## 6.D. The Quantum Probability Density Operator

For quantum systems, the expectation value of an operator $\hat{O}$ is related to the (quantum probability) density operator $\hat{\rho}(t)$ by

$$\langle O(t) \rangle = \mathrm{Tr}\, \hat{O}\, \hat{\rho}(t) \tag{6.47}$$

with

$$\mathrm{Tr}\, \hat{\rho}(t) = 1 \qquad \forall\ t \tag{6.48}$$

Consider two sets of orthonormal and complete eigenstates given by

$$\hat{O}\ |\ o_i \rangle = o_i\ |\ o_i \rangle \qquad \hat{A}\ |\ a_i \rangle = a_i\ |\ a_i \rangle$$

with

$$\langle o_i\ |\ o_j \rangle = \delta_{ij} \qquad \langle a_i\ |\ a_j \rangle = \delta_{ij}$$

$$\sum_i |\ o_i \rangle \langle o_i\ | = \hat{I} \qquad \sum_i |\ a_i \rangle \langle a_i\ | = \hat{I}$$

then

$$\begin{aligned} \langle O(t) \rangle &= \sum_{i,j} \left\langle o_i\ |\ \hat{O}\ |\ o_j \right\rangle \left\langle o_j\ |\ \hat{\rho}(t)\ |\ o_i \right\rangle \\ &= \sum_{i,j} o_i\, \delta_{ij} \left\langle o_j\ |\ \hat{\rho}(t)\ |\ o_i \right\rangle \\ &= \sum_{i} o_i \left\langle o_i\ |\ \hat{\rho}(t)\ |\ o_i \right\rangle \end{aligned} \tag{6.49a}$$

$$\langle O(t) \rangle = \sum_{i,j} \left\langle a_i\ |\ \hat{O}\ |\ a_j \right\rangle \left\langle a_j\ |\ \hat{\rho}(t)\ |\ a_i \right\rangle \tag{6.49}$$

Since the trace of an operator is independent of the basis states, (6.49) gives the same value using the eigenstates of any $\hat{A}$, including those of $\hat{O}$.

Since one can only measure expectation values of physical quantities, $\hat{\rho}(t)$ contains all the information one can extract from the system.

The numbers $\rho_{ij} = \left\langle a_i\ |\ \hat{\rho}(t)\ |\ a_j \right\rangle$ are the $(i, j)$-elements of the density matrix $\boldsymbol{\rho}(t)$ with respect to the basis $\{\ |\ a_i \rangle \}$. Since $\hat{\rho}$ is a Hermitian operator, $\boldsymbol{\rho}$ is a Hermitian matrix. Furthermore, we take

$$\rho_{ii} = \left\langle a_i\ |\ \hat{\rho}(t)\ |\ a_i \right\rangle = \text{probability of system in state } a_i$$

so that

$$\rho_{ii} = \left\langle a_i\ |\ \hat{\rho}(t)\ |\ a_i \right\rangle \geq 0 \qquad \forall\ a_i$$

i.e., the matrix $\boldsymbol{\rho}$ is positive semi-definite.

Consider a system governed by the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} |\ \psi(t)\ \rangle = \hat{H}\ |\ \psi(t)\ \rangle \tag{6.50}$$

The expectation value of any operator $\hat{O}$ with respect to the state $|\ \psi(t)\ \rangle$ is defined as

$$\langle O(t) \rangle = \left\langle \psi(t)\ |\ \hat{O}\ |\ \psi(t) \right\rangle \tag{6.51a}$$

where we have assumed

$$\langle\ \psi(t)\ |\ \psi(t)\ \rangle = 1$$

(6.51a) can be written in the form (6.47) if we define

$$\hat{\rho}(t) = |\ \psi(t)\ \rangle \langle\ \psi(t)\ | \tag{6.51}$$

Indeed, since there is only 1 state,

$$\mathrm{Tr}\, \hat{A} = \left\langle \psi(t)\ |\ \hat{A}\ |\ \psi(t) \right\rangle$$

so that

$$\text{Tr}\,\hat{\rho}(t) = \langle\, \psi(t) \mid \psi(t)\,\rangle \langle\, \psi(t) \mid \psi(t)\,\rangle = 1$$

$$\begin{aligned}\langle\, O(t)\,\rangle &= \langle\, \psi(t) \mid \hat{O}\; \hat{\rho}(t) \mid \psi(t)\,\rangle \\ &= \langle\, \psi(t) \mid \hat{O} \mid \psi(t)\,\rangle \langle\, \psi(t) \mid \psi(t)\,\rangle \\ &= \left\langle\, \psi(t) \mid \hat{O} \mid \psi(t)\,\right\rangle\end{aligned}$$

as claimed.

The density operator (6.51) is said to describe a system in a pure state and it provides the averaging necessary to deal with the fundamental quantum uncertainty.

Statistical mechanics requires additional, e.g., ensemble, averaging to cope with the uncertainty about the (large number of) constituent parts of the system. For systems in equilibrium or nearly so, this can be achieved by averaging over mixed states that are incoherent mixtures of multiple states. $\hat{\rho}$ then takes the form

$$\hat{\rho}(t) = \sum_i p_i \mid \psi_i(t)\,\rangle \langle\, \psi_i(t) \mid \tag{6.52}$$

where $p_i$ is the probability of finding the system in state $\mid \psi_i(t)\,\rangle$, where $\{ \mid \psi_i(t)\,\rangle \}$ is any basis that span the Hilbert space of the system.

Let $\{ \mid \psi_i(t)\,\rangle \}$ be the solution set of the Schrodinger equation (6.50). Then

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\hat{\rho}(t) &= \sum_i p_i \left( i\hbar \frac{\partial \mid \psi_i(t)\,\rangle}{\partial t} \langle\, \psi_i(t) \mid + \mid \psi_i(t)\,\rangle\, i\hbar \frac{\partial \langle\, \psi_i(t) \mid}{\partial t} \right) \\ &= \sum_i \left( \hat{H} \mid \psi_i(t)\,\rangle \langle\, \psi_i(t) \mid - \mid \psi_i(t)\,\rangle \langle\, \psi_i(t) \mid \hat{H} \right) \\ &= \hat{H}\hat{\rho}(t) - \hat{\rho}(t)\hat{H} \\ &= \left[ \hat{H}, \hat{\rho}(t) \right] \\ &= \hbar \hat{L}\, \hat{\rho}(t) \end{aligned} \tag{6.53}$$

where

$$\hat{L} = \frac{1}{\hbar}\left[ \hat{H},\ \right] \tag{6.53a}$$

is the quantum Liouville operator and (6.53) is known as the Liouville equation.

