Fleming's Quantum-Master-Inequality in Spin-1/2-Systems

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Chapter 1

Introduction

1.1 Introductory remarks

As a continuation to a seminar talk I gave in the winter term of 2009 my thesis shall examine a general inequality in quantum mechanics for the case of spin-1/2-systems. The basis for all my considerations is provided by Gordon N. Fleming's publication entitled "Uses of a quantum master inequality" [1].

My seminar talk was focused on the first four chapters of Fleming's paper, namely the derivation of the inequality itself and a few basic applications including Heisenberg's uncertainty relation as a special case of Fleming's inequality.

In my thesis, however, I would like to examine Fleming's master inequality with special regard to spin-1/2-systems. The reasoning behind this is that spin-1/2-systems can be treated quite comfortably and, most importantly, the time evolution of these systems for arbitrary time-independent dynamics can be calculated exactly which allows for analytic comparison between factual time evolution and its estimate given by the master inequality.

1.2 Quantum Master Inequality

As a first step we will derive Fleming's quantum master inequality (QMIE) from basic quantum-mechanical deliberations. This inequality in a slightly modified form yields an upper bound for the overlap of two different state vectors, ψ and ψ' (with $|\psi| = |\psi'| = 1$), as a function of the expectation value $\langle A \rangle$ and the rms deviation ΔA of an arbitrary self-adjoint operator A

acting on those two states. The QMIE in its most general form looks like

$$|\langle\psi',\psi\rangle|^2 \leq \frac{(\Delta_\psi A + \Delta_{\psi'} A)^2}{(\langle A\rangle_\psi - \langle A\rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2}$$

with $\langle A\rangle_\psi$ and $\langle A\rangle_{\psi'}$ being the expectation values of A under ψ and ψ' and $\Delta_\psi A$ and $\Delta_{\psi'} A$ the respective rms deviations.

In our case, where we consider the time evolution due to an arbitrary time-independent dynamics one of the two state vectors will be the initial state ψ_0 and the other one will be the state ψ_t at a given time t, with the overlap of the two states being the survival probability P of the initial state up until the time t.

$$P(t) := |\langle\psi_t,\psi_0\rangle|^2$$

Moreover, a condition for saturating the QMIE is also presented in this chapter.

1.3 Specialisation to Spin-1/2-Systems

Up until now we have not considered a specialisation to spin-1/2-systems. Doing so will allow us to write the QMIE in a much simpler form due to the fact that any self-adjoint operator with the spectrum $\{1,-1\}$ on a spin-1/2-system can be written as a linear combination of Pauli matrices (excluding the unit matrix) and then has the property that its square is equal to the identity. Hence, the rms deviation can be written as a function of the expectation values

$$\Delta\sigma = \sqrt{1-\langle\sigma\rangle^2},$$

which results, as we will see, in a much more compact expression for the master inequality

$$|\langle\psi',\psi\rangle|^2 \leq \frac{1}{2}\left[1 + \langle\sigma\rangle_\psi\langle\sigma\rangle_{\psi'} + \Delta_\psi\sigma\Delta_{\psi'}\sigma\right].$$

1.4 Expectation value of the σ-operator

Now a quite simple and well arranged calculation of the expectation value of the σ-operator in an arbitrary direction r underlying an arbitrary time-independent dynamic, parameterised by n, with an arbitrary initial preparation in the direction of a is provided, since it became clear that the right-hand side of the QMIE for spin-1/2-systems is only a function of the expectation value of a chosen operator at two different times, in our case. The expectation value can then be expressed as a simple scalar product between the vector a describing the initial state and r_t as

$$\langle \sigma(r) \rangle_{\chi_t} = \langle a, r_t \rangle$$

with

$$r_t = \langle r, n \rangle\, n + \cos(2\omega t)\, (r - \langle r, n \rangle\, n) - \sin(2\omega t)\, (n \times r)\,,$$

which conceptually means that we describe the expectation value of a time-independet operator under a time-dependet wave function as the expectation value of a time-dependent operator acting on the initial time-independet state.

From that we see that the estimate of the factual time evolution given by the QMIE is a function of the three scalar products [1]$\langle n, r \rangle$, $\langle n, a \rangle$ and $\langle a, r \rangle$, since $\langle a, n \times r \rangle$ can be expressed using the scalar products between the three vectors, which is also shown.

1.5 Examples

As a neat example for the visualisation and for the further discussion special choices for a, n and r are made. By setting the y-component of all three vectors to zero the problem is reduced to a two-dimensional one and choosing an initial state in z-direction, the dynamics along the x-axis and varying the vector r along the unit circle in the x-z-plane, parameterised by its z-coordinate named ρ, gives us a demonstrative example for how the factual time evolution is estimated by the QMIE as (see def. 2)

$$Q = \frac{2}{\pi} \sqrt{1 - \rho^2}\; E(\rho)$$

with Q being the quality of the estimate and $E(\rho)$ denoting the elliptic integral of the second kind, which will be discussed in more detail throughout this example.To give a qualitative impression of the estimates fig. 1.1 shows the factual time evolution P and its estimate P_{QMIE}, given by the QMIE, for three different values of ρ.

[1]As we will see, $|r| = |n| = |a| = 1$ can be assumed without loss of generality.

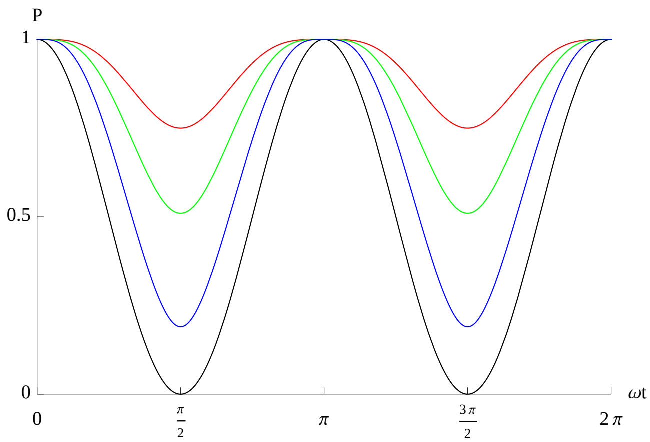

Figure 1.1: P (black) and P_{QMIE} for $\rho = 0.5$ (red), 0.7 (green) and 0.9 (blue)

Chapter 2

The Quantum Master Inequality

The foundation for all our considerations is provided by the Quantum Master Inequality, which shall be derived from basic quantum mechanics.

2.1 Derivation of the QMIE

Definition 1 *Let $\mathcal{H}$ be a Hilbert-space over $\mathbb{C}$ with its associated scalar product being denoted as $\langle\cdot,\cdot\rangle$. The norm induced by this scalar product shall be written as $|\cdot|$. For $\psi \in \mathcal{H}$ with $|\psi| = 1$, the linear mapping $A : \mathcal{H} \to \mathcal{H},\ \psi \mapsto A\psi$ is also called an operator.The expression $\langle A\rangle_\psi := \langle\psi, A\psi\rangle$ is called expectation value of A. $\Delta_\psi A := \sqrt{\langle A^2\rangle_\psi - \langle A\rangle_\psi^2}$ is the rms deviation of A.*

Proposition 1 *Let $\psi,\ \psi' \in \mathcal{H}$ be two normalized vectors in this Hilbert-space, namely $|\psi| = |\psi'| = 1$. Furthermore let $A : \mathcal{H} \to \mathcal{H}$ be a linear, continuos and self-adjoint mapping. Let $\theta \in [0, \pi/2]$ be such that $\cos\theta = |\langle\psi', \psi\rangle|$.Then*

$$|\langle A\rangle_\psi - \langle A\rangle_{\psi'}|\cos\theta \leq (\Delta_\psi A + \Delta_{\psi'} A)\sin\theta. \tag{2.1}$$

Given that $(\langle A\rangle_\psi - \langle A\rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2 \neq 0$, above inequality can be rearranged to

$$\cos^2\theta = |\langle\psi', \psi\rangle|^2 \leq \frac{(\Delta_\psi A + \Delta_{\psi'} A)^2}{(\langle A\rangle_\psi - \langle A\rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2}. \tag{2.2}$$

This inequality is dubbed Quantum Master Inequality (QMIE).

Prop. 1 has been given by Fleming in [1].

Remark 1 *What can be observed in ineq. 2.2 is that the absolute value of the scalar product (the overlap) between the two vectors ψ and ψ' is bounded by an expression involving an arbitrary choice for the operator A. This motivates the assumption that there might be more and less suitable choices for A in terms of how well the left-hand side is estimated by the right-hand side of the inequality.*

Furthermore the QMIE can generalise the observation that two eigenvectors corresponding to different eigenvalues of a self-adjoint operator are orthogonal. To see this, let us first take a look at why the two eigenvectors must be orthogonal. Let $A : \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator and for $\psi, \varphi \in \mathcal{H} \setminus 0$ let

$$(A-a)\,\psi = 0 \ \text{and} \ (A-b)\,\varphi = 0,$$

where $a, b \in \mathbb{R}$ and $a \neq b$. Let us now multiply the equation on the left-hand side with $\langle \varphi, \cdot \rangle$ (one could also multiply the equation on the right-hand side with $\langle \psi, \cdot \rangle$) in order to see

$$0 = \langle \varphi, A\psi \rangle - a\langle \varphi, \psi \rangle = \langle A\varphi, \psi \rangle - a\langle \varphi, \psi \rangle = (b-a)\,\langle \varphi, \psi \rangle,$$

which can only be true if $\langle \varphi, \psi \rangle = 0$, meaning that φ and ψ are orthogonal. Now we go back to the QMIE and rewrite it as

$$|\langle \psi', \psi \rangle|^2 \leq \frac{(\Delta_\psi A + \Delta_{\psi'} A)^2}{(\langle A \rangle_\psi - \langle A \rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2} = \frac{1}{1 + \left(\frac{\delta_A}{2}\right)^2},$$

with

$$\delta_A = \frac{\langle A \rangle_\psi - \langle A \rangle_{\psi'}}{\frac{\Delta_\psi A + \Delta_{\psi'} A}{2}}$$

which measures the difference of the two expectation values in units of the arithmetic average of the two rms deviations. Let us now put down the inequality for δ_A as

$$\frac{|\delta_A|}{2} \leq \sqrt{\frac{1}{|\langle \psi', \psi \rangle|^2} - 1}, \tag{2.3}$$

from which we see that $|\delta_A|$ can become larger as the overlap $|\langle \psi', \psi \rangle|$ gets closer to zero. This means that the more orthogonal two states are the better they can be distinguished, where orthogonal vectors (with an overlap of $|\langle \psi', \psi \rangle| = 0$) are perfectly distinguishable. Fig. 2.1 shows the right-hand side of ineq. 2.3 as a function of $|\langle \psi', \psi \rangle|$.

With the same premise, let us rewrite inequ. 2.1 for ψ and φ as

$$|\langle A \rangle_\psi - \langle A \rangle_\varphi| \cos\theta \leq (\Delta_\psi A + \Delta_\varphi A) \sin\theta.$$

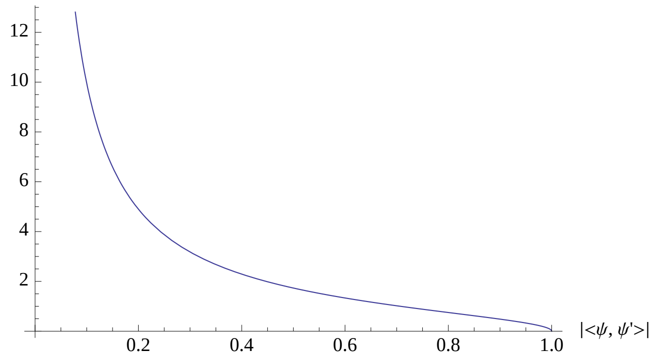

Figure 2.1: Right-hand side of ineq. 2.3

Since ψ and φ are eigenstates of the operator A their rms deviations are zero and their expectation values under A are the respective eigenvalues, hence

$$|a-b|\cos\theta \leq 0,$$

which can only be true if $\cos\theta = 0$, meaning that ψ and φ are orthogonal.

Now we will prove prop. 1.

