightarrow$$

$$\frac{d(\langle\psi|\hat{H}|\psi\rangle)}{db} = \frac{d}{db}\left(\frac{m\omega_0^2}{8b}+\frac{\hbar^2 b}{2m}\right) = \frac{\hbar^2}{2m} - \frac{m\omega_0^2}{8b^2} = 0 \Rightarrow$$

$$\omega_0^2 = \frac{8\hbar^2b^2}{2m} \Rightarrow b = \frac{m\omega_0}{2\hbar} \Rightarrow$$

$$\langle\psi|\hat{T}|\psi\rangle = \frac{\hbar^2 b}{2m} = \frac{1}{4}\hbar\omega_0$$

$$\langle\psi|\hat{V}|\psi\rangle = \frac{m\omega_0^2}{8b} = \frac{1}{4}\hbar\omega_0$$

$$\langle\psi|\hat{H}|\psi\rangle = E_0 = \frac{1}{2}\hbar\omega_0$$ (agrees indeed with harmonic oscillator ground state)

$$A = \left(\frac{2b}{\pi}\right)^{1/4} = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4}$$

e) $\langle T\rangle = \frac{1}{4}\hbar\omega_0$, $\langle\hat{V}\rangle = \frac{1}{4}\hbar\omega_0$ (see d))

Heisenberg states $\Delta x\,\Delta p \geq \hbar/2$, so if the particle was truly at the bottom of the well, this would give $\langle\hat{V}\rangle = 0$ with $\Delta x = 0$. Then, Δp must be very high, so $\langle\hat{T}\rangle$ very high and this high energy cost for $\langle\hat{T}\rangle$ makes that it is not the ground state. Instead, a trade off with both $\langle T\rangle$ and $\langle\hat{V}\rangle$ a bit more than zero gives a state with minimal energy.

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d) Probability P_{LL} for both in the left well at $-a$:

d-i) $$P_{LL} = \left| \langle\varphi_{L1}|\langle\varphi_{L2}|\left(|\Psi_T\rangle_S\right)\right|^2$$

$$= \left| \langle\varphi_{L1}|\langle\varphi_{L2}|\left(\tfrac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle + \tfrac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle\right)\right|^2$$

$$= \left| \langle\varphi_{L1}|\langle\varphi_{L2}|\left(\tfrac{1}{2\sqrt{2}}(|\varphi_{L1}\rangle + |\varphi_{R1}\rangle)(|\varphi_{L2}\rangle - |\varphi_{R2}\rangle) + \tfrac{1}{2\sqrt{2}}(|\varphi_{L1}\rangle - |\varphi_{R1}\rangle)(|\varphi_{L2}\rangle + |\varphi_{R2}\rangle)\right)\right|^2$$

$$= \Big| \langle\varphi_{L1}|\langle\varphi_{L2}|\Big(\tfrac{1}{2\sqrt{2}}\big(|\varphi_{L1}\rangle|\varphi_{L2}\rangle - |\varphi_{L1}\rangle|\varphi_{R2}\rangle + |\varphi_{R1}\rangle|\varphi_{L2}\rangle - |\varphi_{R1}\rangle|\varphi_{R2}\rangle$$
$$+ |\varphi_{L1}\rangle|\varphi_{L2}\rangle + |\varphi_{L1}\rangle|\varphi_{R2}\rangle - |\varphi_{R1}\rangle|\varphi_{L2}\rangle - |\varphi_{R1}\rangle|\varphi_{R2}\rangle\big)\Big)\Big|^2$$

$$= \left|\tfrac{1}{2\sqrt{2}}\left(1 - 0 + 0 - 0 + 1 + 0 - 0 - 0\right)\right|^2 = \left(\frac{2}{2\sqrt{2}}\right)^2 = \frac{1}{2}$$

d-ii) $$P_{LL} = \left| \langle\varphi_{L1}|\langle\varphi_{L2}|\left(|\Psi_T\rangle_{AS}\right)\right|^2$$

$$= \left| \langle\varphi_{L1}|\langle\varphi_{L2}|\left(\tfrac{1}{\sqrt{2}}|\varphi_{g1}\rangle|\varphi_{e2}\rangle + \tfrac{1}{\sqrt{2}}|\varphi_{e1}\rangle|\varphi_{g2}\rangle\right)\right|^2$$

$$= \Big| \langle\varphi_{L1}|\langle\varphi_{L2}|\Big(\tfrac{1}{2\sqrt{2}}\big(|\varphi_{L1}\rangle|\varphi_{L2}\rangle - |\varphi_{L1}\rangle|\varphi_{R2}\rangle + |\varphi_{R1}\rangle|\varphi_{L2}\rangle - |\varphi_{R1}\rangle|\varphi_{R2}\rangle$$
$$- |\varphi_{L1}\rangle|\varphi_{L2}\rangle - |\varphi_{L1}\rangle|\varphi_{R2}\rangle + |\varphi_{R1}\rangle|\varphi_{L2}\rangle - |\varphi_{R1}\rangle|\varphi_{R2}\rangle\big)\Big)\Big|^2$$

$$= \left|\tfrac{1}{2\sqrt{2}}\left(1 - 0 + 0 - 0 - 1 - 0 + 0 + 0\right)\right|^2 = 0$$

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Problem 4

a) $\hat{H} = \hat{T} + \hat{V}$ (kinetic + ~~p~~potential energy)

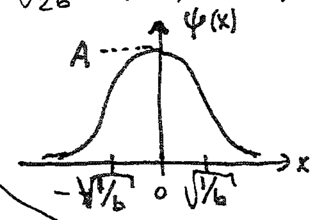
In x-representation, with constants used being $m, \omega_0 \Rightarrow$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2$$

b) $$\int_{-\infty}^{\infty} \varphi^*(x)\,\varphi(x)\,dx = 1 \quad \text{when normalized} \Rightarrow$$

$$\int_{-\infty}^{\infty} A^2 e^{-2bx^2}\,dx = 1 \Rightarrow A^2\int_{-\infty}^{\infty} e^{-(\sqrt{2b}x)^2}\frac{1}{\sqrt{2b}}\,d(\sqrt{2b}x) = 1 \Rightarrow$$

$$A^2\frac{1}{\sqrt{2b}}\sqrt{\pi} = 1 \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$$



c) Say $|\varphi\rangle = \sum_{n=0}^{\infty} c_n|\chi_n\rangle \Rightarrow$

$$\frac{\langle\varphi|\hat{H}|\varphi\rangle}{\langle\varphi|\varphi\rangle} = \frac{\sum_n E_n|c_n|^2}{\sum_n|c_n|^2} > \frac{\sum_n E_0|c_n|^2}{\sum_n|c_n|^2}$$

$$= E_0\frac{\sum_n|c_n|^2}{\sum_n|c_n|^2} = E_0 \qquad \text{q.e.d.}$$

since all $E_n > E_0$ for $n > 0$