The solution to (6.53) is

$$\begin{aligned} \hat{\rho}(t) &= e^{-it\hat{L}}\, \hat{\rho}(0) \\ &= \sum_{n=0}^{\infty} \frac{(-i\,t)^n}{n!} \hat{L}^n\, \hat{\rho}(0) \\ &= \sum_{n=0}^{\infty} \frac{(-i\,t)^n}{n!\,\hbar^n} \overbrace{\left[ \hat{H}, \left[ \hat{H}, \ldots, \right.\right.}^{n} \left[ \hat{H}, \hat{\rho}(0) \right] \ldots \left.\left. \right]\right] \\ &= e^{-\frac{i}{\hbar} t \hat{H}}\, \hat{\rho}(0)\, e^{\frac{i}{\hbar} t \hat{H}} \end{aligned} \tag{6.54}$$

(6.47) thus becomes

$$\begin{aligned} \langle\, O(t)\,\rangle &= \text{Tr}\left[ \hat{O}\, e^{-\frac{i}{\hbar} t \hat{H}}\, \hat{\rho}(0)\, e^{\frac{i}{\hbar} t \hat{H}} \right] \\ &= \text{Tr}\left[ e^{\frac{i}{\hbar} t \hat{H}}\, \hat{O}\, e^{-\frac{i}{\hbar} t \hat{H}}\, \hat{\rho}(0) \right] \\ &= \text{Tr}\left[ \hat{O}(t)\, \hat{\rho}(0) \right] \end{aligned} \tag{6.55}$$

where

$$\hat{O}(t) = e^{\frac{i}{\hbar} t \hat{H}}\, \hat{O}\, e^{-\frac{i}{\hbar} t \hat{H}} \tag{6.56}$$

is the Heisenberg picture version of $\hat{O}$. Taking the time derivative of (6.56) gives

$$i\hbar \frac{\partial}{\partial t}\hat{O}(t) = e^{\frac{i}{\hbar}t\hat{H}}\left(-\hat{H}\hat{O} + \hat{O}\hat{H}\right)e^{-\frac{i}{\hbar}t\hat{H}}$$
$$= \left[\hat{O}(t), \hat{H}\right]$$
$$= -\hbar\hat{L}\,\hat{O}(t) \qquad (6.57)$$

Note the difference between (6.57) for $\hat{O}(t)$ and (6.53) for $\hat{\rho}(t)$.

Using the completeness

$$\sum_i \mid E_i\rangle\langle E_i \mid = \hat{I}$$

of the orthonormal energy eigenstates $\mid E_i\rangle$ of $\hat{H}$, we can write (6.54) as

$$\hat{\rho}(t) = \sum_{i,j,k,l} \mid E_i\rangle\langle E_i \mid e^{-\frac{i}{\hbar}t\hat{H}} \mid E_j\rangle\langle E_j \mid \hat{\rho}(0) \mid E_k\rangle\langle E_k \mid e^{\frac{i}{\hbar}t\hat{H}} \mid E_l\rangle\langle E_l \mid$$
$$= \sum_{i,j,k,l} \mid E_i\rangle e^{-\frac{i}{\hbar}t E_j}\delta_{ij}\langle E_j \mid \hat{\rho}(0) \mid E_k\rangle e^{\frac{i}{\hbar}t E_l}\delta_{kl}\langle E_l \mid$$
$$= \sum_{j,k} \mid E_j\rangle e^{-\frac{i}{\hbar}t E_j}\langle E_j \mid \hat{\rho}(0) \mid E_k\rangle e^{\frac{i}{\hbar}t E_k}\langle E_k \mid$$
$$= \sum_{j,k} \langle E_j \mid \hat{\rho}(0) \mid E_k\rangle e^{-\frac{i}{\hbar}t(E_j - E_k)} \mid E_j\rangle\langle E_k \mid \qquad (6.58)$$

Thus, if the terms with the time factors $e^{-\frac{i}{\hbar}t(E_j - E_k)}$ all vanish, a stationary state is obtained. This means

$$\langle E_j \mid \hat{\rho}(0) \mid E_k\rangle = 0 \qquad \forall\ j \neq k$$

giving

$$\hat{\rho}_s = \sum_j \langle E_j \mid \hat{\rho}(0) \mid E_j\rangle \mid E_j\rangle\langle E_j \mid$$
$$= \sum_j \langle E_j \mid \hat{\rho} \mid E_j\rangle \mid E_j\rangle\langle E_j \mid$$
$$= \hat{\rho}(\hat{H}) \qquad (6.59)$$

which can be any function of $\hat{H}$.

In general, (6.53) indicates that any $\hat{\rho}$ that commutes with $\hat{H}$ is stationary. Thus, we can write

$$\hat{\rho}_s = \hat{\rho}\left(\hat{H}, \hat{I}_1, \ldots, \hat{I}_n\right) \qquad (6.60)$$

where

$$\left[\hat{I}_j, \hat{H}\right] = 0 \qquad \forall\ j$$

Note that the existence of the invariants $\hat{I}_j$ implies the energy eigenstates are degenerate and requires an additional quantum number labelling for each invariant to maintain orthogonality. For the case (6.60), the energy eigenstates take the form $\mid E_j; \alpha_1, \ldots, \alpha_n\rangle$ with

$$\hat{H} \mid E_j; \alpha_1, \ldots, \alpha_n\rangle = E_j \mid E_j; \alpha_1, \ldots, \alpha_n\rangle$$
$$\hat{I}_k \mid E_j; \alpha_1, \ldots, \alpha_n\rangle = \alpha_k \mid E_j; \alpha_1, \ldots, \alpha_n\rangle \qquad k = 1, \ldots, n$$

## Exercise 6.5.

Consider a harmonic oscillator with

$$\hat{H} = \frac{1}{2m}\left(\hat{p}^2 + m\,\omega^2\,\hat{x}^2\right)$$

Assume that

$$\hat{\rho}(0) = \hbar\sqrt{a\,b}\,\left(e^{-a\hat{x}^2}\,e^{-b\hat{p}^2} + e^{-b\hat{p}^2}\,e^{-a\hat{x}^2}\right)$$

where $a$ & $b$ are constants with dimensions $[a] = \left[x^{-2}\right]$ and $[b] = \left[p^{-2}\right]$.

(a) Compute the probability of finding the particle within $(x,\ x + d\,x)$ at $t = 0$.

(b) Write the Liouville equation in the position basis.

(c) Compute the probability of finding the particle within $(x,\ x + d\,x)$ at time $t$.

## Answer (a)

The probability of finding the particle within $(x,\ x + d\,x)$ at $t = 0$ is

$$\begin{aligned} P(x,\,0) &= \left\langle x \mid \hat{\rho}(0) \mid x \right\rangle d\,x \\ &\equiv \rho_{x\,x}(0)\,d\,x \end{aligned}$$

Note: either $\mid x\rangle$ or $\mid p\rangle$ can span the Hilbert space of $\hat{H}$.

