PAPER

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Optimal strategies to infer the width of an infinite square well by performing measurements on the particle(s) contained in the well

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Abstract

We seek the optimal strategy to infer the width a of an infinite potential well by performing measurements on the particle(s) contained in the well. In particular, we address quantum estimation theory as the proper framework to formulate the problem and to determine the optimal quantum measurement, as well as to evaluate the ultimate bounds to precision. Our results show that in a static framework the best strategy is to measure position on a delocalized particle, corresponding to a width-independent quantum signal-to-noise ratio (QSNR), which increases with delocalisation. Upon considering time-evolution inside the well, we find that QSNR increases with time as t^2 (at least for small t). On the other hand, it decreases with a and thus time-evolution is a metrological resource only when the width is not too large compared to the available time evolution. Finally, we consider entangled particles in the well and observe super-additivity of the QSNR: it is the sum of the single-particle QSNRs, plus a positive definite term, which depends on their preparation and may increase with the number of entangled particles. Overall, entanglement represents a resource for the precise characterization of potential wells.

Keywords: quantum estimation, quantum wells, quantum metrology

(Some figures may appear in colour only in the online journal)

1. Introduction

In undergraduate quantum mechanics courses, the potential wells are usually the first examples used to theoretically illustrate quantum effects due to confinement and interference [1–8]. The *particle in a box* is also the subject of basic experiments in the undergraduate physical chemistry laboratory [9–11]. On the other hand, quantum well (QW) potentials are not just an academic exercise. Rather, QWs provide relevant approximate models used in several branches of physics, optoelectronics and chemistry, since they often provide a surprisingly accurate description of different physical systems. At the same time, QWs may be used to illustrate potential drawbacks in canonical standard quantization [12–14].

In physical systems where short range forces are dominant, e.g. nuclei, QW potentials help to illustrate several phenomena at low energy [15]. QWs are also employed to describe the confinement of electrons inside crystals [16], e.g. quantum wells, wires and dots corresponding to confinement in one, two or three dimensions, respectively [17–19]. Those structures may be created by inserting in a given semiconductor a nano sized impurity made of a different one. Quantum dots, in particular, received much attention, because of their applications in nanoelectronics. The size of the quantum dot is a crucial parameter, since it determines the optical properties of the crystal; the smaller the dots, the larger is the intensity of the emitted light. As a consequence, the precise knowledge of the dimensions of the potential well, in particular of its width, is a crucial information for the development of effective light sources.

In this paper, we consider a toy problem with potential applications in the fields mentioned above. We consider an infinite QW in one dimension and seek for the optimal strategy to infer its width, denoted by a, by using *quantum probes* [20–30], i.e performing measurement on the particles subjected to the QW potential. The analogue problem in N dimensions may be then reduced to N problems in one dimension. In particular, we address quantum estimation theory as the proper framework where to formulate the problem, to look for the most suitable quantum measurement, and to evaluate the ultimate quantum bounds to precision. We will consider one or more particles in a QW, and will look for the optimal strategy to infer its width. In other words, we are looking for the best initial preparation, the optimal interaction time, and the more informative measurement, overall providing the highest precision in the determination of the width of the QW. In this optimization procedure, the figures of merit is the so-called quantum Fisher information, which provides a quantitative measure of the information about a parameter, which may be extracted by measurements performed on a family of quantum states.

Our results show that in a static framework, position measurement is the optimal one for any initial state, i.e. its Fisher information is equal to the quantum Fisher information. In other words, position data provides us with all the available information about the width of well. Moreover, we found that before making a measurement it may be convenient to wait for a certain amount of time, because the quantum Fisher information increase with the time evolution as t^2, at least for small t. Finally, we found that entanglement represents a resource, i.e. precision may be enhanced using multi-particle entangled states in the well.