Proof. First we define an auxiliary vector

$$\psi_A := A\psi - \langle A\rangle_\psi\, \psi$$

which has the properties that it is perpendicular to ψ and that its norm is $\Delta_\psi A$:

$$\psi_A \perp \psi : \langle A\psi - \langle A\rangle_\psi\, \psi, \psi\rangle = \langle A\psi, \psi\rangle - \langle A\rangle_\psi \langle \psi, \psi\rangle = 0$$

since $\langle \psi, \psi\rangle = |\psi|^2 = 1$ and $\langle A\psi, \psi\rangle = \langle \psi, A\psi\rangle$ because A is self-adjoint.

$$\begin{aligned}|\psi_A| = \Delta_\psi A : |\psi_A|^2 &= \langle A\psi - \langle A\rangle_\psi\, \psi, A\psi - \langle A\rangle_\psi\, \psi\rangle \\ &= \langle A^2\rangle_\psi - 2\langle A\rangle_\psi^2 + \langle A\rangle_\psi^2 \\ &= \langle A^2\rangle_\psi - \langle A\rangle_\psi^2 = (\Delta_\psi A)^2\,.\end{aligned}$$

Next we form the two expressions $\langle \psi', A\psi\rangle$, $\langle A\psi', \psi\rangle$ and represent them in terms of ψ_A and ψ'_A as

$$\langle \psi', A\psi\rangle = \langle \psi', \psi_A + \langle A\rangle_\psi\, \psi\rangle = \langle \psi', \psi_A\rangle + \langle A\rangle_\psi \langle \psi', \psi\rangle \tag{2.4}$$

and

$$\langle A\psi', \psi\rangle = \langle \psi'_A + \langle A\rangle_{\psi'}\, \psi', \psi\rangle = \langle \psi'_A, \psi\rangle + \langle A\rangle_{\psi'} \langle \psi', \psi\rangle. \tag{2.5}$$

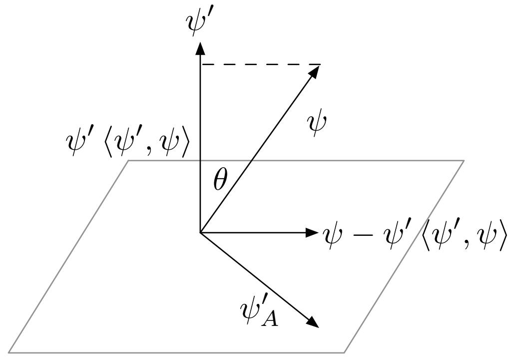

Figure 2.2: Geometric relations among the occurring vectors

As the left-hand sides of eq. 2.4 and eq. 2.5 are equal, rearranging terms yields

$$(\langle A \rangle_\psi - \langle A \rangle_{\psi'}) \langle \psi', \psi \rangle = \langle \psi'_A, \psi \rangle - \langle \psi', \psi_A \rangle.$$

Taking absolute values on both sides leaves us with

$$|\langle A \rangle_\psi - \langle A \rangle_{\psi'}| \, |\langle \psi', \psi \rangle| = |\langle \psi'_A, \psi \rangle - \langle \psi', \psi_A \rangle| \tag{2.6}$$

where the right-hand side can be estimated by (triangle inequality)

$$|\langle \psi'_A, \psi \rangle - \langle \psi', \psi_A \rangle| \leq |\langle \psi'_A, \psi \rangle| + |\langle \psi', \psi_A \rangle|$$

which is quickly commented on in rmk. 2.

Now, we take care of the two expressions $|\langle \psi'_A, \psi \rangle|$ and $|\langle \psi', \psi_A \rangle|$. To do this we first split up the vector ψ in a portion parallel to ψ' and one perpendicular to the direction of ψ' (see fig. 2.2), so that

$$\psi = (\psi - \psi' \langle \psi', \psi \rangle) + \psi' \langle \psi', \psi \rangle,$$

with the first summand being the perpendicular and the second being the parallel part. This decomposition is unique. Considering the norm square of ψ we obtain

$$\begin{aligned} 1 = |\psi|^2 &= |(\psi - \psi' \langle \psi', \psi \rangle) + \psi' \langle \psi', \psi \rangle|^2 \\ &= |\langle \psi', \psi \rangle|^2 + |\psi - \psi' \langle \psi', \psi \rangle|^2 \\ &= \cos^2 \theta + \sin^2 \theta, \end{aligned}$$

because the mixing terms $\langle \psi - \psi' \langle \psi', \psi \rangle, \psi' \langle \psi', \psi \rangle \rangle$ and its complex conjugate are zero, as they are the scalar product of two orthogonal vectors. From that, applying the relation $\cos\theta = |\langle \psi', \psi \rangle|$ from above , it is evident that

$$|\psi - \psi' \langle \psi', \psi \rangle|^2 = \sin^2\theta.$$

Finally with the Cauchy-Schwartz inequality (see rmk. 3 below) we can put down

$$|\langle \psi - \psi' \langle \psi', \psi \rangle, \psi'_A \rangle| \le |\psi - \psi' \langle \psi', \psi \rangle| \, |\psi'_A| = (\sin\theta) \, (\Delta_{\psi'} A) \, ,$$

which implies

$$|\langle \psi, \psi'_A \rangle| \le (\sin\theta) \, (\Delta_{\psi'} A)$$

since ψ' is perpendicular to ψ'_A. Repeating these calculations from the point where we considered the absolute square of ψ, this time interchanging ψ and ψ' yields

$$|\langle \psi', \psi_A \rangle| \le (\sin\theta) \, (\Delta_{\psi} A) \, .$$

Going back to eq. 2.6 and applying all the steps we have picked up in the meantime we obtain the Quantum Master Inequality

$$|\langle A \rangle_\psi - \langle A \rangle_{\psi'}| \cos\theta \le (\Delta_\psi A + \Delta_{\psi'} A) \sin\theta, \tag{2.7}$$

which risen to the power of two under application of the relation $\cos^2\theta + \sin^2\theta = 1$ and upon rearranging terms, provided that $(\langle A \rangle_\psi - \langle A \rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2 \neq 0$, gives us

$$|\langle \psi', \psi \rangle|^2 \le \frac{(\Delta_\psi A + \Delta_{\psi'} A)^2}{(\langle A \rangle_\psi - \langle A \rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2}, \tag{2.8}$$

an upper bound for the overlap between ψ and ψ'. $\square$

2.2 Auxiliary relations

As already mentioned, in the course of proving the QMIE two geometric relations come to show, namely the triangle inequality and the Cauchy-Schwartz inequality. These relations shall be looked upon in the context of complex numbers as this is our working ground.

Remark 2 *As the scalar products between two arbitrary vectors in our Hilbert-space $\mathcal{H}$ are complex numbers we can write $\langle \psi'_A, \psi \rangle = \alpha$ and $\langle \psi', \psi_A \rangle = \beta$ with $\alpha, \beta \in \mathbb{C}$. Thus, the relation*

$$|\alpha - \beta| \le |\alpha| + |\beta|$$

upon replacing β by $-\beta$ becomes the triangle inequality

$$|\alpha + \beta| \leq |\alpha| + |\beta|\,,$$

which can be proven analogously to its proof in [2], with $\bar{\alpha}$ and $\bar{\beta}$ being the complex conjugates of α and β, like this:

$$\begin{aligned}
|\alpha + \beta|^2 &= (\alpha + \beta)\left(\bar{\alpha} + \bar{\beta}\right) \\
&= \alpha\bar{\alpha} + \left(\alpha\bar{\beta} + \bar{\alpha}\beta\right) + \beta\bar{\beta} \\
&= |\alpha|^2 + 2\mathbf{R}\left(\alpha\bar{\beta}\right) + |\beta|^2 \\
&\leq |\alpha|^2 + 2\left|\alpha\bar{\beta}\right| + |\beta|^2 \qquad \textit{since } \mathbf{R}\, z \leq |z| \;\; \forall\, z \in \mathbb{C} \\
&= |\alpha|^2 + 2\,|\alpha|\,|\beta| + |\beta|^2 \qquad \textit{as } \; |\bar{z}| = |z| \\
&= (|\alpha| + |\beta|)^2\,.
\end{aligned}$$

Above yields

$$|\alpha + \beta|^2 \leq (|\alpha| + |\beta|)^2$$

which, upon taking the square root, since both sides are positive real numbers, results in the triangle inequality, as claimed.

Remark 3 *Besides the triangle inequality the Cauchy-Schwartz inequality is also relevant in proving the QMIE. Thus, this inequality shall be proven as presented in [3]. With x, y being two vectors in a Hilbert-space the Cauchy-Schwartz inequality reads*

$$|\langle x, y\rangle|^2 \leq \langle x, x\rangle\,\langle y, y\rangle \qquad x, y \in \mathcal{H}.$$

Suppose now that $y \neq 0$ and $\alpha \in \mathbb{C}$. With that we can write down

$$\begin{aligned}
0 \leq \langle x - \alpha\, y, x - \alpha\, y\rangle =&\langle x, x\rangle - 2\mathbf{R}\langle x, \alpha\, y\rangle + |\alpha|^2\,\langle y, y\rangle \\
=&\langle x, x\rangle - 2\mathbf{R}\left(\alpha\langle x, y\rangle\right) + |\alpha|^2\,\langle y, y\rangle.
\end{aligned}$$

Setting

$$\alpha := \frac{\langle y, x\rangle}{\langle y, y\rangle}$$

yields

$$\begin{aligned}
0 \leq&\langle x, x\rangle - 2\mathbf{R}\left(\frac{\langle y, x\rangle}{\langle y, y\rangle}\langle x, y\rangle\right) + \frac{|\langle x, y\rangle|^2}{\langle y, y\rangle^2}\langle y, y\rangle \\
=&\langle x, x\rangle - \frac{|\langle x, y\rangle|^2}{\langle y, y\rangle},
\end{aligned}$$

where we obtain

$$|\langle x, y\rangle|^2 \leq \langle x, x\rangle \langle y, y\rangle$$

from, which after taking the square root, again since both sides are positive real numbers, leaves us with

$$|\langle x, y\rangle| \leq |x|\, |y| \,,$$

which is exactly what we have used in proving the QMIE. The strict inequality is valid if and only if x and y are linearly independent.

In the case of linearly dependent vectors, $x, y \in \mathcal{H}$ with $\alpha, \beta \in \mathbb{C}\backslash 0$ such that $\alpha\, x + \beta\, y = 0$ we can write $x = -\,(\beta/\alpha)\, y$ and we have

$$|\langle x, y\rangle|^2 = \left|\frac{\beta}{\alpha}\right|^2 \langle y, y\rangle^2 = \left\langle -\frac{\beta}{\alpha} y, -\frac{\beta}{\alpha} y \right\rangle \langle y, y\rangle = \langle x, x\rangle\langle y, y\rangle$$

as the saturation of the Cauchy-Schwartz inequality.

2.3 Deviance from Fleming's proof

Remark 4 *The proof that was presented here slightly deviates from Fleming's original proof in "Uses of a Quantum Master Inequality" [1]. In his proof Fleming defines ψ_A as*

$$\psi_A := \frac{A\psi - \langle A\rangle_\psi\, \psi}{\Delta_\psi A}$$

demanding the exclusion of the case $\Delta_A \psi = 0$ as this induces an artificial singularity in ψ_A. This problem can be circumvented as we did in our proof, setting aside the ostensive disadvantage that ψ_A is not normalised. The rest of the derivation basically utilises the same methods, except that Cauchy-Schwartz do not appear explicitly in finding an expression for $|\langle \psi_A, \psi' \rangle|$ and $|\langle \psi_A', \psi \rangle|$.

2.4 Quality of the estimate

Definition 2 *(Quality of the estimate) Let $[0, \tau] = I \subset \mathbb{R}$ be an interval in the domain of real numbers. Furthermore, let $\gamma : I \to \mathcal{H}$, $t \mapsto \gamma(t)$ be a continuous function and let A be an arbitrary linear, continuous and self-adjoint operator. With this we define the transition probability from the state $\gamma(0) =: \varphi$ at $t = 0$ to the state $\gamma(t) =: \gamma_t$ as*

$$P(t) = |\langle \gamma_t, \varphi \rangle|^2$$

and, given that $(\langle A\rangle_\varphi - \langle A\rangle_{\gamma_t})^2 + (\Delta_\varphi A + \Delta_{\gamma_t} A)^2 \neq 0$*, rewrite the right-hand side of the QMIE as*

$$P_{QMIE}(t) = \frac{(\Delta_\varphi A + \Delta_{\gamma_t} A)^2}{(\langle A\rangle_\varphi - \langle A\rangle_{\gamma_t})^2 + (\Delta_\varphi A + \Delta_{\gamma_t} A)^2},$$

which gives us $P, P_{QMIE} : I \to \mathbb{R}$ *as two real-valued functions of the real parameter* t*. From that we define*

$$Q := \frac{2}{\tau}\int_0^\tau (P_{QMIE}(t) - P(t))\,\mathrm{d}t \tag{2.9}$$

as the quality of the estimate of the transition probability by the QMIE in the interval $[0,\tau]$ *with respect to the operator* A*. The scaling factor of* 2 *in the definition of* Q *is included for later convenience only.*

Since $P_{QMIE}(t) \geq P(t)\ \forall\, t$ *we can conclude that for* $Q = 0$ *the estimate given by the QMIE in the chosen interval exactly equals* P*.*

2.5 Saturation of the QMIE

As discussed in rmk. 1 we have seen that there ought to be more and less suitable choices for the operator A in terms of how good the estimate can become. In fact, we will now give a condition the operator A has to adhere to, that leads to the saturation of the QMIE.

