Suggested Solutions, FY2045 2019

December 2019

Problem 1)

Which of the following statements are correct ?
Velg ett eller flere alternativer:

- [ ] The (time-dependent) Schrödinger equation is not deterministic
- [ ] Quantum mechanics can always predict the outcome of a single experiment
- [x] The (time-dependent) Schrödinger equation is determenistic ✓
- [ ] Quantum mechanics can never predict the outcome of a single experiment
- [x] Quantum mechanics can sometimes predict the outcome of a single experiment ✓

The time-dependet Schrödinger equation is deterministic. $\Psi(t_0 + t)$ is fully determined by $\Psi(t_0)$ evolving in time according to the Schrödinger equation. So this is trivially true. If a system is in a known eigenstate with respect to a given observable then measurement of that observable will yield the eigenvalue of that eigenstate. E.g. if the a fermion is in the spin up state (z_+, eigenvalue equals $+1$) then measuring the spin will give the eigenvalue $+1$ with certainty. Hence sometimes the outcome of a single experiment is predictable.

Problem 2)

The dimension of the Hilbert space of a particle in a two-dimensional infinite square well is

infinite ✓ .

The dimension of the Hilbert subspace for the spin degrees of freedom for a system of 3 spin 1/2 particles is

8 ✓ .

If two angular momenta with J_1 = 3/2 and J_2 = 3 are coupled. The resulting dimension of the Hilbert space of the angular momentum of the coupled system is 28 ✓ .

The dimension of the Hilbert space equals the possible states a system can be found by measurment. For a particle in a box there are is a infinite number of bound states so the dimension of the Hilbert space is infinite. 3 spin 1/2 particles can be found in 8 different states (2^n), hence the dimension of the subspace for the spin degrees of freedom is 8. For $J_1 = 3/2$ and $J_2 = 3$ the Hilbert space dimension of each are given by the multiplicity (2J+1), i.e. 4 and 7. The dimension for the coupled system is then given by 4 time 7 which equals 28.

Problem 3) If you checked answer three here no points were subtracted.

Considering a time dependent Hamiltonian of the form $\hat{H}(t) = \hat{H}_0 + V(t)$, choose the correct statements below.

Velg ett eller flere alternativer:

- [x] If the Hamiltonian is time-dependent, it is not possible to find stationary solutions, i.e. there are no solutions where it is possible to write the wavefunction as a product of a time-dependent part and a time-independent part. ✔
- [x] Time-dependent perturbation theory is valid for small perturbation and/or for short times. ✔
- [ ] If the Hamiltonian depends on time, the time dependence of the wavefunction can be written as:

  $\Psi(x,t) = \sum_n c_n \psi_n \exp[-iE_n t/\hbar]$

  where ψ_ns are solution of the time-independent (unperturbed) Hamiltonian.
- [ ] If the Hamiltonian is time-dependent, time evolution is no longer given by the Schrödinger equation and one may use time-dependent perturbation theory to find approximate describtion of the time evolution.

Problem 4) Here it is important to remember that there are three quantum number (n,l,m) and

The state of a particle in a sperical box with the potential:

$$V(r) = \begin{cases} 0 & \text{for} \quad r < a \\ \infty & \text{for} \quad r > a \end{cases}$$

is characterized my the three quantum numbers n, l and m. If five non-interacting identical spin 1/2-fermions with mass m, are put into a box with radius a, what is the total ground state energy (rounded) of the system? (Check the formula sheet)

Velg ett alternativ:

- ( ) $E_{tot} = \frac{5\hbar^2\pi^2}{2ma^2}$
- ( ) $E_{tot} = \frac{33\hbar^2}{2ma^2}$
- (•) $E_{tot} = \frac{80\hbar^2}{2ma^2}$ ✔
- ( ) $E_{tot} = \frac{93\hbar^2}{2ma^2}$

thus a m-degeneracy, as hinted in the problem description. Thus the correct result is obtained by $2 * \pi^2 + 3 * 4.5^2 \approx 80$.

