Problem set 2

2.1 Heisenberg's equation of motion

Starting out with the equation of motion for $\hat{x}$, this can be done without the explicit expressions for $\hat{x}$ and $\hat{p}$ in the coordinate representation.

$$\frac{d}{dt}\hat{x} = \frac{i}{\hbar}\left[\hat{H},\hat{x}\right] = \frac{i}{\hbar}\left[\frac{\hat{p}\hat{p}}{2m}+V(\hat{x}),\hat{x}\right] = \frac{i}{\hbar}\left(\left[\frac{\hat{p}\hat{p}}{2m},\hat{x}\right]+\underbrace{[V(\hat{x}),\hat{x}]}_{=0}\right) = \frac{i}{\hbar}\left[\frac{\hat{p}\hat{p}}{2m},\hat{x}\right]$$

Using the relation$[AB,C] = A\,[B,C]+[A,C]\,B$, and $[\hat{x},\hat{p}] = i\hbar$ we get:

$$\frac{d}{dt}\hat{x} = \frac{i}{2m\hbar}\left(\hat{p}\,[\hat{p},\hat{x}]+[\hat{p},\hat{x}]\,\hat{p}\right) = \frac{i}{2m\hbar}\left(\hat{p}\,(-i\hbar)-i\hbar\hat{p}\right) = \frac{\hat{p}}{m} \tag{1}$$

On to the equation of motion for $\hat{p}$:

$$\frac{d}{dt}\hat{p} = \frac{i}{\hbar}\left[\hat{H},\hat{x}\right] = \frac{i}{\hbar}\left[\frac{\hat{p}\hat{p}}{2m}+V(\hat{x}),\hat{p}\right] = \frac{i}{\hbar}\left(\underbrace{\left[\frac{\hat{p}\hat{p}}{2m},\hat{p}\right]}_{=0}+[V(\hat{x}),\hat{p}]\right) = \frac{i}{\hbar}\,[V(\hat{x}),\hat{p}]$$

To get further, we choose the coordinate representation and a wavefunction for the commutator to act on:

$$\begin{aligned}\frac{i}{\hbar}\,[V(\hat{x}),\hat{p}]\,\psi(x) &= \frac{i}{\hbar}\left[V(x),-i\hbar\frac{\partial}{\partial x}\right]\psi(x) = V(x)\frac{\partial}{\partial x}\psi(x)-\frac{\partial}{\partial x}\,[V(x)\psi(x)] \\ &= V(x)\frac{\partial\psi}{\partial x}-\frac{\partial V}{\partial x}\psi(x)-V(x)\frac{\partial\psi}{\partial x} = -\frac{\partial V}{\partial x}\psi(x)\end{aligned}$$

Since the wavefunction $\psi(x)$ was arbitrary, we may remove it and get:

$$\frac{d}{dt}\hat{p} = -\frac{\partial V}{\partial x} \tag{2}$$

Combining (1) and (2), we get:

$$m\frac{d^2\hat{x}}{dt^2} = -\frac{\partial V}{\partial x}$$

Which is on exactly the same form as the classical equation of motion for a particle in a potential $V(x)$.

2.2 Time dependent unitary transform

The states and operators transform under $\hat{U}$ as follows:

$$|\psi(t)\rangle \;\rightarrow\; |\psi'(t)\rangle = \hat{U}(t)|\psi(t)\rangle \tag{3}$$

$$\hat{A} \;\rightarrow\; \hat{A}'(t) = \hat{U}(t)\hat{A}\hat{U}(t)^{-1} \tag{4}$$

We are to show

$$\hat{H} \to \hat{H}'(t) = \hat{U}(t)\hat{H}\hat{U}(t)^{-1} + i\hbar\frac{d\hat{U}}{dt}\hat{U}(t)^{-1}$$

