Chapter 1

Origin of Entanglement

1.1 A brief history of non-classical correlation

Quantum mechanics is a theory devised for the description of microscopic objects and their behavior. Throughout the previous century, the theory was very successful in explaining many experiments on the microscopic scale such as black body radiation [1], atomic spectra [2] and many others [3, 4], where classical models had mostly failed.

The structure of quantum mechanics suggests that nature should be understood in an indeterministic framework *i.e.* by probabilistic description. Such a description made many physicists uncomfortable when the theory was developed and caused many debates over the following century.

1.1.1 The beginning of paradox

In 1935, Einstein, Podolsky and Rosen (EPR) [5] argued that the quantum mechanical description given by wave functions is not complete since the theory implies the lack of objective reality. They gave an example in which noncommuting quantities, such as position and momentum, can both be taken as elements of physical reality from their definition¹ although the quantum mechanical description by a wave function does not allow this. The famous EPR paradox was argued using a two particle state, known as an EPR state, whose wave function is described by

$$\Psi(x_1, x_2) = \int_{-\infty}^{\infty} e^{(2\pi i/h)(x_1 - x_2 + x_0)p} \, dp \tag{1.1}$$

where x_1 and x_2 are the positions of first and second particles. The state can be decomposed into either a momentum eigenstate $u_p(x_1) = e^{(2\pi i/h)px_1}$ or a position eigenstate $v_x(x_1) = \delta(x_1 - x)^2$ of the first particle as

$$\Psi(x_1, x_2) = \int_{-\infty}^{\infty} \psi_p(x_2) u_p(x_1) dp$$
 (1.2)

$$= \int_{-\infty}^{\infty} \varphi_x(x_2) v_x(x_1) dx \qquad (1.3)$$

¹ "If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then their exists an element of physical reality corresponding to this physical quantity."

 $^{{}^{2}\}delta(x_{1}-x)$ is the well-known Dirac delta-function whose integration form is $\delta(x_{1}-x) = \frac{1}{h} \int_{-\infty}^{\infty} e^{(2\pi i/h)(x_{1}-x)p} dp.$

where $\psi_p(x_2) = e^{-(2\pi i/h)(x_2-x_0)p}$ and $\varphi_x(x_2) = h\delta(x - x_2 + x_0)$ are the momentum and the position eigenstates of the second particle. The eigenvalues of the wave functions are the expectation values of the corresponding physical quantities. In the case of the EPR state, they claimed that by measuring the first particle's position x_1 , without disturbing the second particle, one can measure the second particle's position x_2 , with certainty, which corresponds to an "element of physical reality". In the mean time, the second particle's momentum p_2 can also be found by measuring the first particle's momentum without disturbing the second particle and thus, the second particle's momentum p_2 also corresponds to an element of physical reality. Therefore, the position x_2 and the momentum p_2 of the second particle can be elements of physical reality simultaneously and this contradicts the quantum mechanical description by the wave function. They conclude that the wave function does not provide a complete description of physical reality while leaving open the question of whether or not such a description exists.

Shortly after the appearance of the EPR paper, Schrödinger published two papers, one is his famous "cat paradox" paper [6] and the other is a more technical article about the "entanglement" of wave functions [7]. In these pieces of work, he expressed a well-documented skepticism about "the present situation in quantum mechanics"³. In his article, he coined the term "entanglement" to describe the peculiar connection between quantum systems such as the EPR state

When two systems, of which we know the states by their respective representatives, enter into temporary physical interaction due to known forces between them, and when after a time of mutual influence the systems separate again, then they can no longer be described in the same way as before, viz. ... By the interaction the two representatives [the quantum states] have become entangled.

The term "entanglement" later became a key word in the field of quantum information after its precise mathematical definition by Werner [8] in 1989. Reportedly, Schrodinger's point later changed his view of quantum mechanics in 1950's [9].

Even before 1935, the year of the EPR paper, the EPR argument was criticised by Bohr in an article [10], which had the same title as the EPR paper. In his paper, he mentioned that

The criteria of physical reality proposed by EPR contains an ambiguity as regards the meaning of expression "without, in any way, disturbing a system".

³It is the original title of his "cat paradox" paper.

According to Heisenberg's uncertainty principle, due to the uncontrollable interaction between the object and the measuring instrument, a precise measurement of the position of a quantum particle inevitably disturbs the momentum of the particle and vice versa. The fact that precise measurements of conjugate physical quantities are mutually exclusive is called the *complementarity* of physical quantities which characterises the peculiar nature of a quantum particle. In the EPR example, the position x_1 and the momentum p_1 of the first particle are complementary to each other. The act of measuring either x_1 or p_1 , which cannot be executed simultaneously even in principle, is a matter of "free choice" that we want to measure the one or the other. If one chooses to measure one of either measurements on the first particle, say x_1 (or p_1), this precludes the prediction of the conjugate quantity for the second particle p_2 (or x_2). Therefore, no conclusions can be drawn from a comparison of possible results of mutually incompatible measurements, x_1 and p_1 so that x_2 and p_2 cannot be taken as definite elements of reality simultaneously.

However, Bohr's argument did not convince Einstein and this is evident from Einstein's autobiography [11]:

...it becomes evident that the paradox forces us to relinquish one of the following two assertions :

- 1. the description by means of the ψ -function is complete,
- 2. the real states of spatially separate objects are independent of each other.

For Einstein, the second assertion was indisputable as each EPR particle should exist independently from its counterparts, *i.e.* each particle should be localized. Otherwise, causality, which is essential to theories in physics such as the special theory of relativity, is possibly at risk⁴. It was Einstein's belief that there should be a local realistic model for the quantum state.⁵ Furthermore, he believed [11, p.671] that, in time, developments in theoretical physics would replace quantum theory by a deterministic and, therefore, more complete theory. This, afterwards, motivated many physicists to look for proof or disproof of the existence of a complete theory by considering variables, which were possibly missing in the theory, so called "hidden variables". Fig. 1.1 summarizes schematically Einstein's view of quantum theory.

⁴See further discussions in the next chapter about the no-signalling theorem.

⁵ "But on one supposition we should in my opinion, absolutely hold fast: the real factual situation of the system S_2 is independent of what is done with the system S_1 , which is spatially separated from the former." [11]



Figure 1.1: Einstein's view of quantum theory and hidden variable theory.

1.1.2 John S. Bell and inequalities

The argument was settled a few decades later by Irish physicist J. S. Bell in a rather unexpected way [12]. Before the advent of Bell's formulation, the EPR model was reformulated once more by D. Bohm in the early 1950's [13, 14]. Instead of using the zero total momentum state, he considered a zero total angular momentum state, singlet state, which is composed of two spin half particles. The wave function for a system with zero total spin ⁶ is

$$\Psi = \frac{1}{\sqrt{2}} \left[u_+(1)u_-(2) - u_-(1)u_+(2) \right]$$
(1.4)

where u_+ and u_- are the one-particle spin wave functions representing, respectively, spins of $\hbar/2$ and $-\hbar/2$ and the arguments (1) and (2) refer, respectively, to the two particles. For this singlet state, the particles 1 and 2 are strongly correlated since, when one is in a spin up state, the other particle is always in a spin down state and vice versa. Instead of position and momentum measurements as was the case of the original EPR particles, the spin particles are measured by an inhomogeneous magnet, a Stern-Gerlach magnet, which can measure either the x, y, or z component of the spin. The x, y, and z components of the spin measurement are represented by the Pauli spin operators σ_x , σ_y and σ_z which are mutually incompatible measurements⁷. If one measures one of the particles in (1.4) and the measurement result is $\hbar/2$, the measurement of the same spin component for the

⁶Vector representation of the singlet state will be appeared in the next chapter.

⁷More formally, the operators do not commute each other *i.e.* $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$ where $i, j, k \in \{x, y, z\}$ and ϵ_{ijk} is 1 for permutation, -1 for anti-permutation and 0 for the others.

other particle will always yield $-\hbar/2$. On the other hand, when the measurement directions for the two particles are orthogonal, the measurement results for the particles are completely random. Therefore, as in the original EPR argument, the σ_x and σ_y and σ_z components of the spin of the second particle are elements of physical reality in contradiction to their quantum mechanical description by the wave function.

In 1964, J. S. Bell showed that the expectation values of certain local measurements for the states in Eq. (1.4) do not agree with the expectation values produced by any local hidden variable theory [12]. The discovery was quite surprising since it implies that no local hidden variable model for the description of quantum states is allowed by quantum theory.

If we assume that a spin measurement of an arbitrary component $\vec{\sigma} \cdot \vec{a}^{8}$ is completely determined by a parameter λ , a hidden variable, and the local measurement setting \vec{a} , then, we have the value A of the measurement as a function of λ and \vec{a} as $A(\vec{a}, \lambda) = \pm 1^{9}$. This means that the measurement results are independent of anything other than λ and \vec{a} , thus the measurement is completely local. For the local spin measurements of any two spins, the expectation value of the measurements, which corresponds to the correlation between the two spins, can be obtained as

$$E(\vec{a}, \vec{b}) = \int d\lambda \rho(\lambda) A_1(\vec{a}, \lambda) A_2(\vec{b}, \lambda)$$
(1.5)

where $\rho(\lambda)$ is the probability distribution of the hidden variable, λ , satisfying $\int d\lambda \rho(\lambda) = 1$. Generally, for a bipartite spin state, the expectation value can have any value between 1 and -1 as $-1 \leq E(\vec{a}, \vec{b}) \leq 1$. For the singlet state (1.4), the expectation value is -1 whenever the directions of the spin measurements are identical $\vec{a} = \vec{b}$, *i.e.*

$$E(\vec{a}, \vec{a}) = -1,$$
 (1.6)

because the spin states 1 and 2 are always in opposite directions $A_1(\vec{a}, \lambda) = -A_2(\vec{a}, \lambda)$. Now, one can consider the situation where one of the spin half particles is measured in a direction \vec{a} and the other particle is measured in \vec{b} and \vec{c} ¹⁰.

⁸where $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ and \vec{a} is a unit vector.

⁹We normalised the measurement values as ± 1 instead of $\pm \hbar/2$.

¹⁰For a quantum measurement, in general, the two different measurements in the directions \vec{b} and \vec{c} do not commute. Therefore, the measurements in the directions \vec{b} and \vec{c} for a quantum state cannot be performed simultaneously to within an arbitrary precision. However, it does not affect our discussion since (i) we are currently looking for a classical bound which does not need to consider the non-commutability and (ii) for the quantum case, the problem of simultaneous measurement does not change our conclusion for the hidden variable discussion

Then, the expectation value $E(\vec{a}, \vec{b})$ for the local measurements \vec{a} and \vec{b} and the expectation value $E(\vec{a}, \vec{c})$ for \vec{a} and \vec{c} can be obtained and the difference between the expectation values is then,

$$E(\vec{a},\vec{b}) - E(\vec{a},\vec{c}) = -\int d\lambda \rho(\lambda) A(\vec{a},\lambda) \left[A(\vec{b},\lambda) - A(\vec{c},\lambda) \right]$$
(1.7)

$$= \int d\lambda \rho(\lambda) A(\vec{a}, \lambda) A(\vec{b}, \lambda) \left[A(\vec{b}, \lambda) A(\vec{c}, \lambda) - 1 \right] \quad (1.8)$$

where $A(\vec{b}, \lambda)^2 = 1$ was used to obtain the second equality. Furthermore, since $A(\vec{a}, \lambda)A(\vec{b}, \lambda) = \pm 1$ and $A(\vec{b}, \lambda)A(\vec{c}, \lambda) - 1$ is negative, we have an inequality

$$|E(\vec{a},\vec{b}) - E(\vec{a},\vec{c})| \le \int d\lambda \rho(\lambda) \left[1 - A(\vec{b},\lambda)A(\vec{c},\lambda)\right]$$
(1.9)

and, after a little rearrangement, it has the form

$$|E(\vec{a}, \vec{b}) - E(\vec{a}, \vec{c})| - E(\vec{b}, \vec{c}) \le 1$$
(1.10)

which is the famous Bell's inequality [15]. It is notable that, for the derivation of Bell's inequality, any theories for the state are not considered. The only assumptions made in deriving the inequality are local measurement and the existence of a hidden variable. Thus, if the inequality is violated by any experiment, the state cannot be described by any local hidden variable theory. Surprisingly, quantum mechanics predicts such experimental results which violate the inequality. In quantum mechanics, the expectation value of the local measurements [15] for the singlet state (1.4) is given by¹¹

$$E(\vec{a}, \vec{b}) = \langle \vec{\sigma} \cdot \vec{a} \otimes \vec{\sigma} \cdot \vec{b} \rangle = -\vec{a} \cdot \vec{b} = -\cos\theta_{ab}$$
(1.11)

where θ_{ab} is the angle between the measurement directions \vec{a} and \vec{b} . Using the correlation functions of the singlet state, the function on the left hand side of Eq. (1.10) becomes

$$B(\vec{a}, \vec{b}, \vec{c}) = |E(\vec{a}, \vec{b}) - E(\vec{a}, \vec{c})| - E(\vec{b}, \vec{c})$$

= $|-\cos\theta_{ab} + \cos\theta_{ac}| + \cos\theta_{bc},$ (1.12)

and when $\theta_{ab} = \theta_{bc} = \pi/3$ and $\theta_{ac} = 2\pi/3$, the function $B(\vec{a}, \vec{b}, \vec{c})$ clearly violates

once the measured statistics violate the proposed bound, *i.e.* Bell's inequality.