Problem 5)

5a)

$$\begin{aligned}\frac{d\langle\hat{A}\rangle}{dt} = \frac{d}{dt}\langle\Psi|\hat{A}|\Psi\rangle = \frac{d}{dt}\int \Psi^*\hat{A}\Psi d\Gamma \\ = \int\left(\frac{d\Psi}{dt}\right)^*\hat{A}\Psi d\Gamma + \underbrace{\int\Psi^*\left(\frac{d\hat{A}}{dt}\right)\Psi d\Gamma}_{=\left\langle\frac{d\hat{A}}{dt}\right\rangle} + \int\Psi^*\hat{A}\left(\frac{d\Psi}{dt}\right)d\Gamma = \\ = \left\langle\frac{d\hat{A}}{dt}\right\rangle + \int\left[\left(\frac{d\Psi}{dt}\right)^*\hat{A}\Psi + \Psi^*\hat{A}\left(\frac{d\Psi}{dt}\right)\right]d\Gamma\end{aligned} \tag{1}$$

From the Schrödinger equation we have:

$$\frac{d\Psi}{dt} = \frac{1}{i\hbar}\hat{H}\Psi = -\frac{i}{\hbar}\hat{H}\Psi \tag{2}$$

Inserting into (1) gives:

$$\frac{d\langle\hat{A}\rangle}{dt} = \left\langle\frac{d\hat{A}}{dt}\right\rangle + \int\left[\left(-\frac{i}{\hbar}\hat{H}\Psi\right)^*\hat{A}\Psi + \Psi^*\hat{A}\left(-\frac{i}{\hbar}\hat{H}\Psi\right)\right]d\Gamma \tag{3}$$

Using that the Hamiltonian is hermitian:

$$\left(\hat{H}\Psi\right)^* = \Psi^*\hat{H} \tag{4}$$

we find:

$$\begin{aligned}\frac{d\langle\hat{A}\rangle}{dt} &= \left\langle\frac{d\hat{A}}{dt}\right\rangle + \frac{i}{\hbar}\int\Psi^*(\hat{H}\hat{A} - \hat{A}\hat{H})\Psi d\Gamma \\ &= \left\langle\frac{d\hat{A}}{dt}\right\rangle + \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle\end{aligned} \tag{5}$$

.

5b)

Starting from the expression given in 5a), the time evolution of $\langle\hat{x}\rangle$ is given by:

$$\frac{d\langle\hat{x}\rangle}{dt} = \left\langle\frac{d\hat{x}}{dt}\right\rangle + \frac{i}{\hbar}\langle[\hat{H},\hat{x}]\rangle \tag{6}$$

The first term on the r.h.s. is 0 since $\langle\hat{x}\rangle$ does not depend on time. The commutator in the second term on the r.h.s. is:

$$\left\langle[\hat{H},\hat{x}]\right\rangle = \left\langle\left[\frac{\hat{p}^2}{2m} + V(x),\hat{x}\right]\right\rangle = \left\langle\left[\frac{\hat{p}^2}{2m},\hat{x}\right]\right\rangle, \tag{7}$$

since the position operator commutes with $V(x)$. Further:

$$\frac{i}{\hbar}\left\langle\left[\frac{\hat{p}^2}{2m},\hat{x}\right]\right\rangle = -\frac{i}{2m\hbar}\langle[\hat{x},\hat{p}]\hat{p} + \hat{p}[\hat{x},\hat{p}]\rangle = -\frac{2i^2\hbar}{2m\hbar}\langle\hat{p}\rangle = \frac{\langle\hat{p}\rangle}{m} \tag{8}$$

Thus:

$$m\frac{\langle\hat{x}\rangle}{dt} = \langle\hat{p}\rangle \tag{9}$$

In the second last step we used that $[\hat{x},\hat{p}] = i\hbar$ and the commutator relation given in the support sheet:

$$\left[\hat{A},\hat{B}\hat{C}\right] = \left[\hat{A},\hat{B}\right]\hat{C} + \hat{B}\left[\hat{A},\hat{C}\right] \tag{10}$$

For the time evolution of $\langle \hat{p} \rangle$ we have:

$$\frac{d\langle \hat{p}\rangle}{dt} = \left\langle \frac{d\hat{p}}{dt} \right\rangle + \frac{i}{\hbar}\langle [\hat{H}, \hat{p}] \rangle = \frac{i}{\hbar}\left\langle \left[\frac{\hat{p}^2}{2m} + V(x), \hat{p}\right] \right\rangle = \frac{i}{\hbar}\langle [V(x), \hat{p}] \rangle \tag{11}$$

The operator for momentum is:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \tag{12}$$