First off, we write down the Schrödinger equation in both frames:

$$\hat{H}|\psi(t)\rangle = i\hbar\frac{d}{dt}|\psi(t)\rangle \tag{5}$$

$$\hat{H}'|\psi'(t)\rangle = i\hbar\frac{d}{dt}|\psi'(t)\rangle \tag{6}$$

Here, the total derivative is used as our states are not in the position representation. Starting with the transformed equation (6), we wish to rewrite the right hand side in terms of $|\psi(t)\rangle$ and $\hat{H}$:

$$\begin{aligned}\hat{H}'|\psi'(t)\rangle &= i\hbar\frac{d}{dt}|\psi'(t)\rangle = i\hbar\frac{d}{dt}\left(\hat{U}(t)|\psi(t)\rangle\right) = i\hbar\frac{d\hat{U}}{dt}|\psi(t)\rangle + i\hbar\hat{U}(t)\frac{d}{dt}|\psi(t)\rangle \\ &\overset{(5)}{=} i\hbar\frac{d\hat{U}}{dt}|\psi(t)\rangle + \hat{U}(t)\hat{H}|\psi(t)\rangle\end{aligned}$$

Next, we wish to get rid of the states, we use (3) and rewrite $|\psi(t)\rangle = \hat{U}(t)^{-1}|\psi'(t)\rangle$ such that our equation becomes:

$$\hat{H}'|\psi'(t)\rangle = i\hbar\frac{d\hat{U}}{dt}\hat{U}(t)^{-1}|\psi'(t)\rangle + \hat{U}(t)\hat{H}\hat{U}(t)^{-1}|\psi'(t)\rangle$$

From where it directly follows that:

$$\hat{H}' = \hat{U}(t)\hat{H}\hat{U}(t)^{-1} + i\hbar\frac{d\hat{U}}{dt}\hat{U}(t)^{-1}$$

Thus, if we assume $|\psi(t)\rangle$ are energy eigenstates in the Schrödinger picture, then equation (5) is turned into: $\hat{H}|\psi(t)\rangle = E|\psi(t)\rangle$, now transforming the state and letting the transformed hamiltonian act on the state gives:

$$\begin{aligned}\hat{H}' &= \left(\hat{U}(t)\hat{H}\hat{U}(t)^{-1} + i\hbar\frac{d\hat{U}}{dt}\hat{U}(t)^{-1}\right)|\psi'(t)\rangle \\ &= E|\psi'(t)\rangle + i\hbar\frac{d\hat{U}}{dt}|\psi(t)\rangle\end{aligned}$$

The transformation changed the Hamiltonian such that the transformed energy eigenstates no longer are eigenstates of this operator and the Hamiltonian doesn't represent energy anymore. We also see from the above calculation that if $\hat{H}' = \hat{U}(t)\hat{H}\hat{U}(t)^{-1}$, it would satisfy $\hat{H}'|\psi'(t)\rangle = E|\psi'(t)\rangle$. Thus $\hat{U}(t)\hat{H}\hat{U}(t)^{-1}$ is the energy operator in the transformed picture, while the one calculated above governs time evolution.

Problem 4.2 (Midtterm exam 2010)
Solutions

a) Assume orthogonality, $\langle\psi_L|\psi_R\rangle = 0$. In this basis the Hamiltonian has the matrix form

$$H = \begin{pmatrix} E_0 & \lambda \\ \lambda & E_0 \end{pmatrix} \tag{1}$$

The eigenvalues E are found from the equation,

$$\begin{vmatrix} E_0 - E & \lambda \\ \lambda & E_0 - E \end{vmatrix} = 0 \quad \Rightarrow \quad (E - E_0)^2 - \lambda^2 = 0 \tag{2}$$

Solutions

$$E_0^\pm = E_0 \pm \lambda \tag{3}$$

Eigenvectors in matrix form

$$\psi_0^\pm = \begin{pmatrix} \alpha_0^\pm \\ \beta_0^\pm \end{pmatrix}, \quad |\alpha_0^\pm|^2 + |\beta_0^\pm|^2 = 1 \tag{4}$$