In order to do this we have to find a way to saturate the two inequalities that come to show in proving the QMIE, the triangle inequality and the Cauchy-Schwartz inequality as these two inequalities are the only estimates that appear in deriving the QMIE and by saturating those, we saturate the QMIE.

Proposition 2 *Let* $A : \mathcal{H} \to \mathcal{H}$ *be a linear, self-adjoint and continuos operator,* $\psi, \psi' \in \mathcal{H}$ *with* $|\psi| = |\psi'| = 1$*. Furthermore let* θ *be defined as above. Then if and only if (i)*

$$\langle \psi', A\psi\rangle = \lambda\langle \psi, \psi'\rangle,$$

with

$$\min\{\langle A\rangle_\psi, \langle A\rangle_{\psi'}\} \leq \lambda \leq \max\{\langle A\rangle_\psi, \langle A\rangle_{\psi'}\}$$

and (ii) the operator A *stabilises the subspace* $\mathbb{C}\,\psi + \mathbb{C}\,\psi'$*, namely*

$$A\,(\mathbb{C}\,\psi + \mathbb{C}\,\psi') \subseteq (\mathbb{C}\,\psi + \mathbb{C}\,\psi'),$$

the QMIE becomes saturated, so that

$$|\langle A\rangle_\psi - \langle A\rangle_{\psi'}| \cos\theta = (\Delta_\psi A + \Delta_{\psi'} A)\sin\theta.$$

Proof. As mentioned, by saturating the triangle inequality

$$|\langle A\rangle_\psi - \langle A\rangle_{\psi'}|\, |\langle \psi', \psi\rangle| = |\langle \psi'_A, \psi\rangle - \langle \psi', \psi_A\rangle| \leq |\langle \psi'_A, \psi\rangle| + |\langle \psi', \psi_A\rangle|$$

as well as the two Cauchy-Schwartz inequalities

$$\begin{aligned} |\langle \psi, \psi'_A\rangle| &= |\langle \psi - \psi' \langle \psi', \psi\rangle, \psi'_A\rangle| \leq |\psi - \psi' \langle \psi', \psi\rangle|\; |\psi'_A| \\ |\langle \psi', \psi_A\rangle| &= |\langle \psi' - \psi \langle \psi, \psi'\rangle, \psi_A\rangle| \leq |\psi' - \psi \langle \psi, \psi'\rangle|\; |\psi_A| \end{aligned}$$

the QMIE becomes saturated. So, let us first try to see prop. 2 for the triangle inequality, which becomes saturated if

$$|\langle \psi'_A, \psi\rangle - \langle \psi', \psi_A\rangle| = |\langle \psi'_A, \psi\rangle| + |\langle \psi', \psi_A\rangle|\,.$$

In order to do this we have to find a pair $(\alpha, \beta) \in (\mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0}) \setminus (0, 0)$ such that

$$\alpha \langle \psi'_A, \psi\rangle + \beta \langle \psi', \psi_A\rangle = 0,$$

hence

$$\begin{aligned} 0 &= \alpha \langle A\psi' - \langle A\rangle_{\psi'}, \psi\rangle + \beta \langle \psi', A\psi - \langle A\rangle_\psi \psi\rangle \\ &= \alpha \langle A\psi', \psi\rangle + \beta \langle \psi', A\psi\rangle - \alpha \langle A\rangle_{\psi'} \langle \psi', \psi\rangle - \beta \langle A\rangle_\psi \langle \psi', \psi\rangle \\ &= (\alpha + \beta) \langle \psi', A\psi\rangle - (\alpha \langle A\rangle_{\psi'} + \beta \langle A\rangle_\psi) \langle \psi', \psi\rangle \end{aligned}$$

and as $\alpha + \beta > 0$ we can rewrite this to

$$\langle \psi', \psi\rangle = \lambda \langle \psi', \psi\rangle$$

with

$$\lambda = \frac{\alpha}{\alpha + \beta} \langle A\rangle_{\psi'} + \frac{\beta}{\alpha + \beta} \langle A\rangle_\psi$$

where, since $\frac{\alpha}{\alpha+\beta} + \frac{\beta}{\alpha+\beta} = 1$, λ is a convex combination of the two expectation values $\langle A\rangle_{\psi'}$ and $\langle A\rangle_\psi$ and therefore lies in the interval that is bounded by those.

Let us note that for $\theta = 0$, both sides of the QMIE are zero as $\sin\theta = 0$ and we can write $\psi' = e^{i\alpha}\, \psi$ with $\alpha \in \mathbb{R}$, giving us identical expectation values $\langle A\rangle_{\psi'}$ and $\langle A\rangle_\psi$, so that the left-hand side is zero as well. Thus, the QMIE saturates in a trivial way.

We can now look at the Cauchy-Schwartz inequality for $\theta > 0$: to saturate this inequality the involved vectors have to be complex multiples of each other, i.e.,

$$\begin{aligned} \psi_A &\in \mathbb{C}\left(\psi' - \psi\left\langle\psi, \psi'\right\rangle\right) \\ \psi'_A &\in \mathbb{C}\left(\psi - \psi'\left\langle\psi', \psi\right\rangle\right) \end{aligned}$$

and we note that, since $\theta > 0$, $\psi' - \psi\left\langle\psi, \psi'\right\rangle \neq 0 \neq \psi - \psi'\left\langle\psi', \psi\right\rangle$. As $\psi_A = A\psi - \langle A\rangle_\psi \psi$ the two above equations imply that

$$\begin{aligned} A\psi &\in \mathbb{C}\,\psi + \mathbb{C}\,\psi' \\ A\psi' &\in \mathbb{C}\,\psi + \mathbb{C}\,\psi'. \end{aligned}$$

On the other hand, as $\psi_A \perp \psi$ and $\psi'_A \perp \psi'$

$$\begin{aligned} \psi_A &\parallel \left(\psi' - \psi\left\langle\psi, \psi'\right\rangle\right) \\ \psi'_A &\parallel \left(\psi - \psi'\left\langle\psi', \psi\right\rangle\right) \end{aligned}$$

directly follows from

$$A\left(\mathbb{C}\,\psi + \mathbb{C}\,\psi'\right) \subseteq \left(\mathbb{C}\,\psi + \mathbb{C}\,\psi'\right).$$

This is because the space that is spanned by ψ and ψ' is two-dimensional. We know that $\psi_A \perp \psi$, which defines one of the two directions uniquely. We also know that $\psi \perp \left(\psi' - \psi\left\langle\psi, \psi'\right\rangle\right)$ and therefore it is evident, that $\psi_A \parallel \left(\psi' - \psi\left\langle\psi, \psi'\right\rangle\right)$, which is exactly what we need for saturating the Cauchy-Schwartz inequality.

The same argument can be repeated for ψ'_A and $\left(\psi - \psi'\left\langle\psi', \psi\right\rangle\right)$. $\square$

Chapter 3

Specialisation to spin-1/2-systems

So far we have not applied to the fact that we will be working with spin-1/2-systems. Thus, our next step is to rewrite the QMIE for such a system by considering its special properties, for instance the relation between the expectation value of the σ-operator and its rms deviation.

3.1 Hilbert-space and state vector

Our first step in specialising our generic discussion from above to spin-1/2-systems is to choose our Hilbert-space accordingly. We will from now on be working with $\mathcal{H} = \mathbb{C}^2$, which allows us to write down our most general state as

$$\chi = c_+\chi_+ + c_-\chi_-,$$

where χ_+ and χ_- form an orthonormal basis and c_+, $c_- \in \mathbb{C}$.

3.2 Parametrisation of the observables

Let us now study the σ-operator, since it will replace the operator A in the QMIE for spin-1/2-systems.

Remark 5 *The most general self-adjoint operator one can write down in* $\mathcal{H} = \mathbb{C}^2$ *is*

$$A = s\,\mathbf{1} + \sigma(r)$$

where $s \in \mathbb{R}$*,* $\mathbf{1}$ *is the two-dimensional unit matrix and*

$$\sigma(r) = r_1\,\sigma^1 + r_2\,\sigma^2 + r_3\,\sigma^3 \tag{3.1}$$

with $r = (r_1, r_2, r_3) \in \mathbb{R}^3$ *and*

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Let us examine the constituents of the QMIE for this general operator A*, namely*

$$\begin{aligned} \langle A\rangle_\psi - \langle A\rangle_{\psi'} =& \langle s\,\mathbf{1} + \sigma(r)\rangle_\psi - \langle s\,\mathbf{1} + \sigma(r)\rangle_{\psi'} \\ =& s + \langle \sigma(r)\rangle_\psi - s - \langle\sigma(r)\rangle_{\psi'} \\ =& \langle\sigma(r)\rangle_\psi - \langle\sigma(r)\rangle_{\psi'} \end{aligned}$$

and the rms deviations

$$\begin{aligned} (\Delta_\psi A)^2 =& \langle A^2\rangle_\psi - \langle A\rangle_\psi^2 \\ =& \langle (s\,\mathbf{1} + \sigma(r))^2\rangle_\psi - \langle s\,\mathbf{1} + \sigma(r)\rangle_\psi^2 \\ =& s^2 + 2s\,\langle\sigma(r)\rangle_\psi + \langle(\sigma(r))^2\rangle_\psi - s^2 - 2s\,\langle\sigma(r)\rangle_\psi - \langle\sigma(r)\rangle_\psi^2 \\ =& \langle(\sigma(r))^2\rangle_\psi - \langle\sigma(r)\rangle_\psi^2. \end{aligned}$$

From that it becomes evident that without loss of generality we can restrict ourselves to operators A *of the type*

$$A = \sigma(r).$$

Now we will introduce a very important relation for the product of two σ-matrices.

Proposition 3 *Let* $\sigma(r) = r_1\,\sigma^1 + r_2\,\sigma^2 + r_3\,\sigma^3$ *be a linear combination of the three* σ*-matrices and* $r = (r_1, r_2, r_3), s = (s_1, s_2, s_3) \in \mathbb{R}^3$ *then*

$$\sigma(r)\,\sigma(s) = \langle r, s\rangle + i\,\sigma(r \times s). \tag{3.2}$$

Proof. If we write down the matrix multiplication explicitly as

$$\sigma(r)\,\sigma(s) = \begin{pmatrix} r_3 & r_1 - i\,r_2 \\ r_1 + i\,r_2 & -r_3 \end{pmatrix} \cdot \begin{pmatrix} s_3 & s_1 - i\,s_2 \\ s_1 + i\,s_2 & -s_3 \end{pmatrix} = \begin{pmatrix} \eta_{11} & \eta_{12} \\ \eta_{21} & \eta_{22} \end{pmatrix}$$

we can put down

$$\begin{aligned}
\eta_{11} =& r_3 s_3 + r_1 s_1 + r_2 s_2 + i\,(r_1 s_2 - r_2 s_1)\\
=& \langle r, s\rangle + i\,[r \times s]_3\\
\eta_{12} =& r_3 s_1 - i\,r_3 s_2 - r_1 s_3 + i\,r_2 s_3\\
=& i\,(r_2 s_3 - r_3 s_2) + r_3 s_1 - r_1 s_3\\
=& i\big([r \times s]_1 - i\,[r \times s]_2\big)\\
\eta_{21} =& r_1 s_3 + i\,r_2 s_3 - r_3 s_1 - i\,r_3 s_2\\
=& i\,(r_2 s_3 - r_3 s_2) - r_3 s_1 + r_1 s_3\\
=& i\big([r \times s]_1 + i\,[r \times s]_2\big)\\
\eta_{22} =& r_3 s_3 + r_1 s_1 + r_2 s_2 - i\,(r_1 s_2 - r_2 s_1)\\
=& \langle r, s\rangle - i\,[r \times s]_3
\end{aligned}$$

and therefore write

$$\sigma(r)\,\sigma(s) = \begin{pmatrix} \langle r, s\rangle + i\,[r \times s]_3 & i\big([r \times s]_1 - i\,[r \times s]_2\big) \\ i\big([r \times s]_1 + i\,[r \times s]_2\big) & \langle r, s\rangle - i\,[r \times s]_3 \end{pmatrix}$$

which corresponds to

$$\sigma(r)\,\sigma(s) = \langle r, s\rangle + i\,\sigma(r \times s),$$

where $\langle r, s\rangle$ ist the scalar product and $r \times s$ is the vector product between the two vectors r and s. □

From this and the explicit representation in the matrix form the following properties (see [4], ch. IX §B) can be seen:

(a) If we choose $r = s$ we get

$$\sigma(r)\,\sigma(r) = (\sigma(r))^2 = |r|^2$$

as $\langle r, r\rangle = |r|^2$ and the vector product of a vector with itself is zero.