¹¹One can also calculate the correlation function of the singlet state using vector representation of the singlet state. The representation will be introduced in the next chapter.

the Bell's inequality as $B(\vec{a}, \vec{b}, \vec{c}) = 3/2 > 1$. Thus, we can conclude that the statistics which can be obtained for the quantum state do not allow any local hidden variable model. This provided the evidence that quantum theory could be a complete theory. Moreover, a quantum state, which violates Bell's inequality and precludes any influence of the measurement on the other particle is thus inevitably nonlocal. Therefore, the violation of the inequality requires a complete departure from classical thought in understanding a quantum state and the experimental confirmation of such a result was left for further investigation.

It is also interesting to point out that Bell questioned if the original EPR state in Eq. (1.2), instead of Bohm's singlet state in Eq. (1.4), can violate Bell's inequality [15]. He concluded that since the Wigner function for the EPR state is nowhere negative, there could not be nonlocality argument for the original EPR state as is the case for Bohm's singlet state. The question was revisited in the late 1990's [16]. We discuss the violation of Bell's inequality for the original EPR state in Chapter ??.

After Bell's discovery, generalisations of Bell's inequality were presented for the purpose of applying it to realisable experiments. In 1969, Clauser, Horne, Shimony and Holt (CHSH) generalised Bell's inequality for two measurement settings equally distributed on each side. They found that an array of correlation functions obtained from the measurements have a critical bound which are constrained by local hidden variable theory [17] as

$$B_{CHSH}(\vec{a}, \vec{b}, \vec{a}', \vec{b}') = |E(\vec{a}, \vec{b}) + E(\vec{a}, \vec{b}') + E(\vec{a}', \vec{b}) - E(\vec{a}', \vec{b}')| \le 2$$
(1.13)

where $E(\vec{a}, \vec{b})$ is the same function defined in (1.5). Like Bell's inequality, the CHSH inequality is valid for any set of dichotomic variables, *e.g.* spin up and down for a spin 1/2 particle or vertical and horizontal polarizations of a single photon.

For a bipartite entangled quantum system, such as singlet state which can be realized by π^0 decay ($\pi^0 \rightarrow e^+e^-$) or by atomic radiative cascades (highly correlated photon pairs), the function $B_{CHSH}(\vec{a}, \vec{b}, \vec{a}', \vec{b}')$ in (1.13) can have a value larger than 2 [17]. When the measurement angles are $\theta_{ab} = \theta_{ab'} = \theta_{a'b} = \pi/4$ and $\theta_{a'b'} = 3\pi/4$, with the correlation function in Eq. (1.11), the CHSH-Bell function $B_{CHSH}(\vec{a}, \vec{b}, \vec{a}', \vec{b}')$ has the value, $B_{CHSH}(\vec{a}, \vec{b}, \vec{a}', \vec{b}') = 2\sqrt{2} > 2$. In fact, the largest value for $B_{CHSH}(\vec{a}, \vec{b}, \vec{a}', \vec{b}')$ of any quantum state has been proven to be $2\sqrt{2}$ which is known as the Cirel'son bound [18].¹²

 $^{^{12}}$ Recently, there was a series of studies examining why quantum mechanics is constrained by

In a real experiment, the correlation $E(\vec{a}, \vec{b})$ can be obtained from the probability distributions of the measurement outcomes. If we have sufficiently many pairs of quantum particles, N, which have dichotomic variables, then all the combinations of the joint probabilities for the two two-outcome measurements are measured as

$$p_{ab}(+,+) = \frac{N_{++}}{N}, \quad p_{ab}(-,-) = \frac{N_{--}}{N},$$
 (1.14)

$$p_{ab}(+,-) = \frac{N_{+-}}{N}, \quad p_{ab}(-,+) = \frac{N_{-+}}{N}$$
 (1.15)

where the N_{ij} are the number of pairs which are measured as $i, j \in \{+, -\}$ and the subscripts a and b represent the measurement directions. Since the $E(\vec{a}, \vec{b})$ is defined as the expectation value of the variables $A(\vec{a}, \lambda) = \pm 1^{13}$, from the joint probabilities (1.14), the correlation function (1.5) can be obtained as

$$E(\vec{a}, \vec{b}) = p_{ab}(+, +) + p_{ab}(-, -) - p_{ab}(+, -) - p_{ab}(-, +), \qquad (1.16)$$

where $p_{ab}(i, j)$ is the joint probability that both $i \in \{+, -\}$ and $j \in \{+, -\}$ are registered for the measurement settings \vec{a} and \vec{b} . The correlation functions $E(\vec{a}, \vec{b}'), E(\vec{a}', \vec{b})$ and $E(\vec{a}', \vec{b}')$ can also be obtained from different measurement settings and, as a result, the function $B_{CHSH}(\vec{a}, \vec{b}, \vec{a}', \vec{b}')$ can be constructed from them. Therefore, an experimental test of CHSH-Bell inequality for given pairs can be performed by observing the statistics of the outcomes of the measurements.

Clauser and Horne (CH)[23] developed another set of Bell's inequalities by considering a single photon measurement. For their measurement of the polarization of single photons, the measurement apparatus is composed of a polarizer and a single photon detector. The photons are detected only when they trigger the detector and this requires Bell's inequality with only + outcomes (triggering outcome) probabilities. The marginal probabilities of local measurement outcomes are

$$\sum_{j} p_{ab}(i,j) = p_a(i), \qquad \sum_{i} p_{ab}(i,j) = p_b(j), \qquad (1.17)$$

where $i, j \in \{+, -\}$ and $p_a(i)$ is the probability that the outcome *i* is obtained for the measurement by \vec{a} . With help of the marginal probabilities and the com-

such a bound and the possibility of measuring correlation larger than Cirel'son bound [19, 20, 21, 22].

¹³An expectation value for a set of discrete variables $\{X_i\}$ is defined by $\langle X \rangle = \sum_i p_i X_i$ where p_i is the probability that X_i happens.

pleteness condition $p_a(+) + p_a(-) = p_b(+) + p_b(-) = 1$, the correlation function (1.16), in terms of only triggered count probabilities, becomes

$$E(\vec{a}, \vec{b}) = 4p_{ab}(+, +) - 2p_a(+) - 2p_b(+) + 1$$
(1.18)

which leads to the CH-Bell's inequality

$$-1 \le p_{ab}(+,+) + p_{ab'}(+,+) + p_{a'b}(+,+) - p_{a'b'}(+,+) - p_a(+) - p_b(+) \le 0, \quad (1.19)$$

where we used Eq. (1.13) and Eq. (1.18). This is also consistent with the proof [24] that the local realistic bounds in Bell's inequalities are equivalent to the existence of well-defined joint probabilities. The CH-Bell inequality was tested experimentally in 1976 [25], but the efficiency of the experiment was not sufficient for a reliable conclusion to be drawn even though the results violated the CH-Bell inequalities [26].

1.1.3 Era of nonlocality

In the beginning of controversies, there were no reliable experimental evidences available because of technical difficulties. However, after the first efficient experimental test of the CHSH-Bell inequality by A. Aspect, P. Grangier and G. Roger [27], using an optically pumped atomic cascade, in 1982, there was remarkable progress made in testing Bell's inequality by now. Two major obstacles for a reliable Bell's inequality test are space-like separation of testing sources [15] and detection-inefficiency [28]. They are referred as the locality loophole¹⁴ and the detection loophole ¹⁵ respectively and many experiments have been carried out to close the loopholes $[29, 30]^{16}$. Table 1.1 summarises the experimental progress made in testing Bell's inequality by different groups over the last two decades and they all obtained results in accordance with the prediction of quantum mechanics. These days, it is widely agreed that, leaving aside the fast closing loopholes, no local realistic theory of the type suggested by EPR is compatible with the experimental results showing violations of Bell's inequality. Searching for completely conclusive experimental evidence of the violation is still on going and the most recent idea (July, 2004) for a loophole-free Bell's inequality test is suggested by

 $^{^{14}{\}rm The}$ measuring events for the EPR pairs should happen outside the light cone to avoid any uncontrollable influence between the two measuring apparatus

¹⁵The unwanted losses and decoherence of the EPR states and low efficiency of the detectors hinder us from reaching a reliable conclusion.

¹⁶There are also discussions about recently discovered loopholes [31].

Year	Group	Source	Miscellany
Early 70's	Berkeley, Harvard	Photon pairs by	Single channel polarizer,
	and Texas A&M	atomic cascade	only access the $+$ outcome.
1982	Orsay,	Non-linear laser excitations of	Two channel polarizer.
	Aspect et. al.[27]	atomic cascade of calcium	
1988	Maryland, Shih et. al.[33]	Optical parametric	
	Rochester, Ou et. al.[34]	down conversion	
1992	Caltech,	Optical parametric	EPR state (CV)
	Ou et. al.[35]	down conversion	source is generated.
1994	Melvern,	Optical parametric	4km distance
	Tapster et. al.[36]	down conversion	through optical fiber.
1998	Geneva,	Optical parametric	10.9km distance
	Tittel <i>et. al.</i> [37]	down conversion	through optical fiber.
1998	Innsbruck,	Optical parametric	Closed the
	Weihs et. al.[38]	down conversion	locality loophole.
2001	Boulder & Michigan,	Trapped $^{9}\text{BE}^{+}$ ions	Closed the detection
	Rowe <i>et.</i> al.[39]	entangled by Raman lasers	efficiency loophole.

Table 1.1: Experimental progress of Bell's inequality test. All the experimental results confirmed the impossibility of local hidden variable model for the quantum states within certain precision.

R. Garacia-Patrón, J. Fiurášek and N. J. Cerf [32].

As the predictions of quantum theory are being confirmed by experiments, there have also been many theoretical efforts to generalise the conflict between the local realistic model and the quantum states. Two important questions in that direction are (1) "What are the most general constraints on correlations imposed by local realism?" and (2) "Which quantum states violate these constraints?" The questions provoke us to find a more general class of inequalities, whose violation does not allow any local realistic model, as well as a class of states, which differ from any classically prepared state. Those are, so called, problems of "all the Bell's inequalities" [40] and "entanglement" [8]¹⁷. The two closely related concepts of quantum correlation, nonlocality and entanglement, are not necessarily equivalent [41] except for the pure bipartite state [42].

The generalisation of Bell's inequalities is developed in various ways. For a bipartite two-level system, Braunstein and Caves [43, 44] derived a local realistic bound with an arbitrary number of measurements on each side. When n is the number of two outcome measurements, they found the classical bound to be 2n-2 and the quantum bound to be 2n for $n \to \infty$ which shows a clear discrepancy. Gisin [45] also found a similar type of inequality with n observables, but with a

 $^{^{17}}$ The theory of entanglement will be discussed in Chapter 2.

different array, which showed that increasing the number of observables does not necessarily benefit in terms of higher violation of Bell's inequalities.

Bell's inequalities applied to higher than two level systems were investigated as well. In the early 1990's, Gisin and Peres [42, 46, 47] showed that, using dichotomic observables, any pure N-dimensional bipartite system always violates the CHSH-Bell's inequality if and only if the states are entangled. This result was quite interesting since it implies that a high energy level state cannot necessarily be approximated by a classical state. Later, it is shown that the maximal violation, $2\sqrt{2}$, of the CHSH-Bell's inequality is possible even for an infinite dimensional state, such as the original EPR state [48, 49]. Recently, instead of the dichotomic measurements, Bell's inequalities using the *d* outcome measurements were derived by Collins, Gisin, Linden, Massar and Popescu (CGLMP) [50]. Interestingly, the CGLMP inequality reproduced the numerical simulation which searched for the violation of local realism using the marginal distributions as the amount of noise increased [51]¹⁸.