$$\begin{aligned} \rho_{x\,x'}(0) &= \left\langle x \mid \hat{\rho}(0) \mid x' \right\rangle \\ &= \sqrt{a\,b}\,\left\langle x \,\middle|\, \left(e^{-a\hat{x}^2}\,e^{-b\hat{p}^2} + e^{-b\hat{p}^2}\,e^{-a\hat{x}^2}\right) \,\middle|\, x' \right\rangle \\ &= \sqrt{a\,b}\,\left\langle x \,\middle|\, \left(e^{-a x^2}\,e^{-b\hat{p}^2} + e^{-b\hat{p}^2}\,e^{-a x'^2}\right) \,\middle|\, x' \right\rangle \\ &= \sqrt{a\,b}\,\left(e^{-a x^2} + e^{-a x'^2}\right)\left\langle x \,\middle|\, e^{-b\hat{p}^2} \,\middle|\, x' \right\rangle \\ &= \sqrt{a\,b}\,\left(e^{-a x^2} + e^{-a x'^2}\right)\int_{-\infty}^{\infty} d\,p \left\langle x \,\middle|\, e^{-b\hat{p}^2} \,\middle|\, p \right\rangle \langle p \mid x' \rangle \\ &= \sqrt{a\,b}\,\left(e^{-a x^2} + e^{-a x'^2}\right)\int_{-\infty}^{\infty} d\,p\, e^{-b p^2} \langle x \mid p \rangle \langle p \mid x' \rangle \\ &= \sqrt{a\,b}\,\left(e^{-a x^2} + e^{-a x'^2}\right)\int_{-\infty}^{\infty} \frac{d\,p}{2\,\pi}\, e^{-b p^2}\, e^{i p (x - x')/\hbar} \end{aligned}$$

where

$$\langle x \mid p \rangle = \frac{1}{\sqrt{2\,\pi}}\, e^{i p x/\hbar}$$

With the help of the *Mathematica* code

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Assuming[b > 0 && x > 0 && ℏ > 0, ∫_{-∞}^{∞} e^(i p x/ℏ) / ((2 π) e^(b p^2)) ⅆp]
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we get

$$\rho_{x\,x'}(0) = \frac{1}{2}\sqrt{\frac{a}{\pi}}\,\left(e^{-a x^2} + e^{-a x'^2}\right)e^{-\frac{(x - x')^2}{4 b \hbar^2}} \qquad (1)$$

Hence,

$$P\,(x,\,0) = \sqrt{\frac{a}{\pi}}\, e^{-a x^2}\, d\,x \qquad (2)$$

## Answer (b)

In the position basis, the Liouville equation

$$i\hbar \frac{\partial}{\partial t}\hat{\rho}(t) = \left[\hat{H}, \hat{\rho}(t)\right] \qquad (2a)$$

becomes

$$i\hbar \frac{\partial}{\partial t}\langle x \mid \hat{\rho}(t) \mid x'\rangle = \left\langle x \,\middle|\, \left[\hat{H}, \hat{\rho}(t)\right] \,\middle|\, x'\right\rangle$$

$$\rightarrow \quad i\hbar \frac{\partial \rho_{x x'}(t)}{\partial t} = \int_{-\infty}^{\infty} d x'' \left\{ \left\langle x \,\middle|\, \hat{H} \,\middle|\, x''\right\rangle \left\langle x'' \,\middle|\, \hat{\rho}(t) \,\middle|\, x'\right\rangle - \left\langle x \,\middle|\, \hat{\rho}(t) \,\middle|\, x''\right\rangle \left\langle x'' \,\middle|\, \hat{H} \,\middle|\, x'\right\rangle \right\}$$

$$= \int_{-\infty}^{\infty} d x'' \left\{ \left\langle x \,\middle|\, \hat{H} \,\middle|\, x''\right\rangle \rho_{x'' x'}(t) - \rho_{x x''}(t) \left\langle x'' \,\middle|\, \hat{H} \,\middle|\, x'\right\rangle \right\} \qquad (2b)$$

Using

$$\langle x \mid \hat{H} \mid x'\rangle = \langle x \mid \frac{1}{2m}\left(\hat{p}^2 + m\,\omega^2 \hat{x}^2\right) \mid x'\rangle$$

$$= \frac{1}{2m}\langle x \mid \hat{p}^2 \mid x'\rangle + \frac{1}{2}\omega^2 x'^2 \langle x \mid x'\rangle$$

$$= \frac{1}{2m}\int_{-\infty}^{\infty} d p \langle x \mid \hat{p}^2 \mid p\rangle\langle p \mid x'\rangle + \frac{1}{2}\omega^2 x'^2\, \delta(x - x')$$

$$= \frac{1}{2m}\int_{-\infty}^{\infty} d p\, p^2 \langle x \mid p\rangle\langle p \mid x'\rangle + \frac{1}{2}\omega^2 x'^2\, \delta(x - x')$$

$$= \frac{1}{2m}\int_{-\infty}^{\infty} \frac{d p}{2\pi} p^2 e^{i p (x - x')/\hbar} + \frac{1}{2}\omega^2 x'^2\, \delta(x - x')$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty} \frac{d p}{2\pi} e^{i p (x - x')/\hbar} + \frac{1}{2}\omega^2 x'^2\, \delta(x - x')$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2\right)\delta(x - x')$$

and

$$\int_{-\infty}^{\infty} d x'\, f(x') \frac{\partial^2}{\partial x'^2}\delta(x - x') = \int_{-\infty}^{\infty} d x'\, f(x') \frac{\partial^2}{\partial x^2}\delta(x - x')$$

$$= \frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty} d x'\, f(x')\, \delta(x - x')$$

$$= \frac{\partial^2 f(x)}{\partial x^2}$$

we have

$$\int_{-\infty}^{\infty} d x'' \left\langle x \,\middle|\, \hat{H} \mid x''\right\rangle \rho_{x'' x'}(t)$$

$$= \int_{-\infty}^{\infty} d x''\; \rho_{x'' x'}(t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2\right)\delta(x - x'')$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2\right)\rho_{x x'}(t)$$

and

$$\int_{-\infty}^{\infty} d x''\; \rho_{x x''}(t) \langle x'' \mid \hat{H} \mid x'\rangle$$

$$= \int_{-\infty}^{\infty} dx'' \; \rho_{x x''}(t) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x''^2} + \frac{1}{2} \omega^2 x''^2 \right) \delta(x'' - x')$$

$$= \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x'^2} + \frac{1}{2} \omega^2 x'^2 \right) \rho_{x x'}(t)$$

(2b) thus becomes

$$i\hbar \frac{\partial \rho_{x x'}(t)}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \rho_{x x'}(t)}{\partial x^2} - \frac{\partial^2 \rho_{x x'}(t)}{\partial x'^2} \right) + \frac{1}{2} \omega^2 \left( x^2 - x'^2 \right) \rho_{x x'}(t) \qquad (4)$$

## Answer (c)

Instead of solving (4) directly, we shall solve first the Liouville equation in the energy eigenstate basis and then transform the result to the position eigenstate basis.

For the harmonic oscillator, it is well known that

$$\hat{H} \,|\, n \rangle = E_n \,|\, n \rangle \qquad\qquad E_n = \left( n + \frac{1}{2} \right) \hbar \omega$$

$$\langle x \,|\, n \rangle = \sqrt{\frac{\alpha}{2^n n! \sqrt{\pi}}} \, H_n(\alpha x) \, e^{\alpha^2 x^2/2} \qquad\qquad \alpha = \sqrt{\frac{m\omega}{\hbar}} \qquad (5)$$

where $H_n$ is the $n^{\text{th}}$ order Hermite polynomial.

Note that since $\langle x \,|\, n \rangle$ is real, $\langle x \,|\, n \rangle = \langle n \,|\, x \rangle$.