The coefficients are determined by the eigenvalue equation

$$\begin{aligned} \begin{pmatrix} E_0 & \lambda \\ \lambda & E_0 \end{pmatrix} \begin{pmatrix} \alpha_0^\pm \\ \beta_0^\pm \end{pmatrix} &= E_0^\pm \begin{pmatrix} \alpha_0^\pm \\ \beta_0^\pm \end{pmatrix} \\ &\Rightarrow \\ (E_0 - E_=^\pm)\alpha_0^\pm &= -\lambda\beta_0^\pm \\ &\Rightarrow \\ \alpha_0^\pm = \pm\beta_0^\pm &= \frac{1}{\sqrt{2}} \end{aligned} \tag{5}$$

In bra-ket formulation

$$|\psi_0^\pm\rangle = \frac{1}{\sqrt{2}}(|\psi_L\rangle \pm |\psi_R\rangle) \tag{6}$$

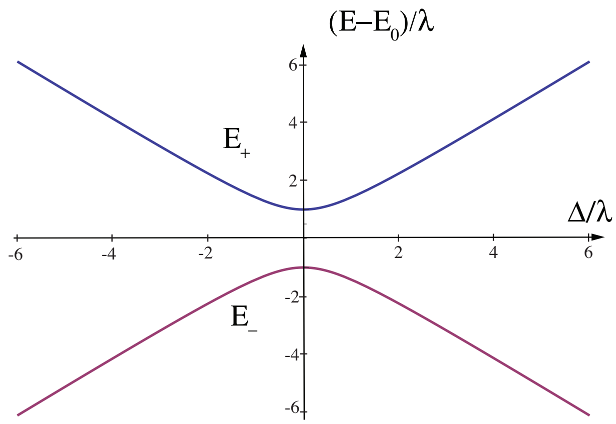
The eigenvectors are the symmetric and antisymmetric combinations of $|\psi_L\rangle$ og $|\psi_R\rangle$. The antisymmetric superposition is lowest in energy. This can be understood as due to a lower possibility for $|\psi_0^-\rangle$ than for $|\psi_0^+\rangle$, to find the N-atom within the potential barrier, where the potential energy is high.

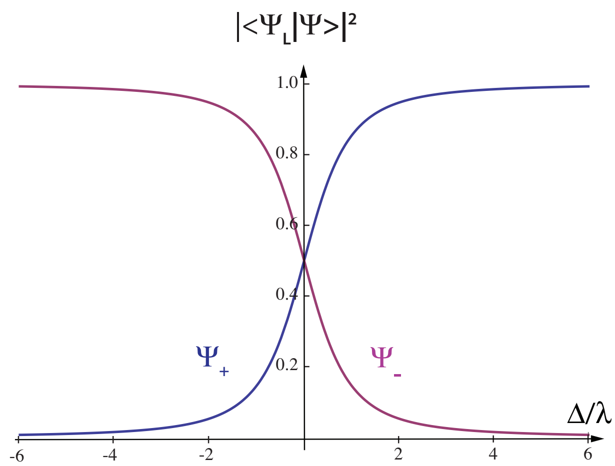
b) New eigenvalue equation

$$\begin{vmatrix} E_0 + \Delta - E & \lambda \\ \lambda & E_0 - \Delta - E \end{vmatrix} = 0 \quad \Rightarrow \quad (E - E_0)^2 = \lambda^2 + \Delta^2 \tag{7}$$

Solutions

$$E_\pm = E_0 \pm \sqrt{\lambda^2 + \Delta^2} \tag{8}$$





c) Eigenvectors, matrix elements

$$\begin{aligned}(E_0 + \Delta - E_\pm)\alpha_\pm + \lambda\beta_\pm &= 0 \quad \Rightarrow \\ (\Delta \mp \sqrt{\lambda^2 + \Delta^2})\alpha_\pm + \lambda\beta_\pm &= 0\end{aligned} \tag{9}$$