Moreover, the nonlocality of systems which have more than two parties was widely studied. In 1986, Svetlichny [52] derived an inequality violated by quantum mechanics for a three-body system. The inequality was found to detect threebody correlations that cannot be reduced to mixtures of two-body ones. In 1989, Greengerger, Horne and Zeilinger (GHZ) [53] produced an argument, even without inequalities, that the state of three or more quantum particles can conflict with any local realistic model. After their characterisation, the states which have genuine multi-body quantum correlations were called as GHZ states. For an arbitrary number M of spin-1/2 particles, Mermin, in 1990 [54], and Klysko, in 1993 [55], developed more general sets of Bell's inequalities, which violate the classical bound by an amount that grows exponentially with M. Therefore, it has been proven that increasing the number of particles does not lead to a classical limit. In 1998, Gisin and Bechmann-Pasquinucci [56] obtained another set of inequalities by means of a recursive argument from Klysko's inequality. They found bounds which discriminate genuine multi-partite entanglement from any pairwise entanglement. Recently, stronger inequalities for the genuine multipartite entanglement of M $\frac{1}{2}$ states were discussed by several authors [57, 58, 59]. Furthermore, in 2001, Werner and Wolf [60] and Zukowski and Brukner [61] found, independently, the set of all possible Bell's inequalities, of which there are 2^{2^M} , for the M spin-1/2 particles with two measurements per site.

 $^{^{18}}$ More discussion can be found in chapter ??

Chapter 2

Modern theory of entanglement

In this chapter, the preliminary quantum theory and entanglement are presented. They are intended to introduce the mathematical notation of the theory and their meanings which will be used throughout the rest of this thesis.

In quantum theory, it is believed that the description of a physical system is possible by a simple mathematical structure called Hilbert space. The structure describes many possible physical systems, which are in the quantum realm, including two-level systems, arbitrary dimensional systems and infinite dimensional systems. A spin-1/2 particle, an angular momentum state of an atom and a quantized light field are specific examples of the physical systems. As basic units of quantum information processing, they are also referred to as qubits, qudits and continuous variable states, respectively.

A composite state which is composed of many subsystems is said to be "entangled" if its mathematical representation satisfies certain criteria. The criteria are derived from the peculiar quantum nature of the composite quantum system. It was Werner [8] who firstly introduced such a criterion for any general mixed state, in 1989. The entanglement of a pure quantum state is well understood whereas the entanglement of general mixed state is still under investigation. For a given mixed state, it is only the 2×2 , 2×3 quantum states [62, 63] and Gaussian state [64, 65] whose entanglement criteria are fully understood.

Moreover, the problem of entanglement measure [66, 67], which characterizes entanglement by enquiring "how much entanglement does the system have", is an important problem in the fast progressing area of quantum information processing (QIP). The problem was approached in several different ways, such as, entanglement of formation (EoF)¹ [69], entanglement of distillation (EoD)²[69], relative entropy (RE) [67, 70] and negativity of partial transposition (NPT) [71, 72]. These measures of entanglement agree with each other for certain asymptotic cases but there are also some discrepancies [73]. The measures of entanglement have their own merits and deficit. For example, EoF, EoD and RE are not only directly linked to the purification of entanglement [74] for a quantum communication but also show useful physical meaning such as additivity and irreversibility of entanglement even though they are not easy to compute for a general quantum system. On the contrary, NPT is a computable measure of entanglement although partial transposition for a composite system is a physically impossible operation.

¹see also entanglement cost [68]

 $^{^{2}}$ It is called entanglement concentration for a partially entangled pure state.

2.1 Quantum state and entanglement

Any pure quantum state, which is isolated from the beginning, can be represented by a *state vector*, ket $|\psi\rangle$ which is defined in an abstract mathematical space, Hilbert space \mathcal{H} . Hilbert space is a complex vector space which have positive inner product and is linear and complete in the norm ³. The state vectors satisfy the rule of linearity, under the name of *superposition*, that is, a linear summation of any two vectors is also a vector as

$$|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle \tag{2.1}$$

where the coefficients a_1 and a_2 are complex numbers. A bra vector, $\langle \psi |$, is defined as the complex conjugate of the ket vector $|\psi\rangle$ and an inner product of a vector is well defined as, $\langle \psi | \psi \rangle = 1$, which results in, $|a_1|^2 + |a_2|^2 = 1$, for $\langle \psi_1 | \psi_2 \rangle = 0$. The coefficients a_1 and a_2 are interpreted as probability amplitudes, giving the likelihoods that the quantum state $|\psi\rangle$ can be found in states $|\psi_1\rangle$ or $|\psi_2\rangle$ respectively.

The superposition principle describes that a quantum system can exist in a state of a combination of mutually independent states *simultaneously* and this does not have any counter part within the framework of classical physics. The principle can be illustrated as, if one were to toss a quantum mechanically prepared coin, the coin can be in a state whose result gives heads and tails simultaneously before its measurement. The phenomenon is also known by the name of Schrodinger's Cat [6], a cat which can be in the state of dead and alive at the same time when it is connected to a microscopic object. This implausible phenomenon is taken as an essence of quantum state.

The superposition principle should be distinguished from a simple statistical mixture of any two possible results since there is a probability that the two independent results can interfere each other. It implies that except in the case $a_1 = 0$ or $a_2 = 0$, the measurement of the state irrevocably disturbs the state and modifies the probabilities for the independent states. After the measurement, the state is prepared in a known state-either $|\psi_1\rangle$ or $|\psi_2\rangle$ -that differs (in general) from its previous state. As a result, if the value of the state is initially unknown, then there is no way to determine a_1 and a_2 with that single measurement, or any other conceivable measurement. In this respect, a quantum state differs from a classical mixture of state; we can measure a classical mixture without disturbing

³Inner product of vector defined as $\langle \psi | \psi \rangle$ and the norm of a vector is $||\psi|| = \langle \psi | \psi \rangle^{\frac{1}{2}}$

it, and we can decipher all the information that it encodes.

A more rigorous definition of the state vector may give rise to the problem of the *interpretation of quantum mechanics*. There are various points of view about the meaning of the state vector and quantum theory. The interpretation of quantum mechanics becomes important especially when someone tries to make a correspondence between the theory and an experiment. However, this is not the subject of this thesis and I left it as a reference.⁴

The smallest nontrivial Hilbert space is two dimensional. Any two orthonormal basis, for example $\{|0\rangle, |1\rangle\}$ is sufficient for a two-level quantum system. Then, the most general normalized pure state can be expressed as

$$|\psi\rangle = a_1|0\rangle + a_2|1\rangle \tag{2.2}$$

where a_1 and a_2 are complex numbers and the overall phase is physically irrelevant⁵. Analogous with the basic unit in classical information theory, the *bit*, this two-level quantum state is called the *quantum bit* or *qubit* which is a basic ingredient in quantum information theory. After a proper parameterization, a qubit can also be represented as a point in a three dimensional unit sphere, called the *Bloch sphere*. Fig. 2.1 shows the Bloch vector representation of a qubit for the parameterization, $(a_1, a_2) = (\cos \varphi, e^{i\theta} \sin \varphi)$. One should be careful to note that the orthogonal states $|0\rangle$ and $|1\rangle$ do not appear orthogonal in the configuration.

In general, a higher dimensional quantum system has spectrum of its measurement outcomes corresponding to its dimensionality. With a given orthonormal basis set $\{|i\rangle\}$, defined in a *d*-dimensional Hilbert space \mathcal{H} , a pure quantum state can be represented as

$$|\psi\rangle = \sum_{i=0}^{d-1} a_i |i\rangle \tag{2.3}$$

where d is the dimensionality of the quantum system and a_i are complex numbers having a constraint $\sum_{i=0}^{d-1} |a_i|^2 = 1$. One possible parameterization for the

⁴According to C. A. Fuchs[75], there are the Bohmians[76], the Consistent Historians[77], the Transactionalists[78], the Spontaneous Collapseans[79], the Einselectionists[80], the Contextual Objectivitist[81], the outright Everettics[82, 83] and many more beyond those.

⁵This is because only measurable physical quantity is probability of measuring outcome, $\langle \psi | \hat{O} | \psi \rangle$, where the overall phase factor is always cancelled. This is why the state vector is called a ray.



Figure 2.1: Qubit representation in the Bloch sphere

coefficient a_i is

$$\left\{a_{i} = e^{i\varphi_{i}}\cos\theta_{i}\prod_{j=0}^{i-1}\sin\theta_{j} \mid 1 \le i \le d-2, \ a_{0} = \cos\theta_{0} \text{ and } a_{d-1} = e^{i\varphi_{d-1}}\prod_{j=0}^{d-2}\sin\theta_{j}\right\}.$$
(2.4)

This clearly shows that a state vector defined in *d*-dimensional Hilbert space has its real vector counterpart defined in a 2d - 1 dimensional real Euclidian space. When there is no constraint, a transformation of the state vector is possible by a unitary operation defined in a *d*-dimensional Hilbert space. An orthonormal basis vector $|i\rangle$ can be transformed by a unitary operator \hat{U} into another orthogonal basis

$$|i\rangle \xrightarrow{\hat{U}} |u_i\rangle = \hat{U}|i\rangle = \sum_{j=0}^{d-1} |j\rangle\langle j|\hat{U}|i\rangle$$
 (2.5)

$$= \sum_{j=0}^{d-1} u_{ij} |j\rangle \tag{2.6}$$

where u_{ij} is the matrix element of the $d \times d$ unitary operator and we use the identity $\mathbb{1} \equiv \sum_{j=0}^{d-1} |j\rangle\langle j|$ for the matrix element representation. It is not difficult to see that the bases $|u_i\rangle$ are orthogonal and that the inverse transformation is

always possible as $|i\rangle = \sum_{j=0}^{d-1} u_{ji}^* |u_j\rangle$. Thus, the state in Eq. (2.3) can be rewritten in a different basis

$$|\psi\rangle = \sum_{j=0}^{a-1} b_j |u_j\rangle \tag{2.7}$$

where $b_j = \sum_{i=0}^{d-1} u_{ji}^* a_i$. This implies that the choice of basis vectors is arbitrary for the description of a quantum state and it is as if there are an infinite number of possible choices of coordinates for the description of a physical object. However, if a basis is given, then the expression of a quantum state is uniquely determined in terms of the coefficients $\{b_j\}$.

It is called a continuous variable (CV) state when the dimensionality of a quantum state is infinite. The CV state utilizes the infinite dimensional Hilbert space even if all the vectors defined in the infinite dimensional Hilbert space are not realistic.⁶ It is the uncertainty principle [84] which gives the restriction on the CV state. There are several examples of CV states which satisfy the minimum uncertainty relation

$$\Delta X \Delta P = \frac{\hbar}{2} \tag{2.8}$$

where $\hat{X} = \frac{1}{\sqrt{2}}(\hat{a}^{\dagger} + \hat{a})$ and $\hat{P} = \frac{i}{\sqrt{2}}(\hat{a}^{\dagger} - \hat{a})$. The spectral representation of the Bosonic annihilation operator, \hat{a} , and creation operator, \hat{a}^{\dagger} , is possible in an orthomormal basis $\{|n\rangle\}$ as

$$\hat{a} = \sum_{n=0}^{\infty} \sqrt{n} |n\rangle \langle n+1|$$
(2.9)

and \hat{a}^{\dagger} is the self-adjoint operator of \hat{a} . The annihilation operator \hat{a} and the creation operator \hat{a}^{\dagger} are defined as the operators which are lowering and raising the number of the basis $|n\rangle$ as $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle$. They satisfy the commutation relation $[\hat{a}, \hat{a}^{\dagger}] = 1$.

An orthonormal basis $|n\rangle$ is called the number state when it represents the total number of bosonic particles such as the total photon number for quantized field. The number state gives information about the total photon number for a quantized field at the expense of information about the phase of the field.

A coherent state [85] is a state which satisfies the minimum uncertainty relation with same fluctuations for all quadratures. The state has a Possonian

 $^{^6\}mathrm{See}$ [44, chapter 4] about the common pitfall for the CV representation.

distribution over the photon numbers as

$$\begin{aligned} \alpha \rangle &= \hat{D}(\alpha) |0\rangle \\ &= e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \end{aligned}$$
(2.10)

where α is an arbitrary complex number whose absolute value represents the mean photon number of the system. The state can be generated from a vacuum state by making an excitation through displacement $\hat{D}(\alpha) \equiv \exp(\alpha \hat{a}^{\dagger} - \alpha^* \hat{a})$. The displacement operator, $\hat{D}(\alpha)$, is unitary, satisfying $\hat{D}(\alpha)\hat{D}(\alpha)^{\dagger} = 1$, and $\hat{D}(\alpha)^{\dagger} =$ $\hat{D}(-\alpha)$. The coherent state is also defined as an eigenstate of the annihilation operator \hat{a} as $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$.