(b) If we set $s = r$ and $r = e_1$ or $r = e_2$ or $r = e_3$ we find

$$\left(\sigma^1\right)^2 = \left(\sigma^2\right)^2 = \left(\sigma^3\right)^2 = \mathbf{1}.$$

(c) For $r = e_j$ and $s = e_k$ for $j, k \in \{1, 2, 3\}$ and $j \neq k$ we get

$$\sigma^j\,\sigma^k + \sigma^k\,\sigma^j = 0$$

since the scalar product of two orthogonal vectors is zero and the vector product cancels, because it is antisymmetric.

(d) In the same manner, for $j, k \in \{1, 2, 3\}$

$$\left[\sigma^j, \sigma^k\right] := \sigma^j \, \sigma^k - \sigma^k \, \sigma^j = 2i \sum_{l=1}^{3} \epsilon^{jkl} \, \sigma^l,$$

because the scalar products again are zero, the vector product is anti-symmetric which in combination with the minus in the definition gives us the term $\sigma^j \, \sigma^k$ twice, and lastly $e_j \times e_k = \sum_{l=1}^{3} \epsilon^{jkl} \, e_l$.

(e) From the previous item, one can almost instantly see for $j, k \in \{1, 2, 3\}$ and $j \neq k$

$$\sigma^j \, \sigma^k = i \sum_{l=1}^{3} \epsilon^{jkl} \, \sigma^l.$$

(f) Finally, from the matrix representation we obtain

$$\operatorname{tr}(\sigma(r)) = \operatorname{tr} \begin{pmatrix} r_3 & r_1 - i \, r_2 \\ r_1 + i \, r_2 & -r_3 \end{pmatrix} = 0$$

and

$$\det(\sigma(r)) = \det \begin{pmatrix} r_3 & r_1 - i \, r_2 \\ r_1 + i \, r_2 & -r_3 \end{pmatrix} = -r_3^2 - (r_1^2 + r_2^2) = - |r|^2$$

Next, we examine a relation between the expectation value $\langle \sigma(r) \rangle_\psi$ and the rms deviation $\Delta_\psi \sigma(r)$ of the σ-operator under an arbitrary wave function ψ. Since the rms deviation is defined (see ch. 2) as

$$\Delta_\psi \sigma(r) = \sqrt{\langle (\sigma(r))^2 \rangle_\psi - \langle \sigma(r) \rangle_\psi^2},$$

using prop. 3 we can rewrite $\Delta_\psi \sigma(r)$ as

$$\begin{aligned} \Delta_\psi \sigma(r) &= \sqrt{\langle |r|^2 \, \mathbf{1} \rangle_\psi - \langle \sigma(r) \rangle_\psi^2} \\ &= |r| \sqrt{1 - \frac{\langle \sigma(r) \rangle_\psi^2}{|r|^2}}, \end{aligned} \tag{3.3}$$

which if we set $|r| = 1$, which we can do without loss of generality (see rmk. 6), becomes even more simple, namely

$$\Delta_\psi \sigma(r) = \sqrt{1 - \langle \sigma(r) \rangle_\psi^2}. \tag{3.4}$$

Remark 6 *In regards to the above observation we should examine whether or not the upper bound given by the QMIE remains the same if we demand that $|r| = 1$. For that we look at the rescaling of an arbitrary self-adjoint operator A and its consequences for the master inequality. Let us write down our operator for the inequality as $\lambda \cdot A$, where $\lambda \in \mathbb{R}_{>0}$. Now putting down the right-hand side of the QMIE as*

$$P_{QMIE} = \frac{(\Delta_\psi \lambda A + \Delta_{\psi'} \lambda A)^2}{(\langle \lambda A \rangle_\psi - \langle \lambda A \rangle_{\psi'})^2 + (\Delta_\psi \lambda A + \Delta_{\psi'} \lambda A)^2},$$

where

$$\langle \lambda A \rangle_\psi = \langle \psi, \lambda A \psi \rangle = \lambda \cdot \langle A \rangle_\psi$$

and therefore also

$$\Delta_\psi \lambda A = \sqrt{\langle (\lambda A)^2 \rangle_\psi - \langle \lambda A \rangle_\psi^2} = \lambda \cdot \sqrt{\langle A^2 \rangle_\psi - \langle A \rangle_\psi} = \lambda \cdot \Delta_\psi A,$$

we see that λ does not alter the upper bound given by the QMIE because

$$P_{QMIE} = \frac{\lambda^2}{\lambda^2} \frac{(\Delta_\psi A + \Delta_{\psi'} A)^2}{(\langle A \rangle_\psi - \langle A \rangle_{\psi'})^2 + (\Delta_\psi A + \Delta_{\psi'} A)^2},$$

where it is needless to say that $\lambda^2 / \lambda^2 = 1$.

If we now set $A = \sigma(r)$ and $\lambda = 1/|r|$ we can properly motivate why we are able to choose $|r| = 1$ without loss of generality.

3.3 QMIE for a spin-1/2-system

Taking advantage of the relation we obtained in the previous section we can now rewrite the QMIE to give it a much more compact form.

Proposition 4 *Let $\mathcal{H} = \mathbb{C}^2$ be the Hilbert-space of a spin-1/2-system, $\psi, \psi' \in \mathcal{H}$ with $|\psi| = |\psi'| = 1$ two normalised state vectors, $r = (r_1, r_2, r_3) \in \mathbb{R}^3$ where $|r| = 1$ and $\sigma : \mathcal{H} \to \mathcal{H}$ $\psi \mapsto \sigma(r)\,\psi = (r_1\,\sigma^1 + r_2\,\sigma^2 + r_3\,\sigma^3)\;\psi$, then*

$$|\langle \psi', \psi \rangle|^2 \leq \frac{1}{2} \left[1 + \langle \sigma \rangle_\psi \langle \sigma \rangle_{\psi'} + \Delta_\psi \sigma \Delta_{\psi'} \sigma \right].$$

Proof. Departing from the right-hand side of ineq. 2.2 and using eq. 3.4 with the abbreviations $x := \langle\sigma(r)\rangle_\psi$ and $y := \langle\sigma(r)\rangle_{\psi'}$ we can write

$$\begin{aligned}
P_{QMIE} &= \frac{\left(\Delta_\psi\sigma + \Delta_{\psi'}\sigma\right)^2}{\left(\langle\sigma\rangle_\psi - \langle\sigma\rangle_{\psi'}\right)^2 + \left(\Delta_\psi\sigma + \Delta_{\psi'}\sigma\right)^2} \\
&= \frac{\left(\sqrt{1-x^2}+\sqrt{1-y^2}\right)^2}{(x-y)^2 + \left(\sqrt{1-x^2}+\sqrt{1-y^2}\right)^2} \\
&= \frac{\left(\sqrt{1-x^2}+\sqrt{1-y^2}\right)^2}{x^2 - 2xy + y^2 + 1 - x^2 + 2\sqrt{1-x^2}\sqrt{1-y^2} + 1 - y^2} \\
&= \frac{1}{2}\,\frac{\left(\sqrt{1-x^2}+\sqrt{1-y^2}\right)^2}{1 - xy + \sqrt{1-x^2}\sqrt{1-y^2}}
\end{aligned}$$

Now defining $a := \sqrt{1-x^2}$ and $b := \sqrt{1-y^2}$ with $\epsilon \in \{-1, 1\}$ we rewrite the last expression as

$$\frac{1}{2}\,\frac{(a+b)^2}{1 + ab - \epsilon\sqrt{1-a^2}\sqrt{1-b^2}}$$

and extend the fraction by $1 + ab + \epsilon\sqrt{1-a^2}\sqrt{1-b^2} = 1 + ab + xy$ in order to get rid of the square roots in the denominator, which leaves us with

$$\frac{1}{2}\,\frac{(a+b)^2}{(1+ab)^2 - (1-a^2)(1-b^2)}\left[1 + ab + xy\right],$$

where

$$\frac{(a+b)^2}{(1+ab)^2 - (1-a^2)(1-b^2)} = \frac{(a+b)^2}{1 + 2ab + a^2b^2 - 1 + a^2 + b^2 - a^2b^2} = 1.$$

Replacing the abbreviations with their actual values again we obtain

$$P_{QMIE} = \frac{1}{2}\left[1 + \langle\sigma\rangle_\psi\langle\sigma\rangle_{\psi'} + \Delta_\psi\sigma\Delta_{\psi'}\sigma\right],$$

where, as noted, $\Delta\sigma$ is a function of $\langle\sigma\rangle$. □

Fig. 3.1 and fig. 3.2 show $P_{QMIE} : [-1, 1] \times [-1, 1] \to [0, 1]$,

$$(x, y) \mapsto \frac{1}{2}\left[1 + xy + \sqrt{1-x^2}\sqrt{1-y^2}\right].$$

As it has become clear from these considerations the only value of interest for the QMIE in a spin-1/2-system is the expectation value of the σ-operator under ψ and ψ'. Hence, our next step is to find a suitable expression for the expectation value $\langle\sigma\rangle$.

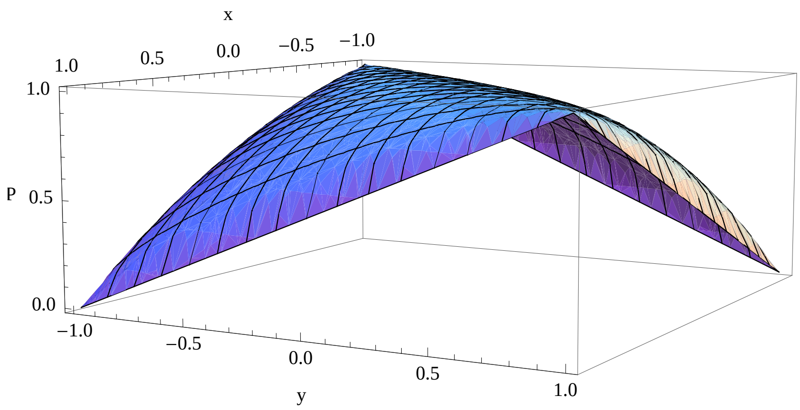

Figure 3.1: P_{QMIE} in the square $[-1, 1] \times [-1, 1]$ (seen from above)

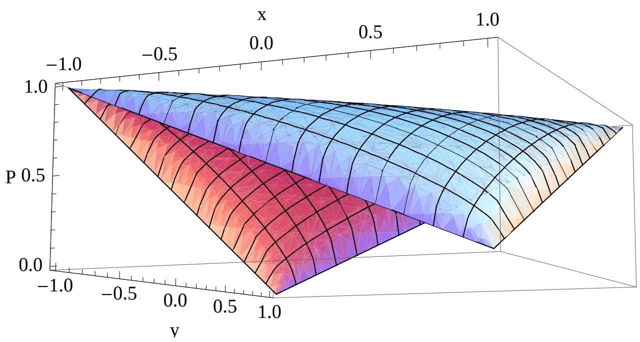

Figure 3.2: P_{QMIE} in the square $[-1, 1] \times [-1, 1]$ (seen from below)

3.4 Expectation value of the σ-operator

We will now consider the expectation value of the σ-operator under a time-evolving wave function due a general time-independent dynamics, since, as mentioned above, this is the only quantity of interest in our case.

Proposition 5 *Let $\mathcal{H} = \mathbb{C}^2$ be the Hilbert-space of a spin-1/2-system exposed to the dynamics $H = \hbar\omega\sigma(n)$ with $\sigma(n) = n_1\,\sigma^1 + n_2\,\sigma^2 + n_3\,\sigma^3$ where $n \in \mathbb{R}^3$ and $|n| = 1$. Furthermore let $a \in \mathbb{R}^3$ with $|a| = 1$ and $\chi_a \in \mathcal{H}$ shall satisfy $\sigma(a)\chi_a = \chi_a$, then for $\chi_t = U(t)\,\chi_a = \exp\left(-i\omega\sigma(n)t\right)\,\chi_a$ and $r \in \mathbb{R}^3$ with $|r| = 1$*

$$\langle\sigma(r)\rangle_{\chi_t} = \langle a, r_t\rangle,$$

where

$$r_t = \langle r, n\rangle\, n + \cos(2\omega t)\,(r - \langle r, n\rangle\, n) - \sin(2\omega t)\,(n \times r)\,.$$

Here the Euclidian scalar product is also denoted as $\langle\cdot,\cdot\rangle$ and it should be clear from the context which scalar product the notation refers to.