Normalized solutions

$$\begin{aligned}\alpha_\pm &= \frac{1}{\sqrt{2\sqrt{\lambda^2+\Delta^2}}}\sqrt{\sqrt{\lambda^2+\Delta^2} \pm \Delta} \\ \beta_\pm &= \pm\frac{1}{\sqrt{2\sqrt{\lambda^2+\Delta^2}}}\sqrt{\sqrt{\lambda^2+\Delta^2} \mp \Delta}\end{aligned} \tag{10}$$

The states in the ket form

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2\sqrt{\lambda^2+\Delta^2}}}\left(\sqrt{\sqrt{\lambda^2+\Delta^2} \pm \Delta}\,|\psi_L\rangle \pm \sqrt{\sqrt{\lambda^2+\Delta^2} \mp \Delta}\,|\psi_R\rangle\right) \tag{11}$$

Overlap

$$|\langle\psi_L|\psi_\pm\rangle|^2 = \frac{1}{2}\left(1 \pm \frac{\Delta}{\sqrt{\lambda^2+\Delta^2}}\right) \tag{12}$$

Avoided crossing: When Δ increases from negative to positive values, the energy difference between the levels decreases, but a direct crossing is avoided by an effective repulsion between the two levels. The minimum energy difference is determined by λ. The eigenvectors are interchanged between the two levels during the avoided crossing, so that the ground state $|\psi_-\rangle$ corresponds to $|\psi_L\rangle$ for large negative Δ and to $|\psi_R\rangle$ for large positive Δ.

d) The Hamiltonian and the states $|\psi_0^\pm\rangle$ in the $\{|\psi_L\rangle, |\psi_R\rangle\}$ basis,

$$\hat{H} = \begin{pmatrix} E_0 + \Delta & \lambda \\ \lambda & E_0 - \Delta \end{pmatrix}, \quad \psi_0^\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \tag{13}$$

Matrix elements of $\hat{H}$ in the $|\psi_0^\pm\rangle$ basis,

$$\begin{aligned} \psi_0^{\pm\dagger} \hat{H} \psi_0^\pm &= \frac{1}{2}(1 \ \pm 1) \begin{pmatrix} E_0 + \Delta & \lambda \\ \lambda & E_0 - \Delta \end{pmatrix} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = E_0 \pm \lambda \\ \psi_0^{\pm\dagger} \hat{H} \psi_0^\mp &= \frac{1}{2}(1 \ \pm 1) \begin{pmatrix} E_0 + \Delta & \lambda \\ \lambda & E_0 - \Delta \end{pmatrix} \begin{pmatrix} 1 \\ \mp 1 \end{pmatrix} = \Delta \end{aligned} \tag{14}$$

In matrix form,

$$\hat{H} = \begin{pmatrix} E_0 + \lambda & \Delta \\ \Delta & E_0 - \lambda \end{pmatrix} = E_0 \mathbb{1} + \lambda \sigma_z + \Delta \sigma_x \tag{15}$$

which in the oscillating electric field, where $\Delta = \Delta_0 \cos \omega t$, gives

$$\hat{H} = E_0 \mathbb{1} + \lambda \sigma_z + \Delta_0 \cos \omega t \sigma_x \tag{16}$$

e) In the rotating wave approximation H takes the following form

$$\begin{aligned} \hat{H} &= E_0 \mathbb{1} + \lambda \sigma_z + \frac{1}{2} \Delta_0 (e^{i\omega t} \sigma_- + e^{-i\omega t} \sigma_+) \\ &= E_0 \mathbb{1} + \lambda \sigma_z + \frac{1}{2} \Delta_0 (\cos \omega t \sigma_x + \sin \omega t \sigma_y) \end{aligned} \tag{17}$$