A squeezed state [86] is another example of a CV state which satisfies the minimum uncertainty relation. The state does not generally have the same amount of fluctuation in each quadrature. The single mode squeezed state is defined as

$$|\zeta\rangle = \hat{S}(\zeta)|0\rangle \tag{2.11}$$

$$= \sqrt{\operatorname{sech} r} \sum_{n=0}^{\infty} \frac{\sqrt{(2n)!}}{n!} \left(-\frac{\mathrm{e}^{i\varphi}}{2} \tanh r \right)^n |2n\rangle \qquad (2.12)$$

where the squeezing operator $\hat{S}(\zeta) = \exp(-\frac{\zeta}{2}\hat{a}^{\dagger 2} + \frac{\zeta^*}{2}\hat{a}^2)$ and the complex number $\zeta = r e^{i\varphi}$. The squeezed states are sometimes referred to as two-photon coherent states since the squeezing operator has the same form as the displacement operator on replacing the \hat{a} with \hat{a}^2 . The squeezing parameter r specifies the ratio between the fluctuations in the quadratures \hat{X} and \hat{P} in a given direction where the phase φ determines the direction of squeezing or equivalently the rotation of the principle axes in the phase space.

2.1.1 Entanglement and superposition

The consequences of the mathematical structure of superposition for a composite system are very intriguing. Consider a system which is composed of two subsystems A and B where $|\psi\rangle_A \in \mathcal{H}_A$ and $|\varphi\rangle_B \in \mathcal{H}_B$. Then, with the state vectors, the vector of a total composite system can be written as $|\Phi\rangle \equiv |\psi\rangle_A \otimes |\varphi\rangle_B \in$ $\mathcal{H}_A \otimes \mathcal{H}_B \equiv \mathcal{H}_{AB}$ ⁷ where it is called the tensor product of two vectors. Further, one can consider a possibility that a composite state exists in a specific state

⁷Without confusion, $|\psi\rangle_A \otimes |\varphi\rangle_B$ is also denoted as $|\psi\rangle|\varphi\rangle$ or $|\psi,\varphi\rangle$.

 $|\psi_1\rangle|\varphi_1\rangle$ or $|\psi_2\rangle|\varphi_2\rangle$ and also the superposition of the possible states as

$$|\Psi\rangle = \alpha |\psi_1\rangle |\varphi_1\rangle + \beta |\psi_2\rangle |\varphi_2\rangle \tag{2.13}$$

where $|\Psi\rangle \in \mathcal{H}_{A\mathcal{B}}$. Except for a trivial case, this state cannot be written as a tensor product of any two vectors⁸. For an ideal measurement, the state can be found in the state $|\psi_1\rangle|\varphi_1\rangle$ with probability $|\alpha|^2$ or in $|\psi_2\rangle|\varphi_2\rangle$ with $|\beta|^2$. Such a composite state whose state vector cannot be decomposed into a direct product of its subsystems is said to be an entangled state (or non-separable state), such states play a fundamental role in quantum mechanics.

Interestingly, in the state (2.13), the two different systems A and B are strongly correlated in a sense that the measurement on one system, say A, will determine the state of the other system B. If one finds that the system A is in $|\psi_1\rangle$ from its measurement, then the system B is always in $|\varphi_1\rangle$ and vice versa. In contrast to the state of B before the measurement on A, which is probabilistic, the state of system B is determined as either $|\varphi_1\rangle$ or $|\varphi_2\rangle$ after the measurement on A. It implies that the state of B is influenced by the action of the measurement on A and this may be taken as a serious problem in deploying the theories in physics. If measuring action at a distance changes the state of a system which is outside of the light cone, then it can conflict with special relativity. However, it is after Bob receives the information of the measurement results from Alice that the quantum state of Bob reduces to one of the two states. Therefore, since the speed of communication between Alice and Bob is restricted by the speed of light so that superluminal communication via quantum states is not possible [79] and quantum mechanics and relativity can harmoniously coexist [87]⁹.

2.1.2 Vector transformation and entanglement

A formal way of generating entanglement is through the direct interaction between two quantum systems. An interaction between quantum systems is described by the dynamics of the composite system and any dynamics of a pure state can be expressed in terms of unitary operations of state vectors *i.e.* vector transformation. Without any constraint, a state vector can be transformed into another vector by an operator defined in the Hilbert space \mathcal{H}

$$|\psi\rangle \xrightarrow{\hat{U}} |\psi'\rangle = \hat{U}|\psi\rangle,$$
 (2.14)

⁸Such a state is called separable state.

⁹See also [88, 89] for the relation between the quantum mechanics and no-signalling theorem.

where the operator \hat{U} satisfies the unitary condition $\hat{U}\hat{U}^{\dagger} = \mathbb{1}_{\mathcal{H}}^{10}$ from $\langle \psi' | \psi' \rangle = 1$. The unitary operation on a quantum state describes time-evolution of the state by mapping a state vector into another vector. A unitary operator can be represented in terms of an Hermitian operator \hat{H} as $\hat{U}(t) = e^{-it\hat{H}}$ where the unitarity is guaranteed by the self-adjoint condition of the Hermitian operator, *i.e.* $\hat{H} = \hat{H}^{\dagger}$. In the Schrödinger picture of dynamics, the transformed vector $|\psi'\rangle \equiv |\psi(t)\rangle = e^{-it\hat{H}} |\psi(0)\rangle$ is the solution of the Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -i\hat{H}|\psi(t)\rangle \tag{2.15}$$

where \hat{H} is the Hamiltonian for the dynamics of the system, which is a Hermitian operator. Thus, the dynamics of a quantum system can be represented by a transformation of a state vector and the Hamiltonian specifies the vector transformation which is unitary.

Consider a transformation of a state vector which describes a bipartite quantum system. For a bipartite quantum system, their interactions are governed by the type of Hamiltonian which corresponds to the evolution of the total composite system. When two initially separable states interact with each other by a Hamiltonian, the total system is transformed into another state and can be entangled as

$$|\Psi\rangle = |\psi\rangle|\varphi\rangle \xrightarrow{U} |\Psi'\rangle = \hat{U}|\Psi\rangle \qquad (2.16)$$

$$= \alpha |\psi_1\rangle |\varphi_1\rangle + \beta |\psi_2\rangle |\varphi_2\rangle \qquad (2.17)$$

where the transformation creates a superposition of the composite system. This is a typical way to make two initially separate pure states entangled.

However, a local unitary operation on each subsystem cannot make the systems entangled. This is due to the fact that the local operation on the state vector maps the vector into another vector while the tensor product structure of the total state is conserved as

$$|\psi\rangle \otimes |\varphi\rangle \xrightarrow{\hat{U}_A \otimes \hat{U}_B} |\psi'\rangle \otimes |\varphi'\rangle \equiv \hat{U}_A |\psi\rangle \otimes \hat{U}_B |\varphi\rangle.$$
(2.18)

The example is when the two systems A and B do not interact with each other. For the local operation, the Hamiltonian is written as $\hat{H} = \hat{H}_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \hat{H}_B$ which corresponds to the free evolution of the local systems. Thus, any unitary operation

 $^{{}^{10}\}mathbb{1}_{\mathcal{H}}$ is the identity operator which is defined in \mathcal{H} and \dagger represents the adjoint of an operator (complex conjugate and transposition).

 $\hat{U}_{AB} \in \mathcal{B}(\mathcal{H}_{A\mathcal{B}})^{11}$ on a product state cannot create entanglement between two quantum systems when the \hat{U}_{AB} can be factorized into $\hat{U}_A \otimes \hat{U}_B$.

Without loss of generality, for a bipartite quantum system whose subsystems are both in \mathcal{H}_d , it is possible to write

$$|\Psi\rangle = \sum_{i=0}^{d-1} \sum_{j=0}^{d-1} c_{ij} |i,j\rangle$$
(2.19)

where c_{ij} is the $d \times d$ complex numbers with unit norm ¹². For a particular choice of the basis, any $d \times d$ bipartite pure quantum system can be transformed into a simple form, called the *Schmidt decomposition* (see for example [44, 90]),

$$|\Psi\rangle = \sum_{k=0}^{d-1} g_k |u_k, v_k\rangle \tag{2.20}$$

where $|u_k\rangle$ and $|v_k\rangle$ are orthonormal Schmidt basis and the g_k are the Schmidt coefficients satisfying $\sum_{k=0}^{d-1} |g_k|^2 = 1$. The Schmidt decomposition can be proven with help of local basis transformations as

$$|u_k\rangle = \sum_{i=0}^{d-1} u_{ik}|i\rangle \text{ and } |v_k\rangle = \sum_{j=0}^{d-1} v_{jk}|j\rangle$$
(2.21)

and they lead Eq. (2.20) into Eq. (2.19) with $c_{ij} = \sum_{k=0}^{d-1} g_k u_{ik} v_{jk}$. Thus, the Schmidt decomposition of a pure bipartite state is obtained by a local basis transformation and the bipartite state is separable if and only if there is only one non zero Schmidt coefficient.

2.1.3 Density matrix for a mixed state

A state vector represents a pure quantum system. However, the state vector representation is not enough to describe a general quantum system. If we consider a bipartite system which is entangled as in Eq. (2.20), $|\Psi\rangle \in \mathcal{H}_{A\mathcal{B}}$, a measurement which is performed on a system A only is given by

$$P(M) = \langle \Psi | \hat{M}_A \otimes \mathbb{1} | \Psi \rangle \tag{2.22}$$

¹¹A bounded operator space is call Banach space. Basic definitions for the Banach space are given in Appendix B. $\mathcal{B}(\mathcal{H})$ is the operator space defined in \mathcal{H} .

 $^{^{12}\}text{Norm}$ of a matrix is defined as $||\hat{C}|| \equiv \sqrt{\text{Tr}(\hat{C}\hat{C}^{\dagger})}$

where P(M) is the expectation value for a measurement M and \hat{M}_A is the measurement operator acting only on the system A *i.e.* $\hat{M}_A \in \mathcal{B}(\mathcal{H}_A)$. The entangled state in Eq. (2.20) is expanded in an orthogonal basis and it allows one to calculate the expectation value P(M) as

$$P(M) = \sum_{k,l=0}^{d-1} g_k^* g_l \langle u_k | \hat{M}_A | u_l \rangle \delta_{kl}$$
 (2.23)

$$= \sum_{k=0}^{d-1} |g_k|^2 \langle u_k | \hat{M}_A | u_k \rangle = \text{Tr}(\hat{\rho} \hat{M}_A)$$
(2.24)

where the density operator $\hat{\rho} \equiv \sum_{k=0}^{d-1} |g_k|^2 |u_k\rangle \langle u_k|$ and the trace of an operator $\operatorname{Tr}(\hat{O}) \equiv \sum_{i=0}^{d-1} \langle i | \hat{O} | i \rangle$. This implies that a general quantum system, specially a mixed state, which is entangled with another system, cannot be represented by a state vector but must be represented by a operator called a density operator. For a trivial case when only one Schmidt coefficient g_k is non-zero, the density matrix is reduced to a rank one projector which is a pure quantum state. In this case, $\hat{\rho}^2 = \hat{\rho}$, which is the condition for a pure state density operator.

The density matrix for a general mixed state can be written in a spectrally decomposed form with rank one projectors, $|u_k\rangle\langle u_k|$ as well as a $d \times d$ matrix in an arbitrary orthonormal basis $\{|i\rangle\}$,

$$\hat{\rho} = \sum_{k=0}^{d-1} |g_k|^2 |u_k\rangle \langle u_k|$$
(2.25)

$$= \sum_{ij} \rho_{ij} |i\rangle \langle j|.$$
 (2.26)

where the matrix element $\rho_{ij} = \sum_{k=0}^{d-1} u_{ik} u_{jk}^* |g_k|^2$ and u_{ik} are the elements of a unitary operator. This means that, for a given mixed state, there are infinitely many possible representations. As a simple example, an identity operator $\frac{1}{2}\mathbb{1}_2$, which describes an equal statistical mixture of two possible states, can be decomposed as $\frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ or $\frac{1}{2}(|+\rangle\langle +|+|-\rangle\langle -|)$ with $|\pm\rangle = \frac{1}{2}(|0\rangle \pm |1\rangle)$, or even $\frac{1}{2}|\psi(\theta)\rangle\langle\psi(\theta)|$ where $|\psi(\theta)\rangle \equiv \cos\theta|0\rangle + \sin\theta|1\rangle$. This also implies that, unlike a pure state, for any mixed state there are infinitely many different ways to prepare it and the differently prepared mixed states are identical if they can be represented by the same density operator. Physically, two quantum states are identical if it is completely impossible to distinguish the two states by any possible measurement.