In order to prove prop. 5 let us examine step by step the expressions it is made up of: first we have $U(t)$, the time evolution operator and secondly, we need to rewrite the expression for the expectation value in terms of a trace of a projection operator in order to obtain the result in this simple form, as presented. Therefore these two objects shall be discussed.

Remark 7 *(Time evolution operator, see [6], ch. 4, §3) The basic time-evolution of our system is given by the Schrödinger equation,*

$$i\hbar\dot{\psi} = H\psi,$$

where ψ is our wave function with $|\psi| = 1$ and H ("Hamiltonian") describes the dynamics the system is exposed to. With the family of evolution operators $\{U(t) : t \in \mathbb{R}\}$ it follows that

$$\psi(t) = U(t)\,\psi(0) =: U(t)\psi_0.$$

Thus we have a Schrödinger equation for $U(t)$

$$i\hbar\dot{U}(t) = HU(t).$$

This linear homogeneous first-order differential equation for $U(t)$ has the maximal solution

$$U(t) = \exp\left[\frac{-iHt}{\hbar}\right]\,U(0).$$

Since $\psi(t=0) = U(0)\psi_0 = \psi_0$ implies $U(0) = 1$, we obtain

$$U(t) = \exp\left[\frac{-iHt}{\hbar}\right].$$

Remark 8 *(Expectation value via trace of a projection operator) Next, a way to rewrite the expectation value shall be discussed. Up until now the expectation value of an operator A (under the wave function ψ) has been defined as*

$$\langle A\rangle_\psi := \langle \psi, A\psi\rangle.$$

Now we will introduce the orthogonal projection operator onto the subspace of the Hilbert-space $\mathcal{H}$ that is spanned by ψ as

$$\Pi^\psi := \psi\,\langle \psi, \cdot\rangle.$$

With this we can rewrite the expectation value, analogously to [7], §5.2 as

$$\langle A\rangle_\psi = \mathrm{tr}\left(\Pi^\psi A\right).$$

The last thing to do now is to write down the projection operator for the state χ_a, which satisfies $\sigma(a)\chi_a = \chi_a$ as

$$\Pi^{\chi_a} =: P^a = \frac{1+\sigma(a)}{2},$$

which is also presented in [7], §5.2 in the context of density and projection operators on a Hilber-space $\mathcal{H} = \mathbb{C}^2$. It is easy to see that

$$P^a\chi_a = \frac{(1+\sigma(a))\,\chi_a}{2} = \frac{\chi_a + \chi_a}{2} = \chi_a$$

and with $\sigma(a)\varphi_a = -\varphi_a$ where $\langle \varphi_a, \chi_a\rangle = 0$ we get

$$P^a\varphi_a = \frac{(1+\sigma(a))\,\varphi_a}{2} = \frac{\varphi_a - \varphi_a}{2} = 0.$$

So P^a is clearly the orthogonal projection on the subspace of $\mathcal{H}$, spanned by χ_a, our initial state.

One more final thing we have to look at before being able to prove prop. 5 is the expression

$$U(t) = \exp\left(-i\omega\sigma(n)t\right).$$

What we do here is to write out the exponential function as a sum explicitly and then use prop. 3, i.e. $(\sigma(n))^2 = 1$, since we already specified that $|n| = 1$, therefore

$$\begin{aligned}
U(t) =& \exp\left(-i\omega\sigma(n)t\right) = \sum_{j=1}^{\infty} \frac{1}{j!}(-i)^j (\omega t)^j \left(\sigma(n)\right)^j \\
=& \sum_{j=1}^{\infty} \frac{1}{(2j+1)!}(-i)^{(2j+1)}(\omega t)^{(2j+1)} \left(\sigma(n)\right)^{(2j+1)} + \\
&+ \sum_{j=1}^{\infty} \frac{1}{(2j)!}(-i)^{(2j)}(\omega t)^{(2j)} \left(\sigma(n)\right)^{(2j)}
\end{aligned}$$

By splitting up the sum in two sub-sums for odd and even j we can apply a few identities, namely

$$(-i)^{(2j+1)} = (-i)\,(-i^2)^j = (-i)\,(-1)^j \qquad (-i)^{(2j)} = (-1)^j$$

and

$$\left(\sigma(n)\right)^{(2j+1)} = \sigma(n)\left(\sigma(n)\right)^{(2j)} = \sigma(n) \qquad \left(\sigma(n)\right)^{2j} = \mathbf{1}.$$

From this we get

$$\begin{aligned}
U(t) =& \cdots = \sum_{j=1}^{\infty} \frac{(-1)^j}{(2j)!}(\omega t)^{(2j)}\,\mathbf{1} - i\sum_{j=1}^{\infty} \frac{(-1)^j}{(2j+1)!}(\omega t)^{(2j+1)}\,\sigma(n) \\
=& \cos\omega t - i\sin\omega t\,\sigma(n)
\end{aligned}$$

Having discussed all the necessary tools and equipped with above results we can now prove prop. 5.

Proof. Departing from

$$\begin{aligned}
\langle\sigma(r)\rangle_{\chi_t} =& \langle\chi_t, \sigma(r)\chi_t\rangle = \langle U(t)\chi_a, \sigma(r)U(t)\chi_a\rangle \\
=& \langle\chi_a, U^*(t)\sigma(r)U(t)\chi_a\rangle \\
=& \mathrm{tr}\left(P^a U^*(t)\sigma(r)U(t)\right) = \mathrm{tr}\,\Omega
\end{aligned}$$

we have to find a suitable expression for $\Omega := P^a U^*(t)\sigma(r)U(t)$ in order to calculate its trace. Hence,

$$\begin{aligned}
\Omega =& P^a U^*(t)\sigma(r)U(t) \\
=& P^a\left[\cos\omega t + i\sin\omega t\,\sigma(n)\right]\sigma(r)\left[\cos\omega t - i\sin\omega t\,\sigma(n)\right] \\
=& P^a\left[\cos^2\omega t\sigma(r) + i\sin\omega t\cos\omega t\,\sigma_1(r,n) + \sin^2\omega t\,\sigma_2(r,n)\right],
\end{aligned}$$

where $\sigma_1(r,n) = \sigma(n)\sigma(r) - \sigma(r)\sigma(n)$ and $\sigma_2(r,n) = \sigma(n)\sigma(r)\sigma(n)$. Now simplifying $\sigma_1(r,n)$ we find

$$\begin{aligned}\sigma_1(r,n) =&\sigma(m)\sigma(r) - \sigma(n)\sigma(r)\\ =&\langle n,r\rangle + i\,\sigma(n\times r) - \langle r,n\rangle - i\,\sigma(r\times n)\\ =&2i\,\sigma(n\times r),\end{aligned}$$

since $\langle n,r\rangle = \langle r,n\rangle$ and $r\times n = -\,(n\times r)$. Similarly for $\sigma_2(r,n)$ we obtain

$$\begin{aligned}\sigma_2(r,n) =&\sigma(n)\sigma(r)\sigma(n)\\ =&\sigma(n)\left[\langle r,n\rangle + i\,\sigma(r\times n)\right]\\ =&\sigma(n)\langle r,n\rangle + i\left(\langle n, r\times n\rangle + i\,\sigma(n\times(r\times n))\right)\\ =&\sigma(n)\langle r,n\rangle - \sigma(r - n\langle n,r\rangle)\\ =&2\sigma(n)\langle r,n\rangle - \sigma(r),\end{aligned}$$

as $\langle n, n\times r\rangle = 0$ and $n\times(r\times n) = r\langle n,n\rangle - n\langle n,r\rangle$ (see [5], preface). Moving forward by applying the expressions we found for σ_1 and σ_2 we get

$$\Omega = P^a\left[\left(\cos^2\omega t - \sin^2\omega t\right)\,\sigma(r) - 2\sin\omega t\cos\omega t\,\sigma(n\times r) + 2\sin^2\omega t\,\sigma(n)\langle n,r\rangle\right].$$

With

$$\begin{aligned}\cos^2\omega t - \sin^2\omega t &= \cos(2\omega t)\\ 2\sin\omega t\cos\omega t &= \sin(2\omega t)\\ 2\sin^2\omega t &= 1 - \cos(2\omega t)\end{aligned}$$

as trigonometric identities (see [8]) we can rearrange our expression to

$$\Omega = P^a\left[\langle r,n\rangle\,\sigma(n) + \cos(2\omega t)\left(\sigma(r) - \langle r,n\rangle\,\sigma(n)\right) - \sin(2\omega t)\,\sigma(n\times r)\right],$$

which we will now write as

$$\Omega = P^a\sigma(r_t)$$

with

$$r_t = \langle r,n\rangle\,n + \cos(2\omega t)\left(r - \langle r,n\rangle\,n\right) - \sin(2\omega t)\left(n\times r\right).$$

Using the explicit representation for the projection operator we find

$$\begin{aligned}\Omega =&P^a\sigma(r_t)\\ =&\frac{1+\sigma(a)}{2}\,\sigma(r_t)\\ =&\frac{\sigma(r_t) + \sigma(a)\sigma(r_t)}{2}\\ =&\frac{\langle a, r_t\rangle}{2} + \frac{\sigma(r_t)}{2} + i\frac{\sigma(a\times r_t)}{2},\end{aligned}$$

where upon taking the trace only the first term is nonzero, since $\operatorname{tr}\sigma = 0$ and therefore the expectation value yields

$$\langle\sigma(r)\rangle_{\chi_t} = \operatorname{tr}\Omega = \frac{\langle a, r_t\rangle}{2}\operatorname{tr}\mathbf{1} = \langle a, r_t\rangle,$$

since the trace of the two-dimensional unit matrix is 2. □

3.5 Alternative derivation of $\langle\sigma\rangle$

Besides this simple and well-arranged derivation utilising more sophisticated and elegant methods, as we have seen, there is also the standard way of calculating the expectation value of $\sigma(r)$ under a time-evolving wave function χ_t, namely calculating the expectation value via its definition, as

$$\langle\sigma(r)\rangle_{\chi_t} = \langle\chi_t, \sigma(r)\chi_t\rangle,$$

where still $\chi_t = U(t)\chi_a$ and $\sigma(a)\chi_a = \chi_a$, though we now write the state vectors and operators out explicitly (in matrix form).

Our first thing to do is to find the explicit expression for χ_a as the normalised eigenvector to the eigenvalue 1 of the operator $\sigma(a) = a_1\,\sigma^1 + a_2\,\sigma^2 + a_3\,\sigma^3$ with $a \in \mathbb{R}^3$, $|a| = 1$, and

$$\sigma(a) = \begin{pmatrix} a_3 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 \end{pmatrix}.$$

This can be done by standard means of linear algebra (see app. A.2). For $a_3 > -1$ the normalised eigenvector χ_a is given (up to an arbitrary phase) by

$$\chi_a = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+a_3} \\ \frac{a_1+ia_2}{\sqrt{1+a_3}} \end{pmatrix}.$$

Secondly, we will represent the time-evolution operator in matrix form, so that

$$\begin{aligned} U(t) &= \cos\omega t - i\sin\omega t\,\sigma(n) \\ &= \begin{pmatrix} \cos\omega t - in_3\sin\omega t & -i\sin\omega t\,(n_1 - in_2) \\ -i\sin\omega t\,(n_1 + in_2) & \cos\omega t + in_3\sin\omega t \end{pmatrix} \end{aligned}$$

and lastly, we write $\sigma(r)$ analogously to $\sigma(a)$ as

$$\sigma(r) = \begin{pmatrix} r_3 & r_1 - ir_2 \\ r_1 + ir_2 & -r_3 \end{pmatrix}.$$

Now we can put down $\chi_t = U(t)\chi_a$ as

$$\chi_t = \frac{1}{\sqrt{2}}\begin{pmatrix}(\cos\omega t - in_3\sin\omega t)\sqrt{1+a_3} + (-i\sin\omega t\,(n_1 - in_2))\frac{a_1+ia_2}{\sqrt{1+a_3}} \\ (-i\sin\omega t\,(n_1+in_2))\sqrt{1+a_3} + (\cos\omega t + in_3\sin\omega t)\frac{a_1+ia_2}{\sqrt{1+a_3}}\end{pmatrix},$$

from which it becomes evident that this derivation, though conceptually simpler, is in fact a lot less clear and much harder to follow.