The form is the same as for the Hamiltonian of a spin-half system in a magnetic field with a constant z-component and a rotating component in the xy-plane. In the lecture notes the Hamiltonian is

$$\hat{H} = \frac{1}{2} \omega_0 \hbar \sigma_z + \frac{1}{2} \omega_1 \hbar (\cos \omega t \sigma_x + \sin \omega t \sigma_y) \tag{18}$$

where ω_0 is proportional with the strength of the constant field component, and ω_1 is proportional to the strength of the rotating component. Comparison with these expressions gives the follwing identifications

$$\lambda = \frac{1}{2} \omega_0 \hbar, \quad \Delta_0 = \omega_1 \hbar \tag{19}$$

In the following this identities will be used. The Hamiltonian (17) has in addition a constant term $E_0 \mathbb{1}$, which is, however, unimportant for the evolution of the system, since it only contributes with a common phase factor for all states. In the following we therefore disregard this term, by setting $E_0 = 0$.

The Hamiltonian is transformed to time independent form by the unitary, time dependent operator

$$\hat{T}(t) = e^{\frac{i}{2}\omega t \sigma_z} \tag{20}$$

The transformed $\hat{H}$ is

$$\begin{aligned} \hat{H}_{\hat{T}} &= \hat{T}(t)\hat{H}\hat{T}(t)^\dagger + i\hbar\frac{d\hat{T}}{dt}\hat{T}(t) \\ &= \frac{1}{2}\hbar\Omega(\cos\theta\sigma_z + \sin\theta\sigma_x) \end{aligned} \tag{21}$$

with

$$\Omega = \sqrt{(\omega-\omega_0)^2+\omega_1^2} = \frac{1}{\hbar}\sqrt{(\omega\hbar-2\lambda)^2+\Delta_0^2} \tag{22}$$

as the Rabi frequency, and with θ determined by the equations

$$\begin{aligned} \cos\theta &= \frac{\omega_0-\omega}{\Omega} = \frac{2\lambda-\Delta_0}{\sqrt{(\omega\hbar-2\lambda)^2+\Delta_0^2}} \\ \sin\theta &= \frac{\omega_1}{\Omega} = \frac{\Delta_0}{\sqrt{(\omega\hbar-2\lambda)^2+\Delta_0^2}} \end{aligned} \tag{23}$$

The resonance frequency is

$$\omega_0 = 2\lambda/\hbar \tag{24}$$

The time evolution operator in the transformed picture is

$$\hat{\mathcal{U}}_T(t) = \cos(\frac{\Omega}{2}t)\mathbb{1} - i\sin(\frac{\Omega}{2}t)(\cos\theta\sigma_z+\sin\theta\sigma_x) \tag{25}$$

and in the Schrödinger picture it is

$$\hat{\mathcal{U}}(t) = e^{-\frac{i}{2}\omega t\sigma_z}\hat{\mathcal{U}}_T(t) = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{26}$$

with matrix elements

$$\begin{aligned} A &= (\cos(\frac{\Omega}{2}t) - i\cos\theta\sin(\frac{\Omega}{2}t))e^{-\frac{i}{2}\omega t} \\ D &= (\cos(\frac{\Omega}{2}t) + i\cos\theta\sin(\frac{\Omega}{2}t))e^{\frac{i}{2}\omega t} \\ B &= -i\sin\theta\sin(\frac{\Omega}{2}t))e^{-\frac{i}{2}\omega t} \\ C &= -i\sin\theta\sin(\frac{\Omega}{2}t))e^{\frac{i}{2}\omega t} \end{aligned} \tag{27}$$

(For details about the derivation we refer to the lecture notes.)