Mathematically, the density operator is defined as a Hermitian operator with

unit trace whose eigenvalues are real and positive. The properties of a density operator can be summarised,

- 1. Hermitian operator: $\hat{\rho} = \hat{\rho}^{\dagger}$
- 2. Positive operator: For any $|\psi\rangle$, $\langle\psi|\hat{\rho}|\psi\rangle \geq 0$
- 3. Unit trace : $Tr(\hat{\rho}) = 1$

The convexity¹³ of the density matrix follows immediately from the the conditions above, that is, a convex combination of density operators is also a density operator as

$$\hat{\rho} = \lambda \hat{\rho}_1 + (1 - \lambda)\hat{\rho}_2 \tag{2.27}$$

where $0 \leq \lambda \leq 1$. That is to say that a mixed state can be constructed by mixing the state $\hat{\rho}_1$ with a probability λ and the state $\hat{\rho}_2$ with a probability $1 - \lambda$. There are infinitely many choice of $\hat{\rho}_1$ and $\hat{\rho}_2$ for a given density matrix $\hat{\rho}$. However, a pure state is peculiar in this sense since it cannot be expressed as a convex sum of the other states and this is the reason that a pure state is called an extremal point.

2.1.4 Phase space representation for CV state

For a continuous variable state, the Wigner function [91] which is defined in phase space is advantageous in many respects. The Wigner function is defined as the fourier transformation of a characteristic function as

$$W(\xi) = \frac{1}{\pi^2} \int_{-\infty}^{\infty} d^2 \alpha \ \chi(\alpha) \exp(\xi \alpha^* - \xi^* \alpha)$$
(2.28)

where the characteristic function $\chi(\xi)$ is the expectation value of the displacement operator

$$\chi(\alpha) = \text{Tr}\hat{\rho}\hat{D}(\alpha). \tag{2.29}$$

where the $\hat{D}(\alpha)$ is the displacement operator defined in (2.10). The Wigner function is directly linked to the expectation values of the bosonic operators of arbitrary high order moments [92] as

$$\langle (\hat{a}^{\dagger m} \hat{a}^n)_s \rangle = \int_{-\infty}^{\infty} d^2 \xi \ W(\xi) \ \xi^{*m} \xi^n$$
 (2.30)

 $^{^{13}\}mathrm{A}$ set is said to be convex if the set contains the straight line segment connecting any two points in the set.

where subscript s means the symmetric ordering for the bosonic operators. The symmetric ordering is an expansion of the bosonic operators in every possible symmetric ordering, for example $(\hat{a}^{\dagger}\hat{a}^{2})_{s} \equiv \frac{1}{3}(\hat{a}^{2}\hat{a}^{\dagger} + \hat{a}\hat{a}^{\dagger}\hat{a} + \hat{a}^{\dagger}\hat{a}^{2})$.

From the bosonic operators, the quadrature operators for canonical variables can be obtained, $\hat{X} \equiv \hat{q}_1$ and $\hat{P} \equiv \hat{q}_2$. They can be used to derive the Heisenberg uncertainty relation [84, 93] in terms of the variance matrix as

$$\mathbf{V} + \frac{i}{2}\mathbf{\Omega} \ge 0 \tag{2.31}$$

where the variance matrix **V** is 2×2 real matrix and $\mathbf{\Omega} \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Elements of the variance matrix are the expectation values of second order moments for canonical variables $\langle (\Delta \hat{q}_i \Delta \hat{q}_j)_s \rangle$ and can be obtained from the Wigner function

$$V_{ij} = \langle (\Delta \hat{q}_i \Delta \hat{q}_j)_s \rangle \tag{2.32}$$

$$= \int d^2q \Delta q_i \Delta q_j W(q_i, q_j) \tag{2.33}$$

where $\Delta \hat{q}_i = \hat{q}_i - \langle \hat{q}_i \rangle$. Therefore, a continuous variable state can be fully described by a Wigner function and the second order moments $\langle (\Delta \hat{q}_i \Delta \hat{q}_j)_s \rangle$ of a state for its minimum uncertainty relation can be obtained from the Wigner function.

A transformation of density matrix $\hat{\rho} \to \hat{\rho}' = \Lambda(\hat{\rho})^{-14}$ changes the form of its variance matrix $\mathbf{V} \to \mathbf{V}'$ as well as the Wigner function $W(\xi) \to W'(\xi)$. Especially, for a transformation by a unitary operation $\hat{\rho} \to \hat{\rho}' = \hat{U}\hat{\rho}\hat{U}^{\dagger}$, the variance matrix of the state is also transformed into another variance matrix leaving the uncertainty relation in (2.31) invariant by satisfying

$$\mathbf{V}' + \frac{i}{2}\mathbf{\Omega} \ge 0. \tag{2.34}$$

It is direct consequence that a unitary operation conserves the commutator of the quadrature operators

$$[\hat{q}_{\alpha}, \hat{q}_{\beta}] = i\Omega_{\alpha\beta} \longrightarrow [\hat{q}'_{\alpha}, \hat{q}'_{\beta}] = [\hat{U}^{\dagger}\hat{q}_{\alpha}\hat{U}, \hat{U}^{\dagger}\hat{q}_{\beta}\hat{U}] = i\Omega_{\alpha\beta}$$
(2.35)

where $\alpha, \beta \in \{1, 2\}$ and $\hat{U}^{\dagger}\hat{U} = \mathbb{1}$. Thus, a unitary operation of a density matrix preserves the uncertainty relation for the state whereas it transforms the variance

¹⁴The Λ is a map for a operator which corresponds to a function for an operator.

matrix in a following manner

$$\hat{\rho} \to \hat{\rho}' = \hat{U}(S)\hat{\rho}\hat{U}^{\dagger}(S) \iff \mathbf{V} \longrightarrow \mathbf{V}' = \mathbf{SVS^{T}}$$
 (2.36)

where S in $\hat{U}(S)$ is $S \in Sp(2, \mathbb{R})$ and it can be represented by a 2×2 real matrix **S** which satisfies

$$\mathbf{S}\mathbf{\Omega}\mathbf{S}^{\mathbf{T}} = \mathbf{\Omega} \tag{2.37}$$

which is the condition for symplectic transformation and results in $det(\mathbf{S}) = 1$.

However, the transformation of the Wigner function, corresponding to the unitary operation for the state, is nontrivial in general (see such as [94]). It is only when the Hamiltonian for the unitary operator $\hat{U} = \exp(-i\hat{H}t)$ is quadratic that the Wigner function is transformed by the symplectic transformation of canonical variables

$$\hat{\rho} \to \hat{\rho}' = \hat{U}(S)\hat{\rho}\hat{U}^{\dagger}(S) \iff W(\xi) \longrightarrow W'(\xi) = W(\mathbf{S}^{-1}\xi)$$
 (2.38)

where $\xi \equiv (q_1, q_2)^T$. This can be proven straightforwardly by the transformation of the characteristic function

$$\chi(\alpha) \to \chi'(\alpha) = \operatorname{Tr}\left(\hat{U}(S)\hat{\rho}\hat{U}^{\dagger}(S)\ \hat{D}(\alpha)\right)$$

$$= \operatorname{Tr}\left(\hat{\rho}\ \hat{U}^{\dagger}(S)\hat{D}(\alpha)\hat{U}(S)\right) = \operatorname{Tr}\left(\hat{\rho}\hat{D}(\alpha')\right) = \chi(\alpha').$$
(2.39)

where $\alpha' = \alpha'_r + i\alpha'_i$ and $(\alpha'_r, \alpha'_i)^T = \mathbf{S}(\alpha_r, \alpha_i)^T$. The unitary operation is a linear Bogoliubov operation which transforms a Gaussian state into a Gaussian state. Any linear Bogoliubov operation is obtainable by combining the squeezing transformation together with some rotations [95].

2.1.5 Formal definition of entanglement

Entanglement of a general mixed state is not a simple extension of pure state entanglement. A bipartite mixed state is represented in terms of the density matrix in the extended Hilbert space $\hat{\rho} \in \mathcal{B}(\mathcal{H}_{AB})$. The bipartite mixed state can be generated classically if it can be decomposed as

$$\hat{\rho} = \sum_{r=1}^{n} p_r \hat{\rho}_r^A \otimes \hat{\rho}_r^B \tag{2.41}$$

where $p_r \in [0, 1]$ satisfies $\sum_{r=1}^{n} p_r = 1$ and $\hat{\rho}_r^{A(B)}$ is the density matrix for the Alice's (Bob's) side. The density matrix in (2.41) can be obtained if one considers a device which generates random numbers $r = 1, \dots, n$ and sends the random numbers to Alice and Bob who will prepare their states locally as $\hat{\rho}_r^A$ and $\hat{\rho}_r^B$ based upon the random number they receive. A density matrix is called classically correlated [8] if it can be approximated (*e.g.* in trace norm) by density matrices of the form (2.41). The physical "source" of generated correlations is the random generator which is chosen as a purely classical device. Moreover, the definition of a classically correlated state is equivalent to that of a separable state for a pure state.

A state which cannot be written in the classically correlated form is called an inseparable state or equivalently an entangled state. In other words, entanglement is defined as a correlation which cannot be created in any classical way. However, whether a given bipartite density matrix $\hat{\rho}$ can be decomposed in the form of (2.41) or not is by no means a trivial problem in general. For example, let us consider a density matrix in a 2 × 2 Hilbert space $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$

$$\hat{\rho}_{S} = \frac{1}{20} \left(9|\Phi^{+}\rangle\langle\Phi^{+}| + 5|\Phi^{-}\rangle\langle\Phi^{-}| + 5|\Psi^{+}\rangle\langle\Psi^{+}| + |\Psi^{-}\rangle\langle\Psi^{-}| \right)$$
(2.42)

where $|\Phi^{\pm}\rangle \equiv \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$ and $|\Psi^{\pm}\rangle \equiv \frac{1}{\sqrt{2}}(|01\rangle \pm |01\rangle)$ are the Bell bases¹⁵. The state is a statistical mixture of maximally entangled states. One might conjecture that the state is entangled since, from the state, we can obtain one of the maximally entangled states by a measurement with a nontrivial probability. If we rewrite the density matrix $\hat{\rho}_S$ in matrix form, which is in the orthonormal bases $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\},$

$$\hat{\rho}_S = \frac{1}{20} \begin{pmatrix} 7 & 0 & 0 & 2\\ 0 & 3 & 2 & 0\\ 0 & 2 & 3 & 0\\ 2 & 0 & 0 & 7 \end{pmatrix}.$$
(2.43)

This is not clear whether the state is separable or not. Difficulty in testing its entanglement may arise from the fact that one should consider every possible expression of the density matrix. In fact, the state $\hat{\rho}_S$ can be written as

$$\hat{\rho}_{S} = \frac{1}{4} \left(|00\rangle \langle 00| + |11\rangle \langle 11| \right) + \frac{1}{20} \left(|01\rangle \langle 01| + |10\rangle \langle 10| \right)$$

$$+ \frac{1}{5} \left(|++\rangle \langle ++|+|--\rangle \langle --| \right),$$
(2.44)

¹⁵The Bell bases themselves are maximally superposed pure states (in that sense, maximally entangled state) whose vectors $\{|\Phi^{\pm}\rangle, |\Psi^{\pm}\rangle\}$ constitute complete set of orthogonal basis in 2×2 Hilbert space.

with $|\pm\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$. The method for finding product expansion is introduced in Appendix A. Thus, the state $\hat{\rho}_S$ is a separable state which can be constructed by local operations and classical communications. In general, the problem of determining whether a given mixed state is entangled or not is notoriously difficult to solve and only a partial solution is presently known.

2.2 Characterization of entanglement

There are many problems related to the entanglement of an arbitrary quantum state. Quantification of the amount of entanglement is one of them. Such a quantification would allow one to compare any two different quantum systems in terms of their degree of entanglement.