With respect to the $|\, n \rangle$ basis, (2a) becomes

$$i\hbar \frac{\partial}{\partial t} \langle n \,|\, \hat{\rho}(t) \,|\, n' \rangle = \left\langle n \,\middle|\, \left[ \hat{H}, \hat{\rho}(t) \right] \,\middle|\, n' \right\rangle$$

$$i\hbar \frac{\partial \rho_{n n'}(t)}{\partial t} = \sum_{n''} \left\{ \left\langle n \,\middle|\, \hat{H} \,\middle|\, n'' \right\rangle \left\langle n'' \,\middle|\, \hat{\rho}(t) \,\middle|\, n' \right\rangle - \left\langle n \,\middle|\, \hat{\rho}(t) \,\middle|\, n'' \right\rangle \left\langle n'' \,\middle|\, \hat{H} \,\middle|\, n' \right\rangle \right\}$$

$$= \sum_{n''} \left( E_{n''} \delta_{n n''} \rho_{n'' n'}(t) - \rho_{n n''}(t) E_{n'} \delta_{n'' n'} \right)$$

$$= \left( E_n - E_{n'} \right) \rho_{n n'}(t)$$

$$= \hbar \omega \left( n - n' \right) \rho_{n n'}(t) \qquad (6)$$

where

$$\rho_{n n'}(t) = \left\langle n \,\middle|\, \hat{\rho}(t) \,\middle|\, n' \right\rangle$$

(6) is easily solved:

$$\rho_{n n'}(t) = \rho_{n n'}(0) \, e^{-i\omega(n - n')t} \qquad (7)$$

Now,

$$\rho_{x x'}(t) = \left\langle x \,\middle|\, \hat{\rho}(t) \,\middle|\, x' \right\rangle$$

$$= \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \langle x \,|\, n \rangle \left\langle n \,\middle|\, \hat{\rho}(t) \,\middle|\, n' \right\rangle \langle n' \,|\, x' \rangle$$

$$= \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \langle x \,|\, n \rangle \rho_{n n'}(t) \langle n' \,|\, x' \rangle$$

$$= \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \langle x \,|\, n \rangle \rho_{n n'}(0) \, e^{-i\omega(n - n')t} \langle n' \,|\, x' \rangle \qquad (7a)$$

Using

$$\rho_{n n'}(0) = \left\langle n \,\middle|\, \hat{\rho}(0) \,\middle|\, n' \right\rangle$$

$$= \int_{-\infty}^{\infty} d x_0 \int_{-\infty}^{\infty} d x_0' \langle n \mid x_0 \rangle \langle x_0 \mid \hat{\rho}(0) \mid x_0' \rangle \langle x_0' \mid n' \rangle$$
$$= \int_{-\infty}^{\infty} d x_0 \int_{-\infty}^{\infty} d x_0' \langle n \mid x_0 \rangle \rho_{x_0 x_0'}(0) \langle x_0' \mid n' \rangle$$

(7a) becomes

$$\rho_{x x'}(t) = \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int_{-\infty}^{\infty} d x_0 \int_{-\infty}^{\infty} d x_0' \langle x \mid n \rangle \langle n \mid x_0 \rangle * \rho_{x_0 x_0'}(0) \langle x_0' \mid n' \rangle e^{-i\omega(n-n')t} \langle n' \mid x' \rangle$$
$$= \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int_{-\infty}^{\infty} d x_0 \int_{-\infty}^{\infty} d x_0' \langle x \mid n \rangle \langle n \mid x_0 \rangle \langle x_0' \mid n' \rangle \langle n' \mid x' \rangle * \frac{1}{2}\sqrt{\frac{a}{\pi}} \left( e^{-a x_0^2} + e^{-a x_0'^2} \right) e^{-\frac{(x_0 - x_0')^2}{4 b \hbar^2}} e^{-i\omega(n-n')t} \qquad (7b)$$

where (1) was used.

Now, we can use (5) to write the identity [ see (10) in Exercise 5.8 ]

$$e^{-x^2-y^2} \sum_{n=0}^{\infty} \frac{1}{2^n n!} z^n H_n(x) H_n(y) = \frac{1}{\sqrt{1-z^2}} \exp\left( -\frac{x^2 + y^2 - 2 x y z}{1 - z^2} \right)$$

as

$$\frac{1}{\sqrt{1-z^2}} \exp\left[ -\frac{\alpha^2 (x^2 + y^2 - 2 x y z)}{1 - z^2} \right]$$
$$= \frac{\sqrt{\pi}\, e^{-\alpha^2(x^2+y^2)/2}}{\alpha} \sum_{n=0}^{\infty} \frac{\alpha}{2^n n! \sqrt{\pi}} z^n e^{-\alpha^2(x^2+y^2)/2} H_n(\alpha x) H_n(\alpha y)$$
$$= \frac{\sqrt{\pi}\, e^{-\alpha^2(x^2+y^2)/2}}{\alpha} \sum_{n=0}^{\infty} z^n \langle x \mid n \rangle \langle n \mid y \rangle$$

Setting $z = e^{-i\omega t}$, we have

$$\sum_{n=0}^{\infty} e^{-i\omega n t} \langle x \mid n \rangle \langle n \mid x_0 \rangle$$
$$= \frac{\alpha}{\sqrt{\pi}} e^{\alpha^2(x^2+x_0^2)/2} \frac{1}{\sqrt{1 - e^{-2i\omega t}}} \exp\left[ -\frac{\alpha^2 (x^2 + x_0^2 - 2 x x_0 e^{-i\omega t})}{1 - e^{-2i\omega t}} \right]$$
$$= \frac{\alpha}{\sqrt{\pi}} e^{\alpha^2(x^2+x_0^2)/2} \sqrt{f^*(t)} \exp\left[ -\alpha^2 f^*(t) (x^2 + x_0^2 - 2 x x_0 e^{-i\omega t}) \right]$$
$$= \sqrt{\frac{m\omega}{\hbar\pi}} e^{m\omega(x^2+x_0^2)/2\hbar} \sqrt{f^*(t)} \exp\left[ -\frac{m\omega}{\hbar} f^*(t) (x^2 + x_0^2 - 2 x x_0 e^{-i\omega t}) \right] \qquad (10a)$$

where

$$f(t) = \frac{1}{1 - e^{2i\omega t}} = \frac{e^{-i\omega t}}{e^{-i\omega t} - e^{i\omega t}} = i \frac{e^{-i\omega t}}{2 \sin \omega t}$$

The $x_0$ integral in (7b) becomes

$$\mathcal{I} = \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} d x_0\, e^{-i\omega n t} \langle x \mid n \rangle \langle n \mid x_0 \rangle e^{-a x_0^2} e^{-\frac{(x_0 - x_0')^2}{4 b \hbar^2}}$$

$$= \int_{-\infty}^{\infty} d\,x_0 \,\frac{\alpha}{\sqrt{\pi}}\, e^{\alpha^2 (x^2 + x_0^2)/2} \sqrt{g(t)}\, \exp\left[-\alpha^2 g(t) \left(x^2 + x_0^2 - 2\,x\,x_0\,e^{-i\,\omega\,t}\right)\right] e^{-a\,x_0^2}\, e^{-\frac{(x_0 - x_0')^2}{4\,b\,\hbar^2}}$$

Similarly,

$$\sum_{n'=0}^{\infty} e^{i\,\omega\,n'\,t} \langle x_0' \mid n' \rangle \langle n' \mid x' \rangle$$

$$= \frac{\alpha}{\sqrt{\pi}}\, e^{\alpha^2 (x'^2 + x_0'^2)/2} \frac{1}{\sqrt{1 - e^{2\,i\,\omega\,t}}} \exp\left(-\frac{\alpha^2 \left(x'^2 + x_0'^2 - 2\,x'\,x_0'\,e^{i\,\omega\,t}\right)}{1 - e^{2\,i\,\omega\,t}}\right)$$

$$= \sqrt{\frac{m\,\omega}{\hbar\,\pi}}\, e^{m\,\omega (x'^2 + x_0'^2)/2\,\hbar} \sqrt{f(t)}\, \exp\left[-\frac{m\,\omega}{\hbar} f(t) \left(x'^2 + x_0'^2 - 2\,x'\,x_0'\,e^{i\,\omega\,t}\right)\right] \quad (10)$$