f) We use the relations

$$|\psi_L\rangle = \frac{1}{\sqrt{2}}(|\psi_0^+\rangle + |\psi_0^-\rangle)\,, \quad |\psi_R\rangle = \frac{1}{\sqrt{2}}(|\psi_0^+\rangle - |\psi_0^-\rangle) \tag{28}$$

which in matrix form are

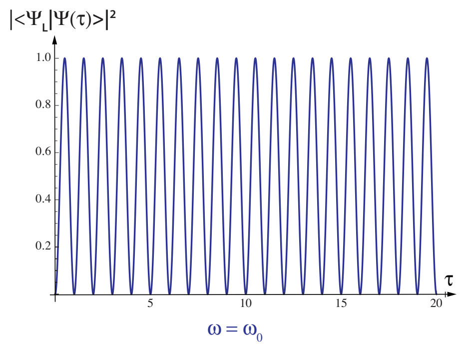
$$\psi_L = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad \psi_R = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \tag{29}$$

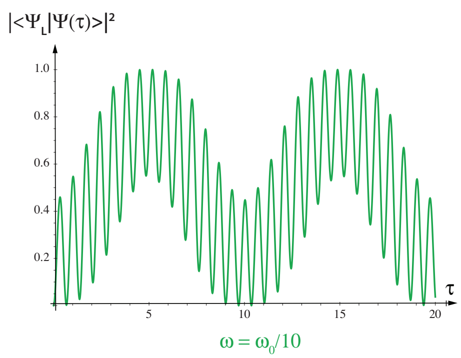
This gives

$$\begin{aligned}\langle\psi_R|\psi(t)\rangle &= \langle\psi_R|\hat{\mathcal{U}}(t)|\psi_L\rangle \\ &= \frac{1}{2}(1\ \ -1)\begin{pmatrix}A & B\\ C & D\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} \\ &= \frac{1}{2}((A-D)+(B-C))\end{aligned} \tag{30}$$

Inserted for A, B, C, D,

$$\langle\psi_R|\psi(t)\rangle = -[\sin\theta\sin(\frac{\Omega}{2}t)\sin(\frac{\omega}{2}t) + i\{\cos(\frac{\Omega}{2}t)\sin(\frac{\omega}{2}t) + \cos\theta\sin(\frac{\Omega}{2}t)\cos(\frac{\omega}{2}t)\}] \tag{31}$$





g) Absolute squared

$$\begin{aligned}|\langle\psi_R|\psi(t)\rangle|^2 &= [\sin\theta\sin(\frac{\Omega}{2}t)\sin(\frac{\omega}{2}t)]^2 + [\cos(\frac{\Omega}{2}t)\sin(\frac{\omega}{2}t) + \cos\theta\sin(\frac{\Omega}{2}t)\cos(\frac{\omega}{2}t)\}]^2 \\ &= \frac{1}{2}[1 - \cos\omega t + \cos^2\theta(1-\cos\Omega t)\cos\omega t + \cos\theta\sin\Omega t\sin\omega t]\end{aligned} \tag{32}$$

Plots of $|\langle\psi_R|\psi(t)\rangle|^2$ with $\tau = 2\pi\lambda t$ as time coordinate:
The two figures correspond to $\omega = \omega_0 = 2\lambda/\hbar$ and $\omega = \omega_0/10 = \lambda/5\hbar$. In both cases we have $\omega_1 = \Delta_0/\hbar = 2\lambda/\hbar = \omega_0$.

Commentary:
At resonance the oscillations are harmonic, with angular frequency ω_0. This is similar to the case with the periodic field component turned off. In this case the frequency ω of the rotating field only influences the complex phase of $\langle\psi_R|\psi(t)\rangle$.

With $\omega = \omega_0/10$ the oscillations are modulated by slower oscillations, with frequency close to ω. The more rapid oscillations in this case are to some extent modified by ω.

The expression (32) shows that more generally the function $|\langle\psi_R|\psi(t)\rangle|^2$ is a linear combination of three periodic functions, with frequencies ω, $\Omega - \omega$ and $\Omega + \omega$.