One may consider a map $\hat{\rho} \longrightarrow \varepsilon(\hat{\rho})$ which characterizes entanglement in the system $\hat{\rho}$. In 1998, Vedral and Plenio [67] suggested that any "successful" measure of entanglement $\varepsilon(\hat{\rho})$ should satisfy the three conditions

- (C.1) $\varepsilon(\hat{\rho}) = 0$ iff $\hat{\rho}$ is separable.
- (C.2) Any local unitary transformation leaves $\varepsilon(\hat{\rho})$ invariant; *i.e.* $\varepsilon(\hat{U}_1^{\dagger} \otimes \hat{U}_2^{\dagger} \hat{\rho} \hat{U}_1 \otimes \hat{U}_2) = \varepsilon(\hat{\rho})$ for some unitary operators \hat{U}_1 and \hat{U}_2
- (C.3) $\varepsilon(\hat{\rho})$ cannot increase under local general measurement(LGM), classical communications (CC), and post selection of sub-ensemble(PSS) with their corresponding operators $\{\hat{V}_i\}$ satisfying the completeness $\sum_i \hat{V}_i^{\dagger} \hat{V}_i = \hat{1}$; *i.e.* $\sum_i p_i \varepsilon(\hat{\rho}_i) \leq \varepsilon(\hat{\rho})$ where $p_i \hat{\rho}_i = \hat{V}_i \hat{\rho} \hat{V}_i^{\dagger}$ with $p_i = \text{Tr} \hat{\rho}_i$.

The first condition is about separability of a system. If it is a proper measure, it should successfully discriminate an entangled state from a separable state.

The second condition is referred to as the local unitary (LU) invariant condition. Entanglement is a correlation which is generated by the interaction of two systems. Any class of density matrices which is LU invariant is taken to be the states which have an equal amount of entanglement since these states can be converted bilaterally by local operations. For the case of a pure state, each class of LU invariant states can be represented by their Schmidt coefficients. That is to say, the states which have identical Schmidt coefficients have LU invariant properties and thus have same amount of entanglement. For a mixed state, Werner [8] found a class of states

$$\hat{\rho}_W = \frac{1-p}{d^2} \mathbb{1}_A \otimes \mathbb{1}_B + p |\Psi\rangle \langle \Psi|$$
(2.45)

where

$$|\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{n=0}^{d-1} |u_n, u_n\rangle_{AB}$$
(2.46)

which is parameterized by a single parameter $0 \leq p \leq 1$. The state is highly symmetric in the sense that partially transposed ¹⁶ state of the Werner state *i.e.* $(\hat{\rho}_W)^{T_A}$ is invariant for the same local unitary operation at each side *i.e.* $\hat{U} \otimes \hat{U}$ invariant. In other words, for a fixed p, the state (2.45) is $\hat{U} \otimes \hat{U}^{\dagger}$ invariant so that p can be taken to be the degree of entanglement of the state.

The third condition is about local operations and classical communications (LOCC). The LOCC includes all possible local operations¹⁷ on the system and all communications by classical channels¹⁸. From its definition, no local operations can increase the average entanglement of the system. However, one should be careful that there is a possibility that the entanglement of a system can be increased by selecting a sub-ensemble of highly entangled states from a given ensemble although the overall entanglement cannot be increased. It is so called entanglement purification [69, 74, 97] which extracts the small number of highly entangled states from a large ensemble of less entangled states.

2.2.1 Entropies for a pure state entanglement

Entanglement of a bipartite pure state can be discussed in terms of Schmidt coefficients. If a state vector of a pure state is transformed into a Schmidt decomposed form Eq. (2.20), the Schmidt coefficient g_k^{19} represents the probability that the composite system is found in a state $|u_k, v_k\rangle$. If a measurement results of the opposite party is not known to the other party *e.g.* when Alice does not know the measurement outcome of Bob, the Schmidt coefficient for Alice simply means the probability that her measurement outcome will be k. Before the measurement and without the information of Bob's measurement, the state of Alice behaves as

 $^{^{16}}$ The precise definition of partial transposition is given in section 2.2.2.

¹⁷Local operations would include local unitary operations, selection of sub-ensemble and generalized measurement for the local systems

 $^{^{18}}$ The role of classical communications and classical information for the quantum correlation is studied in many articles, *e.g.* [96] which is very recent one.

¹⁹Without loss of generality, the real part is enough in this case since the phase part can be absorbed into the defined orthogonal basis.

a random state whose probability distribution depends upon the Schmidt coefficients. The probability distribution describes randomness of Alice's state which is directly related with the amount of correlation for the total state. The same argument can be applied to Bob's side as well. If one considers a partial transposition of the total state Eq. (2.20), then

$$\hat{\rho}_A = \mathrm{Tr}_B |\Psi\rangle \langle \Psi| \qquad (2.47)$$

$$= \sum_{k=0}^{d-1} g_k^2 |u_k\rangle \langle u_k| \tag{2.48}$$

where $\hat{\rho}_A$ is the density matrix for Alice when Bob does nothing to his particle. Before the involvement of measurement, the state is completely random for any possible measurement if the Schmidt coefficients are evenly distributed over the measurement outcomes k i.e. $g_k^2 = \frac{1}{d}$ for $\forall k$. This is where the system has completely lost all information about its own state by the correlation with the particle B and the state is called a maximally entangled state. In contrast to the measurement outcome on the state A is independent of the particle B. The state is a separable state. Thus, the entanglement of a bipartite state can be characterized by the degree of uncertainty or the lack of information about the local state.

In information theory, there is a quantified property of information named Shannon's entropy [98] as

$$S(p) \equiv -\sum_{i} p_i \log_2 p_i.$$
(2.49)

which is a function of the probability distribution $\{p_i\}$. For evenly distributed probabilities $\{p_i = \frac{1}{d}, \text{ for } \forall i\}$, Shannon's entropy is maximized while it is a minimum for a fully concentrated probability distribution. Therefore, it is a property which characterizes the uncertainty of the system. For a binary probability distribution, it is parameterized by a single value as $S(p) = -p \log_2 p - (1-p) \log_2(1-p)$ where $p \in [0, 1]$ and is a monotonically increasing function between $0 \le p \le \frac{1}{2}$.

Meanwhile, entanglement of a bipartite pure state can be characterized by Shannon's entropy of the Schmidt coefficients. The characterization is equivalent to using the von Neumann entropy of the partially traced density matrices, since the Schmidt coefficients are the eigenvalues of the Hermitian operator which is obtained by a partial trace of one of either party. It is written

$$\varepsilon(|\Psi\rangle) = -\mathrm{Tr}\hat{\rho}_A \log_2 \hat{\rho}_A = -\mathrm{Tr}\hat{\rho}_B \log_2 \hat{\rho}_B \qquad (2.50)$$

$$= -\sum_{k=0}^{d-1} g_k^2 \log_2 g_k^2 \tag{2.51}$$

where $\hat{\rho}_{A(B)}$ is the partially traced density matrix for Alice (Bob) $\hat{\rho}_{A(B)} = \text{Tr}_{B(A)}\hat{\rho}$ and g_k is the Schmidt coefficient. The von Neumann entropy which is exploited as a measure of entanglement is defined in terms of the density matrix as $S_V(\hat{\rho}) =$ $-\text{Tr}\hat{\rho}\log_2\hat{\rho}$ whose general properties were found by A. Wehrl [99] as enumerated below

- 1. For a pure state, $S_V(|\phi\rangle\langle\phi|) = 0$ and for a maximally mixed state $S_V(\frac{1}{d}\mathbb{1}_d) = \log_2 d$.
- 2. von Neumann entropy is not changed by a unitary operation : $S_V(\hat{\rho}) = S_V(\hat{U}\hat{\rho}\hat{U}^{\dagger}).$
- 3. Concavity of the von Neumann entropy : $S_V(\sum_i \lambda_i \hat{\rho}_i) \ge \sum_i \lambda_i S_V(\hat{\rho}_i).$
- 4. Subadiditivity and Triangle inequality (Araki-Lieb inequality[100]) : $|S_V(\hat{\rho}_A) - S_V(\hat{\rho}_B)| \le S_V(\hat{\rho}) \le S_V(\hat{\rho}_A) + S_V(\hat{\rho}_B)$
- 5. The von Neumann entropy is always smaller than Shannon entropy which is obtained by the probabilities for the measurement outcome on the system $\hat{\rho}$: $S(\{p_i\}) \geq S_V(\hat{\rho})$, where $p_i \equiv \langle u_i | \hat{\rho} | u_i \rangle$ and equality holds for the observable which commutes with the density matrix.

From the properties 1, 2 and 3, it is not difficult to see that the von Neumann entropy of a partially traced density matrix satisfies the conditions (C.1), (C.2) and (C.3) as a measure of entanglement. The uncertainty or the randomness of each local state measures the amount of entanglement which is generated by the quantum correlations of the two systems.

A physical meaning of von Neumann entropy can be found from the *entangle*ment concentration [69]. Entanglement concentration is a protocol of obtaining a smaller number of maximally entangled states from partially entangled pure states through local operations and measurements. Bennett, Bernstein, Popescu and Schumacher [69] found that the entanglement concentration asymptotically conserves the von Neumann entropy as the average expected entanglement of the concentrated states which are produced from an ensemble of a partially entangled states. These results give a physical meaning to the von Neumann entropy as a measure of entanglement which is the asymptotic number, $n\varepsilon - O(\log_2 n)$, of maximally entangled states obtained from n partially entangled states.

However, the von Neumann entropy cannot be utilized as a measure of entanglement for a mixed state. The separable state defined in Eq. (2.41) does not necessarily have zero von Neumann entropy so that the first condition (C.1) as a measure of entanglement is not satisfied. As a measure of entanglement for mixed states, there are several suggestions such as entanglement of formation (EoF) [97, 101], entanglement of distillation (EoD) [97] and relative entropy (RE) [66, 67] all of which obey the condition (C.1)-(C.3). The EoF, $\varepsilon_F(\hat{\rho})$, is defined as the least expected entanglement of any ensemble of pure states realizing $\hat{\rho}$ as

$$\varepsilon_F(\hat{\rho}) \equiv \min\left\{\sum_i p_i S_V(\hat{\rho}_A^i) \mid \hat{\rho} = \sum_i p_i |\psi_i\rangle \langle \psi_i| \text{ and } \hat{\rho}_A^i = \text{Tr}_B |\psi_i\rangle \langle \psi_i| \right\} \quad (2.52)$$

where $|\psi_i\rangle \in \mathcal{H}_{A\mathcal{B}}$ and the minimum is taken for the possible decompositions of the state $\hat{\rho}$. The EoF agrees with the asymptotic number of maximally entangled states to realize the state $\hat{\rho}$. Meanwhile, the EoD, ε_D , is the amount of entanglement of a state as the asymptotic proportion of singlets that can be distilled using purification procedure which is converse of the EoF. More rigorous definition of EoD can be found at [102]. Differently from the reversibility of entanglement concentration, the purification of entanglement for a mixed state is an irreversible process which implies $\varepsilon_D \leq \varepsilon_F$. In fact, Horodecki *et al.* [103] showed that any entanglement measure ε suitable for the regime of a high number of identically prepared entangled pairs satisfies $\varepsilon_D \leq \varepsilon \leq \varepsilon_F$. The RE is such a measure of entanglement. The RE of a state is defined as a distance between the given state and the nearest separable state. From the fact that a distance between sets of probabilities can be represented by the relative entropy, the RE is defined as

$$\varepsilon_{RE}(\hat{\rho}) \equiv \min_{\hat{\sigma} \in \mathcal{D}} S(\hat{\rho} || \hat{\sigma}) \tag{2.53}$$

where $S(\hat{\rho}||\hat{\sigma})$ is the quantum relative entropy and \mathcal{D} is the set of all separable state. The RE provides an upper bound to the EoD and a lower bound to the EoF [67, 70]. Furthermore, not all entangled states can be distilled. Entangled states which are not distillable are called bound entangled states [104].

2.2.2 Negativity of partial transposition

The separability condition of a mixed quantum state is defined in Eq. (2.41) as the possibility of expanding its density matrix as a convex combination of product density matrices. The separable state which can be prepared only by classical resources is a local state in the sense that every possible local operation on the subsystem,

$$\mathbb{1}_A \otimes \Lambda_B(\hat{\rho}^s_{AB}) = \sum_i p_i \hat{\rho}^A_i \otimes \Lambda_B(\hat{\rho}^B_i), \qquad (2.54)$$

leaves the total state positive definite. The Λ_B^{20} represents a possible physical operation or equivalently a positive map, on the subsystem B. A map is called *positive* if the map transforms a density matrix into a proper density matrix and is called *completely positive* (CP) if the map keeps the positivity even under an extension of Hilbert space. Thus, if one finds a positive map which is not completely positive for a quantum state, then it can be used as a criterion which determines whether the state is entangled with the other system or not. It utilizes the fact that a legitimate operation on a state which is isolated from the external system can be an illegal operation if the state is entangled with another external system. That is because when the states A and B are entangled, an action on system B will modify the state of the whole system.