Hence, (7b) becomes

$$\rho_{x\,x'}(t) = \int_{-\infty}^{\infty} d\,x_0 \int_{-\infty}^{\infty} d\,x_0' \,\frac{1}{2} \sqrt{\frac{a}{\pi}} \left( e^{-a\,x_0^2} + e^{-a\,x_0'^2} \right) e^{-\frac{(x_0 - x_0')^2}{4\,b\,\hbar^2}}$$

$$* \frac{\alpha}{\sqrt{\pi}}\, e^{\alpha^2 (x^2 + x_0^2)/2} \sqrt{f^*(t)}\, \exp\left[-\alpha^2 f^*(t) \left(x^2 + x_0^2 - 2\,x\,x_0\,e^{-i\,\omega\,t}\right)\right]$$

$$* \frac{\alpha}{\sqrt{\pi}}\, e^{\alpha^2 (x'^2 + x_0'^2)/2} \sqrt{f(t)}\, \exp\left[-\alpha^2 f(t) \left(x'^2 + x_0'^2 - 2\,x'\,x_0'\,e^{i\,\omega\,t}\right)\right]$$

$$= \frac{\alpha^2 \sqrt{a}}{2\,\pi^{3/2}} \left| f(t) \right| \exp\left\{ \alpha^2 \left[ \left(\frac{1}{2} - f^*(t)\right) x^2 + \left(\frac{1}{2} - f(t)\right) x'^2 \right] \right\} (\mathcal{I} + \mathcal{I}')$$

$$= \frac{\alpha^2 \sqrt{a}}{4\,\pi^{3/2} \sin \omega\,t} \exp\left[ \frac{1}{2}\, i\,\alpha^2 \left(x^2 - x'^2\right) \cot \omega\,t \right] (\mathcal{I} + \mathcal{I}') \quad (10b)$$

where

$$\mathcal{I} = \int_{-\infty}^{\infty} d\,x_0 \int_{-\infty}^{\infty} d\,x_0' \, \exp\Bigg[ -a\,x_0^2 - \frac{(x_0 - x_0')^2}{4\,b\,\hbar^2} + \frac{1}{2}\alpha^2 x_0^2 - \alpha^2 f^*(t) \left(x_0^2 - 2\,x\,x_0\,e^{-i\,\omega\,t}\right) + \frac{1}{2}\alpha^2 x_0'^2 - \alpha^2 f(t) \left(x_0'^2 - 2\,x'\,x_0'\,e^{i\,\omega\,t}\right) \Bigg] \quad (10c)$$

$$\mathcal{I}' = \int_{-\infty}^{\infty} d\,x_0 \int_{-\infty}^{\infty} d\,x_0' \, \exp\Bigg[ -a\,x_0'^2 - \frac{(x_0 - x_0')^2}{4\,b\,\hbar^2} + \frac{1}{2}\alpha^2 x_0^2 - \alpha^2 f^*(t) \left(x_0^2 - 2\,x\,x_0\,e^{-i\,\omega\,t}\right) + \frac{1}{2}\alpha^2 x_0'^2 - \alpha^2 f(t) \left(x_0'^2 - 2\,x'\,x_0'\,e^{i\,\omega\,t}\right) \Bigg]$$

Since $f^*(t) = f(t) \Big|_{\omega \to -\omega}$ and the integrals are invariant under $x_0 \leftrightarrow x_0'$, we have

$$\mathcal{I}' = \mathcal{I} \Big|_{\omega \to -\omega,\; x \leftrightarrow x'} = \mathcal{I}^* \Big|_{x \leftrightarrow x'}$$

Collecting terms with the same powers, (10c) takes the form

$$\mathcal{I} = \int_{-\infty}^{\infty} d\,x_0 \int_{-\infty}^{\infty} d\,x_0' \, \exp\left( -c_2\,x_0^2 + c_1\,x_0 - c_2'\,x_0'^2 + c_1'\,x_0' + c\,x_0\,x_0' \right) \quad (10d)$$

where

$$c_2 = a + \frac{1}{4\,b\,\hbar^2} + \alpha^2\left[-\frac{1}{2} + f^*(t)\right] \qquad c_2{}' = \frac{1}{4\,b\,\hbar^2} + \alpha^2\left[-\frac{1}{2} + f(t)\right]$$

$$c_1 = 2\,\alpha^2\,f^*(t)\,x\,e^{-i\,\omega\,t} \qquad c_1{}' = 2\,\alpha^2\,f(t)\,x'\,e^{i\,\omega\,t}$$

$$c = \frac{1}{2\,b\,\hbar^2}$$

Using the *Mathematica* code in §Code, we have

$$\mathcal{I} = \frac{2\,\pi}{\sqrt{4\,c_2\,c_2{}' - c^2}}\exp\left(\frac{c\,c_1\,c_1{}' + c_1{}'^2\,c_2 + c_1{}^2\,c_2{}'}{4\,c_2\,c_2{}' - c^2}\right)$$

$$\begin{aligned}4\,c_2\,c_2{}' - c^2 &= \frac{\csc^2\omega\,t}{2\,b\,\hbar^2}\left[a + b\,\alpha^4\,\hbar^2 + \left(-a + b\,\alpha^4\,\hbar^2\right)\cos 2\,\omega\,t + 2\,i\,a\,b\,\alpha^2\,\hbar^2\sin 2\,\omega\,t\right]\\ &= \frac{\csc^2\omega\,t}{b\,\hbar^2}\left[a\sin^2\omega\,t + b\,\alpha^4\,\hbar^2\cos^2\omega\,t + 2\,i\,a\,b\,\alpha^2\,\hbar^2\sin\omega\,t\cos\omega\,t\right]\\ &= \frac{\alpha^4}{\sin^2\omega\,t}\left[\cos^2\omega\,t + \frac{a}{b\,\alpha^4\,\hbar^2}\sin^2\omega\,t + 2\,i\,\frac{a}{\alpha^2}\sin\omega\,t\cos\omega\,t\right]\\ &= \frac{m^2\,\omega^2}{\hbar^2\sin^2\omega\,t}\left[\cos^2\omega\,t + \frac{a}{b\,m^2\,\omega^2}\sin^2\omega\,t + 2\,i\,\frac{a\,\hbar}{m\,\omega}\sin\omega\,t\cos\omega\,t\right]\\ &= \frac{m^2\,\omega^2}{\hbar^2\sin^2\omega\,t}B(t)\end{aligned}$$

where

$$B(t) = \cos^2\omega\,t + \frac{a}{b\,m^2\,\omega^2}\sin^2\omega\,t + 2\,i\,\frac{a\,\hbar}{m\,\omega}\sin\omega\,t\cos\omega\,t \qquad (12)$$