Moving on we calculate the expectation value

$$\langle\sigma(r)\rangle_{\chi_t} = (\chi_t)^\dagger \cdot \sigma(r) \cdot \chi_t$$

as the matrix product between the row vector $(\chi_t)^\dagger$, the matrix $\sigma(r)$ and the column vector χ_t, which gives us (see Mathematica-Code in app. A.2)

$$\begin{aligned}\langle\sigma\rangle &= a_1r_1 + (a_2r_2 + a_3r_3)\cos(2\omega t) \\ &\quad + 2\left[a_2n_2\,(n_1r_1 + n_2r_2 + n_3r_3) + a_3n_3\,(n_1r_1 + n_2r_2 + n_3r_3)\right. \\ &\quad \left.+\, a_1\left(n_1n_2r_2 + n_1n_3r_3 - n_2^2r_1 - n_3^2r_1\right)\right]\sin^2(\omega t) \\ &\quad + (a_3n_2r_1 - a_2n_3r_1 - a_3n_1r_2 + a_1n_3r_2 + a_2n_1r_3 - a_1n_2r_3)\sin(2\omega t),\end{aligned}$$

which at first sight looks pretty long and obscure, but after applying the relations

$$2\sin^2\omega t = 1 - \cos(2\omega t)$$

and, since $|n| = 1$,

$$n_1^2 = 1 - n_2^2 - n_3^2$$

can be written in the same compact form as we have seen in prop. 5.

3.6 Geometric relations among a, n and r

Now that we have seen in two different ways that

$$\langle\sigma(r)\rangle_{\chi_t} = \langle r,n\rangle\langle a,n\rangle + \cos(2\omega t)\,(\langle a,r\rangle - \langle r,n\rangle\langle a,n\rangle) - \sin(2\omega t)\langle a, n\times r\rangle,$$

let us examine the expression

$$\langle a, n\times r\rangle$$

which is called the parallelepipedial product (or scalar triple product) of the three vectors a, n and r and yields the volume of the parallelepiped that is spanned by these (see [9]). It can be written as

$$\langle a, n\times r\rangle = \det(a,n,r) = \det M \qquad M = \begin{pmatrix} a_1 & n_1 & r_1 \\ a_2 & n_2 & r_2 \\ a_3 & n_3 & r_3\end{pmatrix},$$

assuming that a_i, n_i and r_i are the respective coordinates of a, n and r in terms of the cartesian standard base, which has a positive orientation. Now looking at

$$(\langle a, n \times r\rangle)^2 = (\det M)^2 = \det M \ \det M^T = \det\left(MM^T\right),$$

where $MM^T =: G$ is the Gram-matrix of a, n and r and consists of the scalar products between pairs of these three vectors, namely

$$G = \begin{pmatrix} \langle a, a\rangle & \langle a, n\rangle & \langle a, r\rangle \\ \langle n, a\rangle & \langle n, n\rangle & \langle n, r\rangle \\ \langle r, a\rangle & \langle r, n\rangle & \langle r, r\rangle \end{pmatrix},$$

it is easy to see that the parallelepipedial product can be expressed using the scalar products among the vectors of which it is spanned.

Going back to our expectation value we can apply that $|a| = |n| = |r| = 1$ and furthermore note that the scalar product for real vectors is symmetric, therefore reducing G to a matrix of three independent entires

$$G = \begin{pmatrix} 1 & \langle a, n\rangle & \langle a, r\rangle \\ \langle a, n\rangle & 1 & \langle r, n\rangle \\ \langle a, r\rangle & \langle r, n\rangle & 1 \end{pmatrix}$$

and with this we are able to write

$$|\langle a, n \times r\rangle| = \sqrt{\det G} = \sqrt{1 - \alpha^2 - \beta^2 - \gamma^2 + 2\alpha\beta\gamma},$$

where $\alpha := \langle a, n\rangle$, $\beta := \langle a, r\rangle$ ad $\gamma := \langle r, n\rangle$.

This means that the volume of our parallelepiped involving three three-dimensional vectors (9 paramaters) in fact only depends on six different real values, because it is invariant under an arbitrary rotation (G is symmetric). Taking into account that we assume $|a| = |r| = |n| = 1$ we can eliminate three more parameters, leaving us with three independent values. Fig. 3.3 shows the position of the three vectors a, n and r relative to each other.

3.7 Three-parametric QMIE

Having observed that besides the time t the QMIE for a spin-1/2-system underlying time-independet dynamics can be expressed by three parameters we could now rewrite the QMIE in terms of the values α, β and γ.

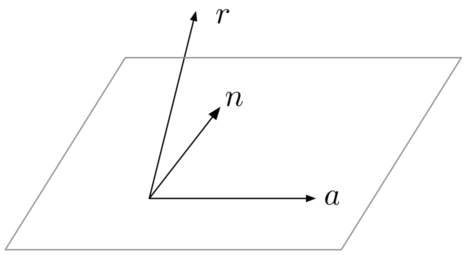

Figure 3.3: Geometry among a, n and r

In order to compare the left- and the right-hand side we need to find an expression involving α, β and γ for the left-hand side as well. This can be done analogously to prop. 5, where we calculated the expectation value of $\sigma(r)$ as a trace over an expression involving the projection operator on our initial state.

Proposition 6 *Let $\mathcal{H} = \mathbb{C}^2$, $a, n \in \mathbb{R}^3$ with $|a| = |n| = 1$ and χ_a shall satisfy $\sigma(a)\chi_a = \chi_a$ then for $\chi_t = U(t)\chi_a$ with $U(t) = \exp(-i\omega\sigma(n)t)$*

$$|\langle\chi_t, \chi_a\rangle|^2 = \cos^2\omega t + \langle a, n\rangle^2 \sin^2\omega t.$$

Proof. Using all the methods we picked up in sec. 3.4 we write

$$|\langle\chi_t, \chi_a\rangle|^2 = |\langle\chi_a, U(t)\chi_a\rangle|^2 = |\mathrm{tr}\,(P^a U)|^2$$

and further

$$\begin{aligned} P^a U &= \frac{1+\sigma(a)}{2}\left(\cos\omega t - i\sin\omega t\sigma(n)\right) \\ &= \frac{1}{2}\left(\cos\omega t - \langle a, n\rangle\; i\sin\omega t + \sigma(\dots)\right), \end{aligned}$$

where taking the absolute value of the trace, since $\mathrm{tr}\,\sigma = 0$ laves us with

$$|\mathrm{tr}\,(P^a U)|^2 = \cos^2\omega t + \langle a, n\rangle^2 \sin^2\omega t,$$

where $\langle a, n\rangle = \alpha$ in congruence with sec. 3.6. □

With this we could now write down the QMIE expressed in α, β and γ. This shall be set aside here, though, since it does not produce any new insights.

Chapter 4

Examples

With the tools and expressions from ch. 3 at hand we can now make special choices for the parameters the QMIE depends on and doing so will allow us to discuss two quite demonstrative examples: we will define a one-and two-dimensional parameter space in order to discuss the quality of the estimate graphically and numerically.

4.1 a, n and r chosen as coplanar

By setting the y-component of all three vectors to zero, our problem is reduced to a two-dimensional one. Additionally, we will now make special choices for a, n and r, i.e.

$$\begin{aligned} a &= (0,0,1) \\ n &= (1,0,0) \\ r &= \left(\sqrt{1-\rho^2}, 0, \rho\right) \end{aligned}$$

with $\rho \in [0,1]$, parametrising the vector r in the first quadrant of the unit circle in the x-z-plane. With this we will now calculate the three scalar products among these vectors as

$$\begin{aligned} \langle a, n\rangle &= 0 \\ \langle r, n\rangle &= \sqrt{1-\rho^2} \\ \langle a, r\rangle &= \rho. \end{aligned}$$

Therefore the expectation value of the σ-operator under χ_t is

$$\langle \sigma \rangle_t = \rho \cos(2\omega t),$$

where we can express the parallelepipedial product $\langle a, n \times r\rangle$ via the three scalar products to note that it is zero, since the volume of a flat parallelepiped (a and r are in the same plane) is zero. We can also observe that $n \times r$ is a vector in y-direction, which upon projection on the vector a along the z-axis returns zero. Or, we could mention that a and r are linearly dependent, therefore the determinant of the matrix M (see sec. 3.6) has to be zero.

From this the right-hand side of the QMIE (P_{QMIE}) can be constructed as

$$\begin{aligned} P_{QMIE}(t) &= \frac{1}{2}\left[1 + \langle\sigma\rangle_0\langle\sigma\rangle_t + \Delta_0\sigma\Delta_t\sigma\right] \\ &= \frac{1}{2}\left[1 + \rho^2\cos(2\omega t) + \sqrt{1-\rho^2}\sqrt{1-\rho^2\cos^2(2\omega t)}\right]. \end{aligned}$$

For the left-hand side we make use of prop. 6 and with $\langle a, n\rangle = 0$ obtain

$$P(t) = \cos^2\omega t = \frac{1}{2}\left(1 + \cos(2\omega t)\right).$$

This yields the QMIE for our example, which looks like

$$cos^2\omega t \le \frac{1}{2}\left[1 + \rho^2\cos(2\omega t) + \sqrt{1-\rho^2}\sqrt{1-\rho^2\cos^2(2\omega t)}\right],$$

where we need a few rearrangements to see that the inequality indeed holds true for all $t \in \mathbb{R}$, namely

$$\begin{aligned} \frac{1}{2}\left(1 + \cos(2\omega t)\right) &\le \frac{1}{2}\left[1 + \rho^2\cos(2\omega t) + \sqrt{1-\rho^2}\sqrt{1-\rho^2\cos^2(2\omega t)}\right] \\ \left(1-\rho^2\right)\cos(2\omega t) &\le \sqrt{1-\rho^2}\sqrt{1-\rho^2\cos^2(2\omega t)}, \end{aligned}$$

where we now raise the inequality to the power of two, which we can do since both sides are non-negative and get

$$\begin{aligned} \left(1 - 2\rho^2 + \rho^4\right)\cos^2(2\omega t) &\le 1 - \rho^2 - \rho^2\cos^2(2\omega t) + \rho^4\cos^2(2\omega t) \\ \left(1-\rho^2\right)\cos^2(2\omega t) &\le 1 - \rho^2, \end{aligned}$$

which is true for any $t \in \mathbb{R}$ and for any $\rho \in [0, 1]$.

In addition to these algebraic considerations fig. 4.1 shows P (black) and P_{QMIE} for $\rho = 0.5$ (red), $\rho = 0.7$ (green) and $\rho = 0.9$ (blue). From this we already get the qualitative impression that the estimate is the better the closer ρ is to 1.

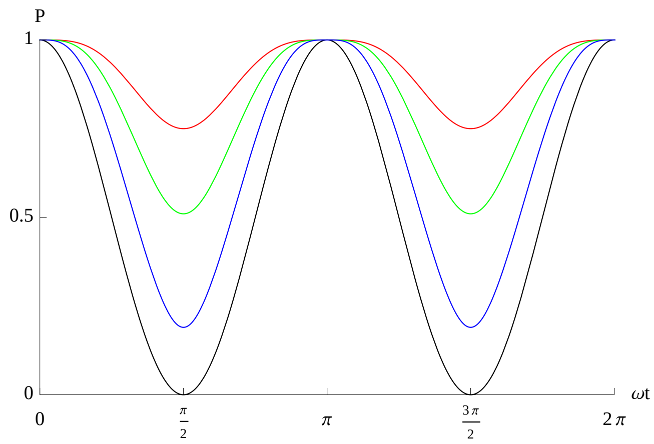

Figure 4.1: P and P_{QMIE} for different ρ

Fig. 4.2 shows $P_{QMIE} - P$ for the same three values of ρ. For $\rho = 0.9$ (blue) a local minium at $\omega t = \pi/2$ can be observed, where for smaller values of ρ the function shows a global maximum at the same point. This shall be discussed more quantitatively now.

First, we define $\tilde{P} : \mathbb{R} \times [0,1] \to [0,1],\ (\omega t, \rho) \mapsto P_{QMIE} - P$ in order to find out at which value ρ_c the global maximum at $\pi/2$ turns into a local minium. For this we try to find $\partial^2_{\omega t}\tilde{P}(\pi/2, \rho_c) = 0$, since we are looking for the point where the curvature shifts from a negative value (maximum) to a positive one (minimum). This can be done analytically and yields

$$\rho_c = \frac{1}{\sqrt{2}},$$

though the occurring expressions are rather unhandy to write down, therefore Mathematica was used to obtain this result (see app. A.3). Fig. 4.3 shows $\tilde{P}$ as a function of $(\omega t, \rho)$ in the domain $[0, \pi] \times [0, 1]$.