Let us consider a so-called time reversal of the Schrödinger equation for a quantum system. The unitary operation in Eq. (2.14) transforms the density matrix for a time evolution of a quantum state. If we consider a *transposition* map on an operator which is defined $[\Lambda^T(\hat{A})]_{ij} = [\hat{A}]_{ji}$, the time evolution rule for the transposed density matrix becomes

$$\hat{\rho}(0)^{T} \rightarrow \hat{U}(t)\hat{\rho}(0)^{T}\hat{U}^{\dagger}(t) = e^{-it\hat{H}}\hat{\rho}(0)^{T}e^{it\hat{H}}$$

$$= \left[e^{it\hat{H}^{T}}\hat{\rho}(0)e^{-it\hat{H}^{T}}\right]^{T} \qquad (2.55)$$

$$\equiv \left[\hat{U}_{T}(-t)\hat{\rho}(0)\hat{U}_{T}^{\dagger}(-t)\right]^{T}$$

$$= \hat{\rho}(-t)^{T}$$

where $\hat{\rho}^T \equiv \Lambda^T(\hat{\rho})$ and $\hat{U}_T(t) \equiv e^{-it\hat{H}^T}$. Note that a transposed Hermitian operator is also Hermitian *i.e.* $\hat{\rho}^T$ and \hat{H}^T are Hermitian operators. Eq. (2.55) shows that

²⁰The notation for the map acts as a function from operator to operator such as $\hat{\rho}_B \to \hat{\rho}'_B = \Lambda_B(\hat{\rho}_B)$ and sometimes it is specified as $\Lambda_B \in \mathcal{M}(\mathcal{H}_{\mathcal{B}}, \mathcal{H}_{\mathcal{B}})$ when it map the operator from $\mathcal{B}(\mathcal{H}_{\mathcal{B}})$ into $\mathcal{B}(\mathcal{H}_{\mathcal{B}})$.

the transposition of a density matrix changes the time evolution rule of density matrices in such a way that the time arrow is reversed. It is not difficult to see that the transposition is a positive map for a density matrix since the eigenvalues of a density matrix are equivalent to those of the transposed density matrix. However, the transposition map is not a completely positive map as we will see shortly.

For the transposition map Λ^T , the Wigner function of an CV state is transformed by conjugation of the canonical parameter. This can be seen from

$$\chi(\alpha) \xrightarrow{\Lambda^T} \chi'(\alpha) = \operatorname{Tr}\left(\hat{\rho}^T \ \hat{D}(\alpha)\right)$$
(2.56)

$$= \operatorname{Tr}\left(\hat{\rho}\ \hat{D}^{T}(\alpha)\right) = \operatorname{Tr}\left(\hat{\rho}\hat{D}(-\alpha^{*})\right) = \chi(-\alpha^{*}) \quad (2.57)$$

which will result the $W(\alpha) \xrightarrow{\Lambda^T} W(\alpha^*)$ from the definition of the Wigner function in (2.28). Therefore, the transposition of a CV state changes the sign of the parameter which corresponds to the momentum.

Although it is a positive map, the transposition is not a complete positive map. The transposition of a subsystem of a composite system which exists in an extended Hilbert space is possible,

$$\mathbb{1}_A \otimes \Lambda_B^T(\hat{\rho}_{AB}) \tag{2.58}$$

is not a positive operator in general, where Λ_B^T is the transposition of the state B. The operation is called a partial transposition for the system B and is sometimes written as $\hat{\rho}_{AB}^{T_B}$. The partial transposition transforms a bipartite density matrix as $\langle i_A, j_B | \hat{\rho}_{AB}^{T_B} | k_A, l_B \rangle = \langle i_A, l_B | \hat{\rho}_{AB} | k_A, j_B \rangle$. If we apply the partial transposition on one of the Bell states, $(\hat{\rho})^{T_B} = (|\phi^+\rangle\langle\phi^+|)^{T_B}$ where $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \in \mathcal{H}_{AB}$, the density matrix is transformed

$$\hat{\rho} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \longrightarrow (\hat{\rho})^{T_B} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(2.59)

and the eigenvalues of the transposed density matrix are $\{\frac{1}{2}, -\frac{1}{2}\}$ and the partially transposed state is not positive definite anymore. Therefore, the partial transposition for its subsystem or local time reversal is not a positive map for density matrices in general.

A separable state is peculiar in that respect. When the state is separable,

the partial transposition preserves the positivity of the total density matrix. It is Peres [62] who observed that a necessary condition for separability is that a matrix, obtained by partial transposition of $\hat{\rho}$, has only non-negative eigenvalues. With the help of the definition (2.41), the partially transposed density matrix of a separable state $\hat{\rho}_{AB} \in \mathcal{B}(\mathcal{H}_{AB})$ is

$$\hat{\sigma} = \hat{\rho}_{AB}^{T_B} = \sum_i p_i \hat{\rho}_i^A \otimes (\hat{\rho}_i^B)^T$$
(2.60)

where $\sum_{i} p_i = 1$. Since the transposed matrices $(\hat{\rho}_i^B)^T$ are non-negative matrices for all *i* with unit trace, they are also legitimate density matrices. It follows that none of the eigenvalues of $\hat{\sigma}$ is negative. This is a necessary condition for Eq. (2.41) to hold. However, the opposite is not necessarily true. In other words, all the entangled states do not necessarily have negative eigenvalues.

The Horodecki family [63] proved that, when the system is in a 2×2 or 2×3 entangled state, the partially transposed density matrix always has a negative eigenvalue. They utilized the fact [105, 106] that any positive map Λ from a two-dimensional state into two or three-dimensional state as well as from a threedimensional state into a two-dimensional state is always decomposable into a completely positive map and transposition, $\Lambda = \Lambda^{CP} + \Lambda^{CP}\Lambda^T$, where Λ^{CP} is a completely positive map and Λ^T is a transposition. Therefore, if a map $\mathbb{1}_A \otimes \Lambda^T_B(\hat{\rho}_{AB})$ is positive, then any possible map $\mathbb{1}_A \otimes \Lambda_B(\hat{\rho}_{AB})$ is positive for 2×2 or 2×3 system. Combining the fact with Hahn-Banach's theorem [107], it is possible to conclude that $\mathbb{1}_A \otimes \Lambda^T_B(\hat{\rho}_{AB})$ is always positive if and only if the state is separable state in a 2×2 or 2×3 Hilbert space.

However, the entangled state does not necessarily have a negative eigenvalue for the partially transposed density matrix for any system other than those in a 2×2 or 2×3 Hilbert space. There are several examples of entangled states which have only positive eigenvalues for the partially transposed density matrix (PPT) and entangled state. Systemic construction of PPT entangled states is possible by employing unextendible product bases (UPB) [108]. The UPB are incomplete orthogonal product bases whose complementary subspace contains no product state. For the 3×3 Hilbert space, we consider the following incomplete

36

 $\begin{aligned} |\psi_1\rangle &\equiv & |0\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |\psi_2\rangle &\equiv & \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |2\rangle \\ |\psi_3\rangle &\equiv & |2\rangle \otimes \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \\ |\psi_4\rangle &\equiv & \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \otimes |0\rangle \\ |\psi_5\rangle &\equiv & \frac{1}{\sqrt{3}}(|0\rangle - |1\rangle + |2\rangle) \otimes \frac{1}{\sqrt{3}}(|0\rangle - |1\rangle + |2\rangle) \end{aligned}$ (2.61)

where $\{|0\rangle, |1\rangle, |2\rangle\}$ are complete orthonormal bases. Again, it is notable that there is no other product basis which is orthogonal to the all $|\psi_i\rangle$'s and the bases are orthogonal each other as $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. A state $\hat{\rho}_B$ which corresponds to the uniform mixture on the space complementary to the UPB $\{|\psi_i\rangle|$ for $\forall i\}$,

$$\hat{\rho}_B = \frac{1}{4} \left(\mathbb{1}_9 - \sum_{j=1}^5 |\psi_j\rangle \langle \psi_j| \right),$$
(2.62)

is an example of PPT state but an entangled state. From its definition, there is no product state $|u_a, v_b\rangle$ in the space orthogonal to all the $|\psi_i\rangle$'s in which the $\hat{\rho}_B$ is defined. Thus, for all the possible product states $|u_a, v_b\rangle$, $\langle u_a, v_b | \hat{\rho}_B | u_a, v_b \rangle = 0$ and this confirms the impossibility of the density matrix $\hat{\rho}_B$ decomposing into any product state. Therefore, the state $\hat{\rho}_B$ is entangled. The PPT of the state (2.62) is trivial to check. Furthermore, it is known that an infinite ensemble of the illustrated mixed entangled state in Eq. (2.62) is not possible to be distilled into a pure singlet state *i.e. bound entangled state*. That is from the proof of Horodecki family [104] that only the states which have a negative eigenvalue for partial transposition (NPT), can be distilled. All the PPT entangled states are bound entangled states which are inseparable but cannot be distilled.

The relation between the entanglement and the eigenvalue of partially transposed density matrix is summarized in Figure 2.2. As we discussed, all the separable states are all PPT states and all distillable states are NPT. A set of states which are entangled but can not be distilled are bound entangled states and the bound entangled states can be split into two different sets of states which are PPT bound entangled states, B^+ , and NPT bound entangled states, B^- . The existence of the different sets of entangled states is comparatively well known for highly symmetric states, but the conditions for general states are still under investigation. In comparison with the example of 3×3 PPT bound entangled states in Eq. (2.62), the B^+ and B^- sets are empty for the 2×2 and 2×3 states [109] such that any 2×2 and 2×3 inseparable states always are NPT and distillable. Bipar-

bases


Figure 2.2: The relation between the separability, distillability and positivity for partial transposition (PPT) of a bipartite state. All the separable states are PPT and all the distillable states are NPT (negative for a partial transposition). The state which is not separable nor distillable is bound entangled state and B^+ is denoted for PPT bound entangled state while B^- is NPT bound entangled state.

tite Gaussian entangled states are also distillable [110] which means the B^+ and B^- sets are empty. For the highly symmetric states, 2×2 and Gaussian states, the negative eigenvalue itself can even be used as a measure of entanglement. For the 2×2 system, one can denote the negative eigenvalues for the partially transposed density matrix as λ_i^- and a map $\varepsilon \in \mathcal{M}(\mathcal{H}_{A\mathcal{B}}, \mathbb{R})$

$$\varepsilon(\hat{\rho}) = -2\sum_{i}\lambda_{i}^{-} \tag{2.63}$$

satisfies the three conditions for a measure of entanglement (C.1), (C.2) and (C.3) [71] which is shown in Appendix C. For a Gaussian state, negative eigenvalues also satisfy the conditions [72] for a measure of entanglement.

Appendices

Appendix A

Finding a separable basis for a 2×2 system

For the purpose of brevity, we will only consider a real vector space for a qubit system. Let us consider an orthogonal basis set expanded in the basis set $\{|0\rangle, |1\rangle\}$ as

$$|+\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + |1\rangle\right) \tag{A.1}$$

$$|-\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle\right). \tag{A.2}$$

The matrix form of the vectors in the fixed basis $\{|0\rangle, |1\rangle\}$ are

$$|+\rangle\langle+| = \frac{1}{2} \begin{pmatrix} 1 & 1\\ 1 & 1 \end{pmatrix} \equiv \hat{P}$$
(A.3)

$$|-\rangle\langle -| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \equiv \hat{M}$$
(A.4)

The following are all the possible diagonal bases for expressing a bipartite quantum system,

As can be seen from the explicit representation, symmetries are found for the diagonal matrices, which are represented in other bases. Using the symmetries, it

is possible to make a choice of elements, such as

$$\hat{P} \otimes \hat{P} + \hat{M} \otimes \hat{M} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$
(A.9)

If we compare this matrix to (2.43), then it is noticeable that by multiplying by some factor and adding more weighted diagonal terms, it will result in the given matrix in Eq.(2.43). In practice, it is not difficult to show that the matrix can be obtained by adding diagonal terms for the bipartite state in a $\{|0\rangle, |1\rangle\}$ bases as

Furthermore, it is more or less true that this method can be used to find more patterns of separable density matrices.