Also,

$$\begin{aligned}&\frac{c\,c_1\,c_1{}' + c_1{}'^2\,c_2 + c_1{}^2\,c_2{}'}{4\,c_2\,c_2{}' - c^2}\\ &= \alpha^4\left[-x^2 + 2\,x\,x' - x'^2\left(1 + 4\,a\,b\,\hbar^2\right) - 2\,i\,b\left(x^2 - x'^2\right)\alpha^2\,\hbar^2\cot\omega\,t\right]\Big/\\ &\quad 2\left[a + b\,\alpha^4\,\hbar^2 + \left(-a + b\,\alpha^4\,\hbar^2\right)\cos 2\,\omega\,t + 2\,i\,a\,b\,\alpha^2\,\hbar^2\sin 2\,\omega\,t\right]\\ &= \frac{1}{4\,b\,\hbar^2\,B(t)}\left(-x^2 + 2\,x\,x' - x'^2\left(1 + 4\,a\,b\,\hbar^2\right) - 2\,i\,b\left(x^2 - x'^2\right)\alpha^2\,\hbar^2\cot\omega\,t\right)\end{aligned}$$

For $x = x'$, this simplifies to

$$\frac{c\,c_1\,c_1{}' + c_1{}'^2\,c_2 + c_1{}^2\,c_2{}'}{4\,c_2\,c_2{}' - c^2} = -\frac{a\,x^2}{B(t)}$$

so that

$$\mathcal{I} = \frac{2\,\pi\sin\omega\,t}{\alpha^2\sqrt{B(t)}}\exp\left[-\frac{a\,x^2}{B(t)}\right] \qquad \mathcal{I}' = \mathcal{I}^*$$

and (10b) becomes

$$\rho_{x\,x}(t) = \sqrt{\frac{a}{\pi}}\ \mathrm{Re}\left\{\frac{1}{\sqrt{B(t)}}\exp\left[-\frac{a\,x^2}{B(t)}\right]\right\} \qquad (11)$$

## Code

In[39]:=
$$f = \frac{1}{1 - e^{2 i \omega t}};$$
$$\text{Assuming}[\omega > 0 \,\&\&\, t > 0,\ f^* f \,//\, \text{ExpToTrig} \,//\, \text{Simplify}]$$

Out[40]=
$$\frac{1}{4} \text{Csc}[t\,\omega]^2$$

In[41]:=
$$\text{Assuming}\left[\omega > 0 \,\&\&\, t > 0,\ \left(\frac{1}{2} - f^*\right) x^2 + \left(\frac{1}{2} - f\right) xp^2 \,//\, \text{ExpToTrig} \,//\, \text{Simplify}\right]$$

Out[41]=
$$\frac{1}{2} i \left(x^2 - xp^2\right) \text{Cot}[t\,\omega]$$

In[1]:=
$$A = \text{Assuming}\Big[c2 > 0 \,\&\&\, c1 > 0 \,\&\&\, c2p > 0 \,\&\&\, c1p > 0 \,\&\&\, c > 0,$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \text{Exp}\left[-c2\, x0^2 + c1\, x0 - c2p\, x0p^2 + c1p\, x0p + c\, x0\, x0p\right] dx0\, dx0p\Big]$$

Out[1]=
$$\text{ConditionalExpression}\left[\frac{2\sqrt{c2}\; e^{-\frac{c\, c1\, c1p + c1p^2\, c2 + c1^2\, c2p}{c^2 - 4\, c2\, c2p}}\, \pi}{\sqrt{c2\left(-c^2 + 4\, c2\, c2p\right)}},\ c^2 \le 4\, c2\, c2p\right]$$

In[2]:=
$$AA = A[[1]] \,//\, \text{PowerExpand}$$

Out[2]=
$$\frac{2\, e^{-\frac{c\, c1\, c1p + c1p^2\, c2 + c1^2\, c2p}{c^2 - 4\, c2\, c2p}}\, \pi}{\sqrt{-c^2 + 4\, c2\, c2p}}$$

In[3]:=
$$par = \Big\{c2 \to a + \frac{1}{4\, b\, \hbar^2} + \alpha^2\left(-\frac{1}{2} + \frac{1}{1 - e^{-2 i \omega t}}\right),\ c1 \to 2\,\alpha^2 \frac{1}{1 - e^{-2 i \omega t}}\, x\, e^{-i \omega t},$$
$$c2p \to \frac{1}{4\, b\, \hbar^2} + \alpha^2\left(-\frac{1}{2} + \frac{1}{1 - e^{2 i \omega t}}\right),\ c1p \to 2\,\alpha^2 \frac{1}{1 - e^{2 i \omega t}}\, xp\, e^{i \omega t},$$
$$c \to \frac{1}{2\, b\, \hbar^2}\Big\};$$

In[18]:=
$$AD = 4\, c2\, c2p - c^2 \ /.\ par \,//\, \text{Simplify}$$

Out[18]=
$$\left(-b\left(1 + e^{2 i t \omega}\right)^2 \alpha^4 \hbar^2 + a\left(1 - 2\, e^{2 i t \omega} + 2\, b\, \alpha^2 \hbar^2 + e^{4 i t \omega}\left(1 - 2\, b\, \alpha^2 \hbar^2\right)\right)\right) \Big/ \left(b\left(-1 + e^{2 i t \omega}\right)^2 \hbar^2\right)$$

In[19]:=
$$AD1 = AD \,//\, \text{ExpToTrig} \,//\, \text{Simplify}$$

Out[19]=
$$\frac{1}{2\, b\, \hbar^2} \text{Csc}[t\,\omega]^2 \left(a + b\, \alpha^4 \hbar^2 + \left(-a + b\, \alpha^4 \hbar^2\right) \text{Cos}[2\, t\, \omega] + 2\, i\, a\, b\, \alpha^2 \hbar^2\, \text{Sin}[2\, t\, \omega]\right)$$

In[21]:=
$$AE = \frac{c\, c1\, c1p + c1p^2\, c2 + c1^2\, c2p}{4\, c2\, c2p - c^2} \ /.\ par \,//\, \text{Simplify}$$

Out[21]=
$$\Big(e^{2 i t \omega} \alpha^4 \Big(2\left(-1 + e^{2 i t \omega}\right) x\, xp + x^2\left(1 + 2\, b\, \alpha^2 \hbar^2 + e^{2 i t \omega}\left(-1 + 2\, b\, \alpha^2 \hbar^2\right)\right) -$$
$$xp^2\left(-1 - 4\, a\, b\, \hbar^2 + 2\, b\, \alpha^2 \hbar^2 + e^{2 i t \omega}\left(1 + 4\, a\, b\, \hbar^2 + 2\, b\, \alpha^2 \hbar^2\right)\right)\Big)\Big) \Big/$$
$$\left(\left(-1 + e^{2 i t \omega}\right)\left(b\left(1 + e^{2 i t \omega}\right)^2 \alpha^4 \hbar^2 + a\left(-1 + e^{2 i t \omega}\right)\left(1 + 2\, b\, \alpha^2 \hbar^2 + e^{2 i t \omega}\left(-1 + 2\, b\, \alpha^2 \hbar^2\right)\right)\right)\right)$$

In[22]:=
$$AE1 = AE \,//\, \text{ExpToTrig} \,//\, \text{Simplify}$$

Out[22]=
$$\left(\alpha^4\left(-x^2 + 2\, x\, xp - xp^2\left(1 + 4\, a\, b\, \hbar^2\right) - 2\, i\, b\left(x^2 - xp^2\right) \alpha^2 \hbar^2\, \text{Cot}[t\,\omega]\right)\right) \Big/$$
$$\left(2\left(a + b\, \alpha^4 \hbar^2 + \left(-a + b\, \alpha^4 \hbar^2\right) \text{Cos}[2\, t\, \omega] + 2\, i\, a\, b\, \alpha^2 \hbar^2\, \text{Sin}[2\, t\, \omega]\right)\right)$$

## Exercise 6.6.

An ensemble of silver atoms (each with spin $\frac{1}{2}$) is prepared so that 60 % of them are in the $S_z = +\frac{\hbar}{2}$ eigenstate of $\hat{S}_z$ and 40 % in the $S_x = -\frac{\hbar}{2}$ eigenstate of $\hat{S}_x$.