Inserting (12) into (11), and writing out the commutator:

$$\frac{i}{\hbar}\langle [V(x), \hat{p}] \rangle = \int \Psi^* V(x) \frac{\partial}{\partial x} \Psi d\Gamma - \int \Psi^* \frac{\partial}{\partial x} V(x) \Psi d\Gamma$$

$$= \int \Psi^* V(x) \frac{\partial}{\partial x} \Psi d\Gamma - \int \Psi^* \left(\frac{\partial V(x)}{\partial x} \right) \Psi d\Gamma - \int \Psi^* V(x) \frac{\partial \Psi}{\partial x} d\Gamma \tag{13}$$

$$= \int \Psi^* \left(\frac{\partial V(x)}{\partial x} \right) \Psi d\Gamma = -\langle V'(x) \rangle = \frac{d\langle \hat{p}\rangle}{dt}$$

5c i) For a free particle the potential is zero we thus have:

$$V(x) = 0 \Longrightarrow \frac{d\langle \hat{p}\rangle}{dt} = 0 \Longrightarrow \langle \hat{p}\rangle_t = \langle p_0 \rangle$$

$$\frac{d\langle \hat{x}\rangle}{dt} = \frac{1}{m}\frac{d\langle \hat{p}\rangle}{dt} \Longrightarrow \langle x\rangle_t = \langle x_0 \rangle + \frac{\langle p_0 \rangle}{m} t \tag{14}$$

The expectation value of position changes linearly in time, analogous to classical mechanics.

ii) In this case we have:

$$V(x) = -Fx \Longrightarrow \frac{d\langle \hat{p}\rangle}{dt} = F \Longrightarrow \langle \hat{p}\rangle_t = \langle p_0 \rangle + Ft$$

$$\langle \hat{x}\rangle_t = \langle x_0 \rangle + \frac{\langle p_0 \rangle}{m} t + \frac{1}{2} F t^2 \tag{15}$$

This shows a constant acceleration, analogous to classical mechanics.

Problem 6

6a)

$$\begin{aligned} &(H_0 + \lambda\delta(x - L/2)) \left(|\psi_n^{(0)}\rangle + \lambda \left|\psi_n^{(1)}\right\rangle + \mathcal{O}\left(\lambda^2\right) \right) \\ &= \left(E_n^0 + \lambda E_n^{(1)} + \mathcal{O}\left(\lambda^2\right) \right) \left(|\psi_n^{(0)}\rangle + \lambda \left|\psi_n^{(1)}\right\rangle + \mathcal{O}\left(\lambda^2\right) \right) \end{aligned} \tag{16}$$

Multiplication and ordering terms according to the power of λ:

$$\left(H_0 - E_n^0\right) |\psi_n^{(0)}\rangle + \lambda \left(H_0 - E_n^0\right) \left|\psi_n^{(1)}\right\rangle + \lambda \left(\delta(x - L/2) - E_n^{(1)} \right) |\psi_n^{(0)}\rangle + (O)\left(\lambda^2\right) = 0 \tag{17}$$

Importantly, the equation has to hold for any choice of lambda, hence we have:

$$\left(H_0 - E_n^0\right) |\psi_n^{(0)}\rangle = 0$$

$$\left(H_0 - E_n^0\right) \left|\psi_n^{(1)}\right\rangle + \left(\delta(x - L/2) - E_n^{(1)} \right) |\psi_n^{(0)}\rangle = 0 \tag{18}$$

6b)

Multiplying the first order equation by $\langle\psi_n^{(0)}|$ from the left:

$$\left\langle \psi_n^{(0)} \left| \left(H_0 - E_n^0\right) \right| \psi_n^{(1)} \right\rangle + \left\langle \psi_n^{(0)} \left| \left(\delta(x - L/2) - E_n^{(1)} \right) \right| \psi_n^{(0)} \right\rangle = 0 \tag{19}$$

Using that $\left\langle \psi_n^{(0)} \right| H_0 = \langle\psi_n^{(0)}| E_n^0$, the first term is zero:

$$\left\langle \psi_n^{(0)} \left| \left(\delta(x - L/2) - E_n^{(1)} \right) \right| \psi_n^{(0)} \right\rangle = 0 \tag{20}$$

Using $\langle n|m\rangle = \delta_{nm}$ we have:

$$E_n^{(1)} = \langle\psi_n^{(0)}|\lambda\delta(x - L/2)|\psi_n^{(0)}\rangle \tag{21}$$

6c)

$$\begin{aligned}
\lambda E_1^{(1)} &= \langle 1|\lambda\delta(x - L/2)|1\rangle \\
&= \lambda\frac{2}{L}\int_0^L \sin\frac{\pi x}{L}\delta(x - L/2)\sin\frac{\pi x}{L}\mathrm{d}x \\
&= \lambda\frac{2}{L}\sin^2\frac{\pi}{2} \\
&= \lambda\frac{2}{L}
\end{aligned} \tag{22}$$

6d)

The first excited state, and all other states where n is an even number, have a zero at x = L/2. Consequently, the particle has zero probability of being at the location of the delta function perturbation, which means that it is unaffected by the perturbation. Hence, the energy corrections are zero.