Appendix B

Banach spaces

 \mathcal{H} denotes a complex separable Hilbert space which has a well-defined scalar product $\langle \phi | \psi \rangle$ and a norm $||\psi|| = \sqrt{\langle \psi | \psi \rangle}$ for $|\phi \rangle, |\psi \rangle \in \mathcal{H}$. A linear operator \hat{A} acting on \mathcal{H} is *bounded* if $\sup_{||\psi|| \leq 1} ||\hat{A}|\psi\rangle|| < \infty$. The set of all bounded operators equipped with a norm $||\hat{A}||_{\infty} = \sup_{||\psi|| \leq 1} ||\hat{A}|\psi\rangle||$ is a Banach space $\mathcal{B}(\mathcal{H})$. $\mathcal{B}(\mathcal{H})$ is an algebra with respect to the composition of operators and with an involution \dagger (adjoint operation) satisfying

$$\langle \psi | \hat{A} | \varphi \rangle = (\hat{A}^{\dagger} | \psi \rangle)^{\dagger} | \varphi \rangle \tag{B.1}$$

where $(\hat{A}^{\dagger})^{\dagger} = \hat{A}$, $(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$, $(\alpha\hat{A} + \beta\hat{B})^{\dagger} = \alpha^{*}\hat{A}^{\dagger} + \beta^{*}\hat{B}^{\dagger}$ and also satisfying

$$||\hat{A}^{\dagger}\hat{A}||_{\infty} = ||\hat{A}||_{\infty}^{2} = ||\hat{A}^{\dagger}||_{\infty}^{2}.$$
 (B.2)

An operator $\hat{A} \in \mathcal{B}(\mathcal{H})$ is self-adjoint if $\hat{A}^{\dagger} = \hat{A}$ and positive $(\hat{A} \ge 0)$ if $\langle \psi | \hat{A} | \psi \rangle \ge 0$ for all $|\psi\rangle \in \mathcal{H}$. For any $\hat{B} \ge 0$, there exists a square root operator $\hat{B}^{\frac{1}{2}} \ge 0$ such that $\hat{B}^{\frac{1}{2}}\hat{B}^{\frac{1}{2}} = \hat{B}$ and if $\hat{B}\hat{A} = \hat{A}\hat{B}$ then $\hat{B}^{\frac{1}{2}}\hat{A} = \hat{A}\hat{B}^{\frac{1}{2}}$.

Let $\hat{A} \in \mathcal{B}(\mathcal{H})$. We define a trace of \hat{A} as a number (if it exists)

$$\mathrm{Tr}\hat{A} = \sum_{n=1}^{\infty} \langle \varphi_n | \hat{A} | \varphi_n \rangle, \tag{B.3}$$

where $\{\varphi_n\}$ is an orthogonal basis in \mathcal{H} . Tr \hat{A} is independent of a choice of $\{\varphi_n\}$.

An operator $\hat{\rho} \in \mathcal{B}(\mathcal{H})$ is called a *trace class* if $\operatorname{Tr}(\hat{\rho}^{\dagger}\hat{\rho})^{1/2}$ exists. The set of all trace class operators $\mathcal{T}(\mathcal{H})$ is a Banach space with a trace norm $||\hat{\rho}||_1 = \operatorname{Tr}(\hat{\rho}^{\dagger}\hat{\rho})^{1/2}$. If $\hat{\rho} = \hat{\rho}^{\dagger} \in \mathcal{T}(\mathcal{H})$, then there exists a spectral representation $\hat{\rho} = \sum_{n=1}^{\infty} \lambda_n |\varphi_n\rangle \langle \varphi_n|$ where $\langle \varphi_n | \varphi_m \rangle = \delta_{nm}$ and $\operatorname{Tr}\hat{\rho} = \sum_{n=1}^{\infty} \lambda_n, ||\hat{\rho}||_1 = \sum_{n=1}^{\infty} |\lambda_n|$. If $\hat{\rho} \in \mathcal{T}(\mathcal{H})$ and $\hat{A} \in \mathcal{B}(\mathcal{H})$, then $\hat{\rho}\hat{A}, \hat{A}\hat{\rho} \in \mathcal{T}(\mathcal{H})$ and $|\operatorname{Tr}(\hat{\rho}\hat{A})| \leq ||\hat{\rho}||_1 ||\hat{A}||_{\infty}$.

For a fixed $A \in \mathcal{B}(\mathcal{H})$, we define a linear and bounded function f_A on $\mathcal{T}(\mathcal{H})$ such that

$$f_A(\hat{\rho}) = \operatorname{Tr}(\hat{\rho}\hat{A}). \tag{B.4}$$

All linear and bounded functionals on $\mathcal{T}(\mathcal{H})$ form a Banach space $\mathcal{T}(\mathcal{H})^*$, dual space, with a norm $||f|| = \sup_{||\hat{\rho}||_1 \leq 1} |f(\hat{\rho})|$. Any functional $f \in \mathcal{T}(\mathcal{H})^*$ is equal to a certain f_A and $||f|| = ||\hat{A}||_{\infty}$. Hence, the two Banach spaces $\mathcal{B}(\mathcal{H})$ and $\mathcal{T}(\mathcal{H})^*$ is isomorphic and isometric. It follows that for any linear and bounded map Λ on $\mathcal{T}(\mathcal{H})$, there exists a dual map Λ^* on $\mathcal{B}(\mathcal{H})$ such that

$$\operatorname{Tr}[(\Lambda \hat{\rho})\hat{A}] = \operatorname{Tr}(\hat{\rho}\Lambda^*\hat{A}) \tag{B.5}$$

for all $\hat{\rho} \in \mathfrak{T}(\mathcal{H})$ and $\hat{A} \in \mathfrak{B}(\mathcal{H})$.

Appendix C

NPT as a measure of entanglement

We will prove that NPT satisfies the three conditions necessary for a measure of entanglement. The proof was first produced by J. Lee [71]. For a 2×2 system, the condition (C.1) is satisfied from the proof of Peres and the Horodecki family. The second condition (C.2), which is invariance of the negative eigenvalues for any local unitary transformation, can be shown by considering the observation of eigenvalues for the partial transposition with arbitrary local unitary operation as

$$\hat{\rho}_{AB}' = \left(\hat{U}_A \otimes \hat{U}_B\right) \hat{\rho}_{AB} \left(\hat{U}_A \otimes \hat{U}_B\right)^{\dagger} \tag{C.1}$$

$$\longrightarrow \left(\hat{\rho}_{AB}^{\prime}\right)^{T_{A}} = \left(\hat{U}_{A}^{*}\otimes\hat{U}_{B}\right)\hat{\rho}_{AB}^{T_{A}}\left(\hat{U}_{A}^{*}\otimes\hat{U}_{B}\right)^{\dagger}.$$
 (C.2)

Note that \hat{U}^* itself is a unitary operator. From now on, we omit the subscript AB by assuming that the density matrices are $\hat{\rho} \in \mathcal{B}(\mathcal{H}_{A\mathcal{B}})$. The eigenvalues for the $(\hat{\rho}')^{T_A}$ are the same as those for $\hat{\rho}^{T_A}$, since the eigenvalues of the Hermitian operator are independent of the unitary transformation. Thus, (C.2) is also true for negative eigenvalues. The proof of the third condition is a little more tricky. First of all, any local operation on a state, including any local generalised measurement, classical communications and post selections can be represented as

$$\hat{\rho}' = \sum_{i} \left(\hat{A}_i \otimes \hat{B}_i \right) \hat{\rho} \left(\hat{A}_i \otimes \hat{B}_i \right)^{\dagger}$$
(C.3)

where \hat{A}_i and \hat{B}_i corresponds to the Krauss operators for the systems A and B respectively, with $\sum_i \left(\hat{A}_i \otimes \hat{B}_i\right) \left(\hat{A}_i \otimes \hat{B}_i\right)^{\dagger} = \mathbb{1}$. The partial transposition for the state transforms the state as

$$(\hat{\rho}')^{T_A} = \sum_i \left(\hat{A}_i^* \otimes \hat{B}_i\right) \hat{\rho}^{T_A} \left(\hat{A}_i^* \otimes \hat{B}_i\right)^{\dagger}$$
(C.4)

$$= \sum_{i} \hat{V}_{i} \hat{\sigma} \ \hat{V}_{i}^{\dagger} = \sum_{i} p_{i} \hat{\sigma}_{i}$$
(C.5)

by setting $\hat{V}_i \equiv \hat{A}_i^* \otimes \hat{B}_i$, $\hat{\rho}^{T_A} \equiv \hat{\sigma}$ and $p_i \hat{\sigma}_i \equiv \hat{V}_i \hat{\sigma} \hat{V}_i^{\dagger}$ with $p_i = \text{Tr}(\hat{V}_i \hat{\sigma} \hat{V}_i^{\dagger})$. From its definition, the operators $\hat{\sigma}$ and $\hat{\sigma}_i$ are Hermitian operators with unit trace, while they can have negative eigenvalues. Thus, one can diagonalises the matrices,

$$\hat{D}_i \equiv \hat{U}_i \hat{\sigma}_i \hat{U}_i = \frac{1}{p_i} \hat{U}_i \hat{V}_i \hat{\sigma} \hat{V}_i^{\dagger} \hat{U}_i^{\dagger}$$
(C.6)

$$= \frac{1}{p_i} \left(\hat{U}_i \hat{V}_i \hat{U}^{\dagger} \right) \left(\hat{U} \hat{D} \hat{U}^{\dagger} \right) \left(\hat{U} \hat{V}_i^{\dagger} \hat{U}_i^{\dagger} \right)$$
(C.7)

$$\equiv \frac{1}{p_i} \hat{W}_i \hat{D} \hat{W}_i^{\dagger} \tag{C.8}$$

where \hat{D}_i and \hat{D} are diagonal matrices of σ_i and σ and $\hat{W}_i \equiv \hat{U}_i \hat{V}_i \hat{U}^{\dagger}$. Since the NPT is defined in terms of negative eigenvalues, the subspace of the negative eigenvalues of the diagonal matrix can be obtained by projection with the help of a projector \hat{P}_- , which satisfies $\hat{P}_+ + \hat{P}_- = \hat{\mathbb{1}}$. Using the fact that the diagonal matrix can be expanded in a diagonal basis as $\hat{D} = \sum_j \lambda_j |\psi_j\rangle \langle \psi_j| = \sum_j \lambda_j^+ |\psi_j^+\rangle \langle \psi_j^+| + \sum_j \lambda_j^- |\psi_j^-\rangle \langle \psi_j^-|$ where λ^+ and λ^- are positive and negative eigenvalues, one finds

$$\begin{split} \sum_{i} p_{i} \varepsilon(\hat{\rho}_{i}) &= -2 \sum_{i} p_{i} \operatorname{Tr}\left(\hat{P}_{-} \hat{D}_{i} \hat{P}_{-}\right) \\ &= -2 \sum_{i} \operatorname{Tr}\left(\hat{P}_{-} \hat{W}_{i} \hat{D} \hat{W}_{i}^{\dagger} \hat{P}_{-}\right) = -2 \sum_{ij} \lambda_{j} \langle \psi_{j} | \hat{W}_{i}^{\dagger} \hat{P}_{-} \hat{P}_{-} \hat{W}_{i} | \psi_{j} \rangle \\ &= -2 \left\{ \sum_{ij} \lambda_{j}^{+} \langle \psi_{j}^{+} | \hat{W}_{i}^{\dagger} \hat{P}_{-} \hat{P}_{-} \hat{W}_{i} | \psi_{j}^{+} \rangle + \sum_{ij} \lambda_{j}^{-} \langle \psi_{j}^{-} | \hat{W}_{i}^{\dagger} \hat{P}_{-} \hat{P}_{-} \hat{W}_{i} | \psi_{j}^{-} \rangle \right\} \\ &\leq -2 \sum_{ij} \lambda_{j}^{-} \langle \psi_{j}^{-} | \hat{W}_{i}^{\dagger} \hat{P}_{-} \hat{P}_{-} \hat{W}_{i} | \psi_{j}^{-} \rangle \end{split}$$

where we use the inequality $\langle \psi_j^+ | \hat{W}_i^\dagger \hat{P}_- \hat{P}_- \hat{W}_i | \psi_j^+ \rangle = |\hat{P}_- \hat{W}_i | \psi_j^+ \rangle|^2 \ge 0$ to obtain the last line. If one considers the fact that $0 \le \sum_i \langle \psi_j^- | \hat{W}_i^\dagger \hat{P}_- \hat{P}_- \hat{W}_i | \psi_j^- \rangle \le 1$, it is possible to show that

$$\sum_{i} p_i \varepsilon(\hat{\rho}_i) \leq -2 \sum_{ij} \lambda_j^- \langle \psi_j^- | \hat{W}_i^\dagger \hat{P}_- \hat{P}_- \hat{W}_i | \psi_j^- \rangle$$
(C.9)

$$\leq -2\sum_{j}\lambda_{j}^{-} = \varepsilon(\hat{\rho}) \tag{C.10}$$

which is the monotonicity for a measure of entanglement demanded by condition 3.

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