(a) Compute $\hat{\rho}(0)$ in the basis of eigenstates of $\hat{S}_z$.

(b) Assume the atoms sit in a magnetic field $\boldsymbol{B} = B_0\,\hat{\boldsymbol{y}}$ and have a magnetic Hamiltonian

$$\hat{H} = \mu\, S \cdot \boldsymbol{B}$$

where $\mu$ is the magnetic moment of a silver atom.

Compute $\hat{\rho}(t)$ in the basis of eigenstates of $\hat{S}_z$.

(c) Compute $\langle S_z(t) \rangle$ at time $t = 0$ and time $t$.

### Answer (a)

Let

$$\hat{S}_k \mid k_\pm \rangle = \pm\frac{\hbar}{2} \mid k_\pm \rangle \qquad\qquad k = x,\, y,\, z$$

where, for a given $k$,

$$\langle k_\alpha \mid k_\beta \rangle = \delta_{\alpha\beta} \qquad \sum_\alpha \mid k_\alpha \rangle\langle k_\alpha \mid = \hat{I} \qquad \alpha,\, \beta = \pm$$

Initially,

$$\hat{\rho}(0) = \frac{6}{10} \mid z_+ \rangle\langle z_+ \mid + \frac{4}{10} \mid x_- \rangle\langle x_- \mid \tag{1}$$

In the basis $\mid z_\pm \rangle$, the $\hat{S}_k$'s are proportional to the Pauli matrices

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

while the eigenstates are column vectors

$$\mid k_\alpha \rangle = \begin{pmatrix} \langle z_+ \mid k_\alpha \rangle \\ \langle z_- \mid k_\alpha \rangle \end{pmatrix}$$

For example,

$$\mid z_+ \rangle = \begin{pmatrix} \langle z_+ \mid z_+ \rangle \\ \langle z_- \mid z_+ \rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \mid z_- \rangle = \begin{pmatrix} \langle z_+ \mid z_- \rangle \\ \langle z_- \mid z_- \rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{4}$$

Using the *Mathematica* code

```
Eigensystem[( 0 1
              1 0 )]
```

```
{{-1, 1}, {{-1, 1}, {1, 1}}}
```

to solve the eigen-equations for $\hat{S}_x$

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \langle z_+ \mid x_\pm \rangle \\ \langle z_- \mid x_\pm \rangle \end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix} \langle z_+ \mid x_\pm \rangle \\ \langle z_- \mid x_\pm \rangle \end{pmatrix}$$

we have

$$\mid x_+ \rangle = \begin{pmatrix} \langle z_+ \mid x_+ \rangle \\ \langle z_- \mid x_+ \rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \mid x_- \rangle = \begin{pmatrix} \langle z_+ \mid x_- \rangle \\ \langle z_- \mid x_- \rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{3a}$$

where the normalization factor $\frac{1}{\sqrt{2}}$ was obtained by inspection.

Similarly, using code

```
Eigensystem[(0 -i
             i  0)]
```

```
{{-1, 1}, {{i, 1}, {-i, 1}}}
```

we get

$$| y_+ \rangle = \begin{pmatrix} \langle z_+ | y_+ \rangle \\ \langle z_- | y_+ \rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix} \qquad | y_- \rangle = \begin{pmatrix} \langle z_+ | y_- \rangle \\ \langle z_- | y_- \rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \tag{3b}$$

Using

$$| z_+ \rangle \langle z_+ | = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \quad 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$| x_- \rangle \langle x_- | = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} (1 \quad -1) = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

(1) becomes

$$\hat{\rho}(0) = \frac{6}{10} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{4}{10} \times \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{4}{5} & -\frac{1}{5} \\ -\frac{1}{5} & \frac{1}{5} \end{pmatrix} \tag{5}$$

## Answer (b)

The Hamiltonian can be written as

$$\hat{H} = \mu \hat{S} \cdot \boldsymbol{B} = \mu B_0 \hat{S}_y$$
$$= \frac{1}{2} \mu \hbar B_0 ( | y_+ \rangle \langle y_+ | - | y_- \rangle \langle y_- | )$$

which, in the basis $| y_\pm \rangle$, takes the simple form

$$\hat{H} = \frac{1}{2} \mu \hbar B_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The Liouville equation thus becomes

$$i \frac{\partial}{\partial t} \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} = \frac{1}{2} \mu B_0 \left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} \right] \tag{6a}$$

where

$$\rho_{\alpha\beta} = \langle y_\alpha | \hat{\rho} | y_\beta \rangle$$

Now,

$$\left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} \right] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} - \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
$$= \begin{pmatrix} \rho_{++} & \rho_{+-} \\ -\rho_{-+} & -\rho_{--} \end{pmatrix} - \begin{pmatrix} \rho_{++} & -\rho_{+-} \\ \rho_{-+} & -\rho_{--} \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 2\rho_{+-} \\ -2\rho_{-+} & 0 \end{pmatrix}$$

Hence, (6a) becomes

$$i \frac{\partial}{\partial t} \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} = \mu B_0 \begin{pmatrix} 0 & \rho_{+-} \\ -\rho_{-+} & 0 \end{pmatrix}$$

or

$$i \frac{\partial \rho_{++}}{\partial t} = 0 \qquad i \frac{\partial \rho_{+-}}{\partial t} = \mu B_0 \rho_{+-}$$
$$i \frac{\partial \rho_{-+}}{\partial t} = -\mu B_0 \rho_{-+} \qquad i \frac{\partial \rho_{--}}{\partial t} = 0 \tag{6}$$

with solutions

$$\rho_{++}(t) = \rho_{++}(0) \qquad \rho_{+-}(t) = \rho_{+-}(0)\, e^{-i\mu B_0 t}$$
$$\rho_{-+}(t) = \rho_{-+}(0)\, e^{i\mu B_0 t} \qquad \rho_{--}(t) = \rho_{--}(0) \tag{6b}$$

Writing the initial condition (1) in the $|\, y_\pm \rangle$ basis gives

$$\rho_{\alpha\beta}(0) = \langle y_\alpha \,|\, \hat{\rho}(0) \,|\, y_\beta \rangle$$
$$= \frac{6}{10} \langle y_\alpha \,|\, z_+ \rangle \langle z_+ \,|\, y_\beta \rangle + \frac{4}{10} \langle y_\alpha \,|\, x_- \rangle \langle x_- \,|\, y_\beta \rangle$$

Since inner products are independent of basis, we can use the result of (a) to evaluate them. With the help of the *Mathematica* code below, we get

$$\hat{\rho}(0) = \begin{pmatrix} \frac{1}{2} & -\frac{3}{10} - \frac{i}{5} \\ -\frac{3}{10} + \frac{i}{5} & \frac{1}{2} \end{pmatrix} \tag{7}$$

so that (6b) becomes

$$\hat{\rho}(t) = \begin{pmatrix} \frac{1}{2} & -\left(\frac{3}{10} + \frac{i}{5}\right) e^{-i\mu B_0 t} \\ -\left(\frac{3}{10} - \frac{i}{5}\right) e^{i\mu B_0 t} & \frac{1}{2} \end{pmatrix} \tag{8}$$

Note: the sign difference of the off-diagonal elements with Reichl's result arises from the different choice of $|\, y_\pm \rangle$. It is immaterial since it doesn't affect the average of any operator.