Next, we will look for the values of ωt, at which the local maxima left (ωt_1) and right (ωt_2) to our minimum at $\pi/2$ are located. For this we examine $\partial_{\omega t}\tilde{P}$ and try to find its zeros for different values of ρ. Unfortunately this cannot be done analytically and therefore we rely on numerical methods in order to construct tbl. 4.1. Fig. 4.4 $(\partial_{\omega t}\tilde{P})$ can be used to guess the starting points $(\omega t_{1i},\ \omega t_{2i})$ for finding the zeros intelligently. See app. A.3 for the source code. Fig. 4.5 shows the points $(\omega t, \rho)$, where $\tilde{P}$ has a maximum.

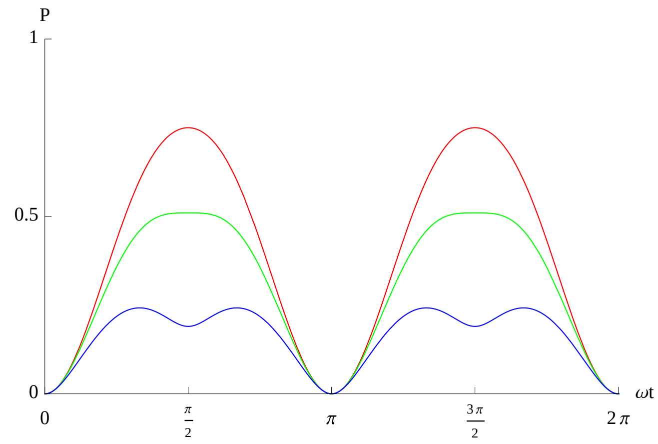

Figure 4.2: $\tilde{P} = P_{QMIE} - P$ for different ρ

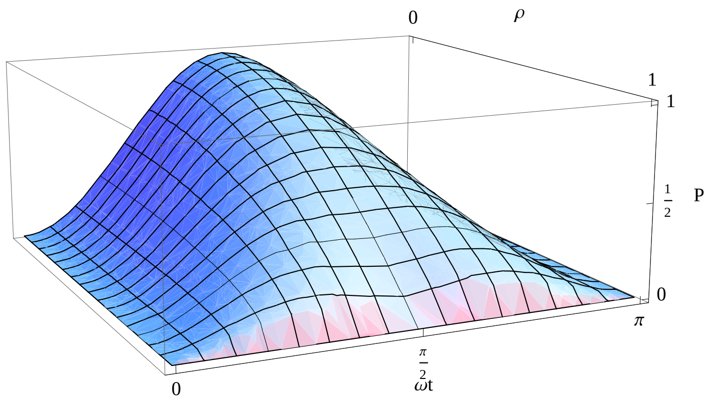

Figure 4.3: $\tilde{P}$ as a function of $(\omega t, \rho)$

ρ	ωt_1	ωt_2	ωt_{1i}	ωt_{2i}
0.75	1.32535	1.81624	1	2
0.80	1.20943	1.93216	1	2
0.85	1.11961	2.02199	1	2
0.90	1.03819	2.1034	1	2
0.95	0.952853	2.18874	1	2

Table 4.1: ωt which the local maxima in $\tilde{P}$ occur at for different ρ

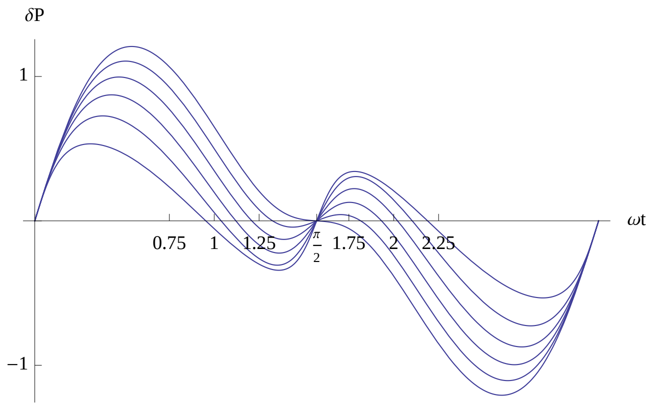

Figure 4.4: $\partial_{\omega t}\tilde{P}$ for $0.7 \leq \rho \leq 0.95$ in steps of 0.05

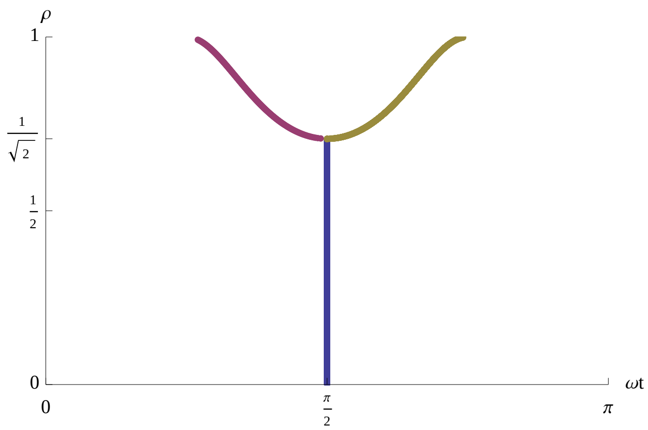

Figure 4.5: Plot of $(\omega t, \rho)$ where $\tilde{P}$ has a maximum

Let us now see how well P is estimated by P_{QMIE} over the entire intervall $[0, \tau]$ with $\tau = \pi/\omega$, where we should remark that the period of the observable is half the period of the dynamics. This brings us back to def. 2, the quality of the estimate. Now, we put down

$$\begin{aligned}
Q &= \frac{2}{\tau}\int_0^{\tau} \left[P_{QMIE}(t) - P(t)\right] \mathrm{d}t \\
&= \frac{2\omega}{\pi}\int_0^{\pi/\omega} \left[P_{QMIE}(t) - P(t)\right] \mathrm{d}t \\
&= \frac{2}{\pi}\int_0^{\pi} \left[P_{QMIE}(t) - P(t)\right] \mathrm{d}\omega t \\
&= \frac{2}{\pi}\cdot\frac{1}{2}\int_0^{\pi} \left[\left(\rho^2 - 1\right)\cos(2\omega t) + \sqrt{1-\rho^2}\sqrt{1-\rho^2\cos^2(2\omega t)}\right] \mathrm{d}\omega t \\
&= \frac{2}{\pi}\sqrt{1-\rho^2}\int_0^{\pi/2} \sqrt{1-\rho^2\cos^2\xi}\,\mathrm{d}\xi,
\end{aligned}$$

where the integral of the first summand is zero and we substitute $\xi = 2\omega t$ in the second part and use that $\cos^2\xi$ is symmetric around $\pi/2$. With $\varphi = \pi/2 - \xi$ the integral becomes $E : [-1, 1] \to \mathbb{R}$,

$$E(\rho) := \int_0^{\pi/2} \sqrt{1-\rho^2\sin^2\varphi}\,\mathrm{d}\varphi,$$

the complete elliptic integral of the second kind, which is discussed in very great detail in [10], §17. A few things from this discussion with special regards to our case shall be extracted and mentioned here.

Firstly, E cannot be expressed by elementary functions, yet for $|\rho| \leq 1$ can be developed in a power series in ρ (see pg. 176 in [11]),

$$E(\rho) = \frac{\pi}{2}\left(1 - \sum_{n=2}^{\infty}\left[\frac{1\cdot 3\cdot 5\cdot\ldots\cdots 2n-1}{2\cdot 4\cdot 6\cdot\cdots\cdot 2n}\right]^2 \frac{\rho^{2n}}{2n-1}\right),$$

allowing us to calculate it with arbitrary accuracy. Secondly, we note two special values, which can be calculated by elementary means, namely

$$E(0) = \frac{\pi}{2} \qquad E(1) = 1.$$

And lastly, the monotony of $E(\rho)$ shall be examined. For that we also need $K(\rho)$, the complete elliptic integral of the first kind, since it appears in the derivative of the complete elliptic integral of the second kind, so

$$\frac{\partial E(\rho)}{\partial\rho} = \frac{E(\rho) - K(\rho)}{\rho},$$

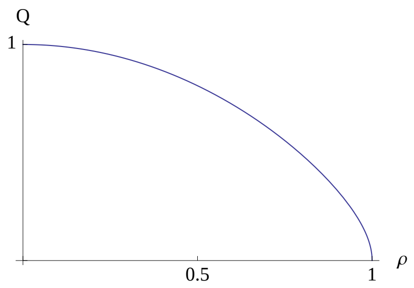

Figure 4.6: Q as a function of ρ

where

$$K(\rho) := \int_0^{\pi/2} \frac{1}{\sqrt{1-\rho^2 \sin^2 \varphi}} \, \mathrm{d}\varphi.$$

With this it is easy to see that for increasing ρ in the domain of $[0, 1]$,

$$\partial_\rho E(\rho) \leq 0$$

(monotonically decreasing) as for $0 < \rho < 1$ the relation

$$E(\rho) < K(\rho)$$

is always valid, since the integrands are positive functions and thus their monotonic behaviour is preserved throughout the integration.

In short, we have a function $E : [0, 1] \to [1, \pi/2]$, $\rho \mapsto E(\rho)$, which monotonically decreases from $E(0) = \pi/2$ to $E(1) = 1$ with its values for arguments $0 < \rho < 1$ only being obtainable through numeric computation.

Going back to the quality of the estimate we can put down

$$Q = \frac{2}{\pi} \sqrt{1-\rho^2} \, E(\rho)$$

for the quality of the estimate, where fig. 4.6 shows a plot of this function and fig. 4.7 gives an example for how Q can be seen in the plot of P and P_{QMIE}. What we see from the expression for Q from above is that the estimate gets the better the closer ρ comes to 1, which can also be observed quite clearly in the plot. This means that the best estimate can be obtained if $a = r$, meaning that the direction of our operator $\sigma(r)$ is parallel to the direction of our initial state, i.e. the preparation.

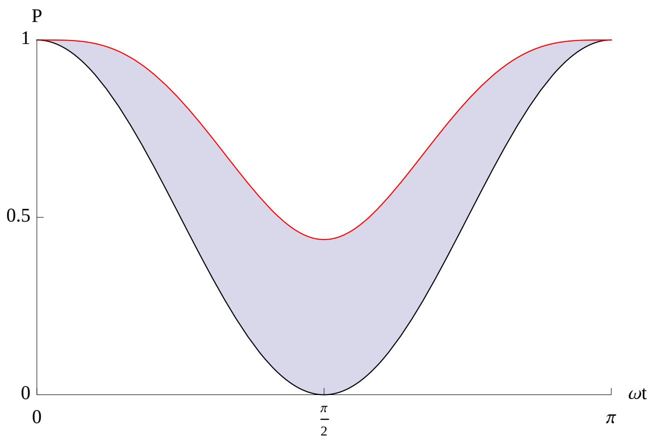

Figure 4.7: Q (area) between P (black) and P_{QMIE} (red, $\rho = 0.75$)

4.2 Varying n and r

Let us stay in this context for a few more deliberations and besides r also vary n in the first quadrant of the unit circle, such that with $\rho, \nu \in [0, 1]$

$$\begin{aligned} a &= (0, 0, 1) \\ n &= \left(\sqrt{1-\nu^2}, 0, \nu\right) \\ r &= \left(\sqrt{1-\rho^2}, 0, \rho\right) \end{aligned}$$

where the scalar products and with this the QMIE are a lot less clear to write down. Therefore the discussion in formulas for this case shall be put aside in favor of a few qualitative, yet quite demonstrative, graphical considerations: fig. 4.8 shows Q as a function of ρ for different values of ν between 0.1 and 0.9 in steps of 0.1, where the lowest function in the plot corresponds to $\nu = 0.1$. We see here, that regardless of the choice of ν, Q goes to zero for $\rho = 1$, again meaning that the best estimate is given when a and r are parallel.

Lastly, fig. 4.9 shows Q in a three-dimensional plot with ν and ρ being the axis of the ground plane, where it is again easy to see that for $\rho = 1$ the quality Q becomes zero.