Problem 7

7a)

$$|x_0\rangle = C\begin{pmatrix} 1+2i \\ 4-2i \end{pmatrix} \tag{23}$$

$$\begin{aligned}
\langle x_0|x_0\rangle &= |C|^2\left\{|1+2i|^2 + |4-2i|^2\right\} \\
&= |C|^2\left\{1^2 + 2^2 + 4^2 + 2^2\right\} = 25|C|^2 \\
\implies C &= \frac{1}{5}
\end{aligned} \tag{24}$$

7b)

$$\begin{aligned}
\left\langle \hat{S}_z \right\rangle_x &= \frac{\hbar}{2}\langle\sigma_z\rangle_{x_0} = \frac{\hbar}{2\cdot 25}(1-2i \quad 4+2i)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1+2i \\ 4-2i \end{pmatrix} \\
&= \frac{\hbar}{50}\{(1-2i)(1+2i) + (4+2i)(-4+2i)\} = -\frac{3}{10}\hbar
\end{aligned} \tag{25}$$

7c) Θ is given to be $\pi/4$ and we can take $\phi = 0$. Thus we have $n_x = \sin\Theta$, $n_y = 0$ and $n_z = \cos\Theta$. From this we have for $\hat{\sigma}_n$:

$$\hat{\sigma}_n = \hat{\sigma}_x\sin\Theta + \hat{\sigma}_z\cos\Theta = \begin{pmatrix} \cos\Theta & \sin\Theta \\ \sin\Theta & -\cos\Theta \end{pmatrix} \tag{26}$$

The eigenvalues must be $\lambda \pm 1$. For $\lambda = 1$ we have:

$$\begin{pmatrix} \cos\Theta & \sin\Theta \\ \sin\Theta & -\cos\Theta \end{pmatrix}|\chi_{n,+}\rangle = \begin{pmatrix} \cos\Theta & \sin\Theta \\ \sin\Theta & -\cos\Theta \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \tag{27}$$

$$a\,(\cos\Theta - 1) + b\sin\Theta = 0$$
$$\Longrightarrow \frac{b}{a} = \frac{1-\cos\Theta}{\sin\Theta} = \frac{\sin\frac{\Theta}{2}}{\cos\frac{\Theta}{2}} \tag{28}$$

Since $\cos^2\alpha + \sin^2\alpha = 1$ it follows that:

$$|\chi_{n,+}\rangle = \begin{pmatrix} \cos\frac{\Theta}{2} \\ \sin\frac{\Theta}{2} \end{pmatrix} \tag{29}$$

$|\chi_{n,-}\rangle$ has to be orthogonal and thus:

$$|\chi_{n,-}\rangle = \begin{pmatrix} \sin\frac{\Theta}{2} \\ -\cos\frac{\Theta}{2} \end{pmatrix} \tag{30}$$

The probabilities of finding the state $|\chi_{n,+}\rangle$ or $|\chi_{n,-}\rangle$ equals the square of the expansion coefficient a_+, a_-:

$$|\chi_{z,+}\rangle = a_+\,|\chi_{n,+}\rangle + a_-\,|\chi_{n,-}\rangle \tag{31}$$

$$\begin{aligned} a_+ &= \langle\chi_{n,+}|\chi_{z,+}\rangle = \cos\tfrac{\Theta}{2} \\ a_- &= \langle\chi_{n,-}|\chi_{z,+}\rangle = \sin\tfrac{\Theta}{2} \end{aligned} \tag{32}$$

Thus the probabilities are:

$$\begin{aligned} P_+ &= \cos^2\tfrac{\pi}{8} = 85\% \\ P_+ &= \sin^2\tfrac{\pi}{8} = 15\% \end{aligned} \tag{33}$$

7d) From the given relations, written in matrix form we have:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0 \tag{34}$$

and

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{35}$$

From eqn. (34) we have:

$$a = -b \quad c = -d \tag{36}$$

From eqn. (35):

$$a - b = 1 \qquad\qquad c - d = 1$$
$$\Longrightarrow \hat{\sigma}_+ = \tfrac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \tag{37}$$