Consider

$$\hat{\rho} = \sum_{\alpha,\beta} \rho^y_{\alpha\beta} \,|\, y_\alpha \rangle \langle y_\beta \,| = \sum_{\alpha,\beta} \rho^z_{\alpha\beta} \,|\, z_\alpha \rangle \langle z_\beta \,|$$
$$= \sum_{\alpha,\beta} \sum_{\alpha',\beta'} \rho^y_{\alpha'\beta'} \,|\, z_\alpha \rangle \langle z_\alpha \,|\, y_{\alpha'} \rangle \langle y_{\beta'} \,|\, z_\beta \rangle \langle z_\beta \,|$$

$\rightarrow$ $$\rho^z_{\alpha\beta} = \sum_{\alpha',\beta'} \rho^y_{\alpha'\beta'} \langle z_\alpha \,|\, y_{\alpha'} \rangle \langle y_{\beta'} \,|\, z_\beta \rangle$$

or $$\hat{\rho}^z = U^+ \hat{\rho}^y U$$

where $U$ is the transformation matrix with elements $U_{\beta'\beta} = \langle y_{\beta'} \,|\, z_\beta \rangle$.

With the help of §Code, we have

$$U = \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}$$

$$\hat{\rho}(t) = \begin{pmatrix} \frac{1}{10}(5 + 3\,\mathrm{Cos}[t\,\mu\,B_0] + 2\,\mathrm{Sin}[t\,\mu\,B_0]) & \frac{1}{10}(-2\,\mathrm{Cos}[t\,\mu\,B_0] + 3\,\mathrm{Sin}[t\,\mu\,B_0]) \\ \frac{1}{10}(-2\,\mathrm{Cos}[t\,\mu\,B_0] + 3\,\mathrm{Sin}[t\,\mu\,B_0]) & \frac{1}{10}(5 - 3\,\mathrm{Cos}[t\,\mu\,B_0] - 2\,\mathrm{Sin}[t\,\mu\,B_0]) \end{pmatrix} \tag{9}$$

## Code

Notations:

xp = $|\, x_+ \rangle$, xm = $|\, x_- \rangle$, etc.

yp* = $\langle x_+ \,|$, etc.

$\rho$pp = $\rho_{++}$, etc.

```
xp = 1/Sqrt[2] {1, 1}; xm = 1/Sqrt[2] {1, -1};
yp = 1/Sqrt[2] {-i, 1}; ym = 1/Sqrt[2] {i, 1};
```

```
zp = {1, 0}; zm = {0, 1};
```

$$\rho pp = \frac{6}{10} (yp^*.zp)\,(zp^*.yp) + \frac{4}{10} (yp^*.xm)\,(xm^*.yp)$$

$$\frac{1}{2}$$

$$\rho pm = \frac{6}{10} (yp^*.zp)\,(zp^*.ym) + \frac{4}{10} (yp^*.xm)\,(xm^*.ym)$$

$$-\frac{3}{10} - \frac{i}{5}$$

$$\rho mp = \frac{6}{10} (ym^*.zp)\,(zp^*.yp) + \frac{4}{10} (ym^*.xm)\,(xm^*.yp)$$

$$-\frac{3}{10} + \frac{i}{5}$$

$$\rho mm = \frac{6}{10} (ym^*.zp)\,(zp^*.ym) + \frac{4}{10} (ym^*.xm)\,(xm^*.ym)$$

$$\frac{1}{2}$$

$$\rho = \begin{pmatrix} \rho pp & \rho pm \\ \rho mp & \rho mm \end{pmatrix};$$

```
ρ // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & -\frac{3}{10} - \frac{i}{5} \\ -\frac{3}{10} + \frac{i}{5} & \frac{1}{2} \end{pmatrix}$$

$$U = \begin{pmatrix} yp^*.zp & yp^*.zm \\ ym^*.zp & ym^*.zm \end{pmatrix};$$

```
U // MatrixForm
```

$$\begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
ρz = U†.ρ.U;
ρz // MatrixForm
```

$$\begin{pmatrix} \frac{4}{5} & -\frac{1}{5} \\ -\frac{1}{5} & \frac{1}{5} \end{pmatrix}$$

$$\rho t = \begin{pmatrix} \rho pp & \rho pm\, e^{-i \mu B_0 t} \\ \rho mp\, e^{i \mu B_0 t} & \rho mm \end{pmatrix};$$

```
ρzt = U†.ρt.U // ExpToTrig // Simplify;
ρzt // MatrixForm
```

$$\begin{pmatrix} \frac{1}{10} (5 + 3\,\mathrm{Cos}[t\,\mu\,B_0] + 2\,\mathrm{Sin}[t\,\mu\,B_0]) & \frac{1}{10} (-2\,\mathrm{Cos}[t\,\mu\,B_0] + 3\,\mathrm{Sin}[t\,\mu\,B_0]) \\ \frac{1}{10} (-2\,\mathrm{Cos}[t\,\mu\,B_0] + 3\,\mathrm{Sin}[t\,\mu\,B_0]) & \frac{1}{10} (5 - 3\,\mathrm{Cos}[t\,\mu\,B_0] - 2\,\mathrm{Sin}[t\,\mu\,B_0]) \end{pmatrix}$$

## Answer (c)

Using the *Mathematica* code below, we have

$$\langle S_z(0) \rangle = \text{Tr}\left[ \hat{S}_z\, \hat{\rho}(t) \right]$$

$$= \text{Tr}\left[ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \frac{4}{5} & -\frac{1}{5} \\ -\frac{1}{5} & \frac{1}{5} \end{pmatrix} \right]$$

$$= \frac{3}{10} \hbar \tag{10}$$

$$\langle S_z(t) \rangle = \text{Tr}\left[ \hat{S}_z\, \hat{\rho}(t) \right]$$

$$= \frac{1}{10} \hbar \left( 3 \,\text{Cos}[t\, \mu\, B_0] + 2 \,\text{Sin}[t\, \mu\, B_0] \right) \tag{11}$$

## Code

```
ħ/2 (1  0
     0 -1).(4/5  -1/5
             -1/5  1/5) // Tr // MatrixForm
```

$$\frac{3\hbar}{10}$$

```
ħ/2 (1  0
     0 -1).ρzt // Tr // Simplify
```

$$\frac{1}{10} \hbar \left(3\,\text{Cos}[t\, \mu\, B_0] + 2\,\text{Sin}[t\, \mu\, B_0]\right)$$