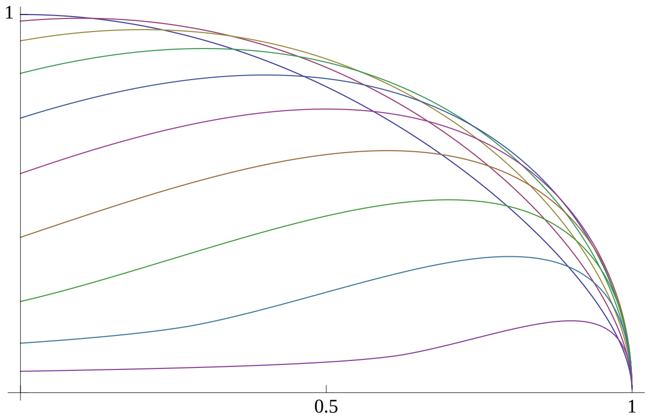

Figure 4.8: Q as a function of ρ for $0.1 \leq \nu \leq 0.9$ in steps of 0.1

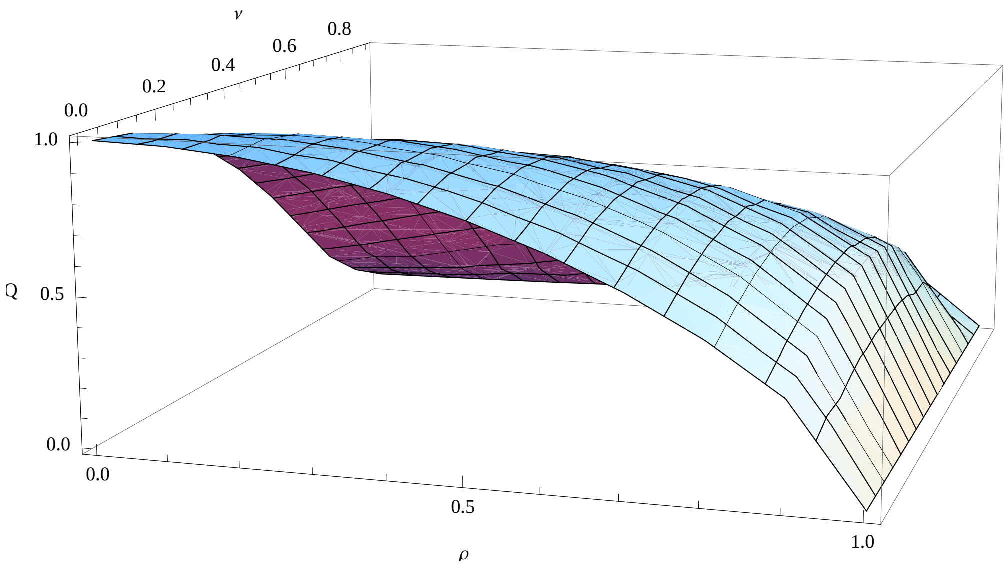

Figure 4.9: $Q(\rho, \nu)$ in a 3D-plot

Appendix A

Source Codes

This chapter lists the source codes for several figures throughout this document and also for a few calculations that have been made using Mathematica (v7.0.0).

A.1 Images

This section shows the source code that was used to produce the various images in this document.

```
n1 = 1; n2 = 0; n3 = 0;   (* direction of the dynamics *)
r1 =
 Sqrt[1 - r^2]; r2 = 0; r3 = r; (* direction of \[Sigma]-operator *)
(* \ initial state vector chosen to be (0, 0, 1) already *)

(* expectation value and rms deviations *)
\[Sigma] =
  2*(-r1*n2 + r2*n1)*Cos[\[Omega]*t]*Sin[\[Omega]*t] +
   2*(r1*n1*n3 + r2*n2*n3 + r3*(n3^2 - 1))*Sin[\[Omega]*t]^2 + r3;
\[Sigma]0 = r3;
\[CapitalDelta]\[Sigma] = Simplify[Sqrt[1 - \[Sigma]^2]];
\[CapitalDelta]\[Sigma]0 = Sqrt[1 - (\[Sigma]0)^2];

(* left- and right-hand side of the qmie *)

inequl = Simplify[Cos[\[Omega]*t]^2 + n3^2*Sin[\[Omega]*t]^2];
inequr = Simplify[((\[CapitalDelta]\[Sigma] + \
\[CapitalDelta]\[Sigma]0)^2)/((\[Sigma] - \[Sigma]0)^2 + (\
\[CapitalDelta]\[Sigma] + \[CapitalDelta]\[Sigma]0)^2)];


\[Omega] = 1;
equplot =
 Plot[{inequl, inequr /. r -> 0.5, inequr /. r -> 0.7,
   inequr /. r -> 0.9}, {t, 0, 4*Pi},
  PlotStyle -> {Black, Red, Green, Blue},
  Ticks -> {Table[n*Pi/2, {n, 0, 8}], {0, 0.5, 1}},
  PlotRange -> {{0, 2*Pi}, {0, 1}}, AxesLabel -> {"\[Omega]t", "P"}]

equplot =
 Plot[{(inequr - inequl) /. r -> 0.5, (inequr - inequl) /.
     r -> 0.7, (inequr - inequl) /. r -> 0.9}, {t, 0, 4*Pi},
  PlotStyle -> {Red, Green, Blue},
  Ticks -> {Table[n*Pi/2, {n, 0, 8}], {0, 0.5, 1}},
  PlotRange -> {{0, 2*Pi}, {0, 1}}, AxesLabel -> {"\[Omega]t", "P"}]
```

Listing A.1: Source code for fig. 1.5.1/4.1 and 4.2

```
n1 = Sqrt[1 - n^2]; n2 = 0; n3 = n;
r1 = Sqrt[1 - r^2]; r2 = 0; r3 = r;

\[Sigma] =
  2*(-r1*n2 + r2*n1)*Cos[\[Omega]*t]*Sin[\[Omega]*t] +
   2*(r1*n1*n3 + r2*n2*n3 + r3*(n3^2 - 1))*Sin[\[Omega]*t]^2 + r3;
\[Sigma]0 = r3;
\[CapitalDelta]\[Sigma] = Simplify[Sqrt[1 - \[Sigma]^2]];
\[CapitalDelta]\[Sigma]0 = Sqrt[1 - (\[Sigma]0)^2];

inequl = Simplify[Cos[\[Omega]*t]^2 + n3^2*Sin[\[Omega]*t]^2];
inequr = Simplify[((\[CapitalDelta]\[Sigma] + \
\[CapitalDelta]\[Sigma]0)^2)/((\[Sigma] - \[Sigma]0)^2 + (\
\[CapitalDelta]\[Sigma] + \[CapitalDelta]\[Sigma]0)^2)];
\[Omega] = 1;


conv = Table[
   Table[{r,
     NIntegrate[inequr - inequl, {t, 0, Pi},
      PrecisionGoal -> 12]}, {r, 0, 0.9999, 0.0001}], {n, 0, 0.9,
    0.1}];
ListLinePlot[conv, Ticks -> {{0, 0.5, 1}, {0, Pi/2, Pi}}]

conv = Flatten[
   Table[{r, n,
     NIntegrate[inequr - inequl, {t, 0, Pi},
       PrecisionGoal -> 12]}, {r, 0, 1, 0.1}, {n, 0, 0.9, 0.1}], 1];
ListPlot3D[conv, AxesLabel -> {"\[Rho]", "\[Nu]", "Q"}]
```

Listing A.2: Source code for images 4.6 and 4.7

```
P = ((r^2 - 1)*Cos[2*t] + Sqrt[1 - r^2]*Sqrt[1 - r^2*Cos[2 t]^2])/2;
ddP = D[D[P, t], t] /. t -> Pi/2;
Solve[ddP == 0, r]
Plot3D[P, {r, 0, 1}, {t, 0, Pi},
 AxesLabel -> {"\[Rho]", "\[Omega]t", "P"},
 Ticks -> {{0, 1}, {0, Pi/2, Pi}, {0, 1/2, 1}}]

A = Table[{t /.
     Last[FindMaximum[P /. r -> s, t, WorkingPrecision -> 12]],
    s}, {s, 0.001, 0.705, 0.001}];
B = Table[{t /.
     Last[FindMaximum[P /. r -> s, {t, 1.45},
       WorkingPrecision -> 12]], s}, {s, 0.706, 0.999, 0.001}];
F = Table[{t /.
     Last[FindMaximum[P /. r -> s, {t, 1.6},
       WorkingPrecision -> 12]], s}, {s, 0.706, 0.999, 0.0001}];
ListPlot[{A, B, F}, PlotRange -> {{0, Pi}, {0, 1}},
 Ticks -> {{0, Pi/2, Pi}, {0, 1/2, 1/Sqrt[2], 1}},
 AxesLabel -> {"\[Omega]t", "\[Rho]"}]
```

Listing A.3: Source code for fig. 4.3 and 4.5

A.2 $\langle\sigma\rangle$ via matrix multiplication

This corresponds to sec. 3.5 ("Alternative derivation of $\langle\sigma\rangle$"), where Mathematica was used to obtain the eigenvectors of $\sigma(a)$ and also to calculate the expectation value of $\sigma(r)$ via matrix multiplication.

```
A = {{a3, a1 - I*a2}, {a1 + I*a2, -a3}};
Eigensystem[A]
```

Listing A.4: Eigenvectors and -values of $\sigma(a)$

```
\[Chi] = (1/Sqrt[2]) {{Sqrt[1 + a3]}, {(a1 + I*a2)/Sqrt[1 + a3]}};
\[Chi]t = (1/Sqrt[2]) {Sqrt[1 + a3], (a1 - I*a2)/Sqrt[1 + a3]};
U = {{Cos[t] - I*n3*Sin[t], -I*Sin[t]*(n1 - I*n2)}, {-I*
     Sin[t]*(n1 + I*n2), Cos[t] + I*n3*Sin[t]}};
Ut = {{Cos[t] + I*n3*Sin[t],
    I*Sin[t]*(n1 - I*n2)}, {I*Sin[t]*(n1 + I*n2),
    Cos[t] - I*n3*Sin[t]}};
\[Chi]time = U.\[Chi];
\[Chi]timet = \[Chi]t.Ut;
R = {{r3, r1 - I*r2}, {r1 + I*r2, -r3}};
FullSimplify[\[Chi]timet.R.\[Chi]time, { a1 >= 0, a2 >= 0, a3 >= 0,
  n1 >= 0, m2 >= 0, n3 >= 0, r1 >= 0, r2 >= 0, r3 >= 0, t >= 0,
  a1^2 + a2^2 + a3^2 == 1, r1^2 + r2^2 + r3^2 == 1,
  n1^2 + n2^2 + n3^2 == 1}]
```

Listing A.5: Expectation value via matrix multiplication

A.3 Discussion of P

This code was used to find ρ_c in section 4.1.

```
P = ((r^2 - 1)*Cos[2*t] + Sqrt[1 - r^2]*Sqrt[1 - r^2*Cos[2 t]^2])/2;
ddP = D[D[P, t], t] /. t -> Pi/2;
Solve[ddP == 0, r]
Plot3D[P, {r, 0, 1}, {t, 0, Pi},
 AxesLabel -> {"\[Rho]", "\[Omega]t", "P"},
 Ticks -> {{0, 1}, {0, Pi/2, Pi}, {0, 1/2, 1}}]

A = Table[{t /.
     Last[FindMaximum[P /. r -> s, t, WorkingPrecision -> 6]],
    s}, {s, 0.001, 0.707, 0.001}];
B = Table[{t /.
     Last[FindMaximum[P /. r -> s, {t, 1.4}, WorkingPrecision -> 6]],
    s}, {s, 0.708, 0.999, 0.001}];
F = Table[{t /.
     Last[FindMaximum[P /. r -> s, {t, 1.6}, WorkingPrecision -> 6]],
    s}, {s, 0.708, 0.999, 0.001}];
ListPlot[{A, B, F}, PlotRange -> {{0, Pi}, {0, 1}},
 Ticks -> {{0, Pi/2, Pi}, {0, 1/2, 1/Sqrt[2], 1}},
 AxesLabel -> {"\[Omega]t", "\[Rho]"}]
```

Listing A.6: Calculation of ρ_c and source for fig. 4.3 and fig. 4.5

```
P = (r^2 - 1)*Cos[2*t] + Sqrt[1 - r^2]*Sqrt[1 - r^2*Cos[2 t]^2];
dP = D[P, t];
Plot[Table[dP , {r, 0.7, 0.95, 0.05}], {t, 0, Pi},
 Ticks -> {{0, 0.75, 1, 1.25, Pi/2, 1.75, 2, 2.25}, {-1, 0, 1}},
 AxesLabel -> {"\[Omega]t", "\[Delta]P"}]
Table[FindRoot[dP, {t, 1}], {r, 0.75, 0.95, 0.05}]
Table[FindRoot[dP, {t, 2}], {r, 0.75, 0.95, 0.05}]
```

Listing A.7: Finding the zeros of $\partial_{\omega t} P$ and source for fig. 4.4

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