The paper is structured as follows. In section 2, we briefly review the infinite square well quantum problem in one dimension and provide an introduction to the ideas and the methods of quantum estimation theory, also evaluating the Fisher information for two relevant observables: position and energy. In section 3, we focus to static situations and evaluate the quantum Fisher information for different families of states, showing that delocalisation is the key feature to gain information about the width of the well. In section 4, we take into account time evolution and evaluate the quantum Fisher information for some class of states. In section 5, we address the use of N-particle probe to infer the width of the QW and describes how

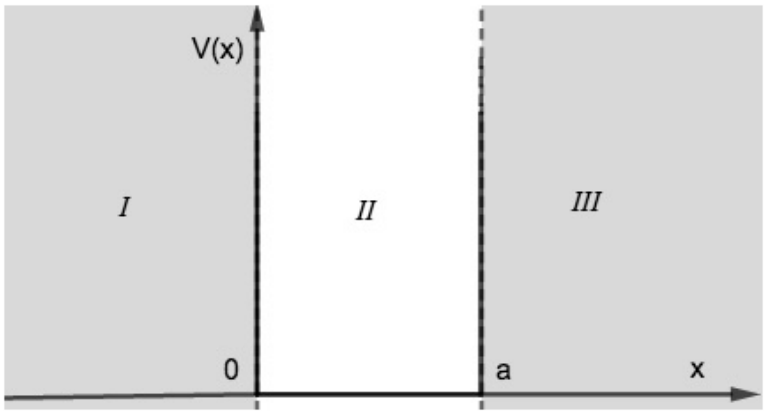

Figure 1. The infinite square well potential, i.e. the model of a particle confined in the region between $x = 0$ and $x = a$. Regions I and III are indeed forbidden because the potential is there infinite. The spectrum is discrete and non-degenerate.

entangled probes may be used to improve precision at fixed number of particles. Section 6 closes the paper by some concluding remarks.

2. Preliminary concepts

In order to introduce the problem and establish notation, let us first review the infinite square well potential problem in non-relativistic quantum mechanics (for the relativistic case, see e.g. [31]), i.e. let us find the eigenvalues and the eigenfunctions of the one-dimensional Hamiltonian $H = \frac{p^2}{2m} + V(x)$, where the potential, of width a, is shown in figure 1, i.e.

$$V(x) = \begin{cases} \infty & \text{for } x < 0 \text{ and } x > a \\ 0 & \text{for } 0 \leqslant x \leqslant a. \end{cases} \tag{1}$$

We look for the eigenvalues and the eigenfunctions of the Hamiltonian H by solving the correspondent eigenvalue equation in the position basis, i.e. solving the Schrodinger equation $-\frac{1}{2}\partial_x^2\psi(x) = [E - V(x)]\psi(x)$ for the wave-function $\psi(x)$, where we use natural unit $\hbar = 1$, and assume unit mass $m = 1$ for the particle. The solution is straightforward upon dividing the space into three regions (see figure 1) to see that regions I and III are forbidden because the potential there is infinite. The eigenfunctions $|\psi_n\rangle$ form a discrete and non-degenerate spectrum of bound states which may be written as [32, 33]

$$|\psi_n\rangle = \int_0^a \mathrm{d}x\, \psi_n(x)\, |x\rangle, \quad \int_0^a \mathrm{d}x\, |\psi_n(x)|^2 = 1,$$

where $n \in \mathbb{N}^+$ and

$$\psi_n(x) = \sqrt{\frac{2}{a}}\, \sin\left(\frac{n\pi}{a}x\right), \tag{2}$$

$$E_n = \frac{n^2\pi^2}{2a^2}. \tag{3}$$

The eigenfunctions exist only in the region II, i.e. all the integrals must be done between 0 and a, and form a complete orthonormal set. We remind that $n \in \mathbb{N}^+$, i.e. it cannot assume the value $n = 0$, because in that case $\psi_0(x) = 0$ and the uncertainty relations would be violated. The ground state has energy $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$.

According to the Stone–Von Neumann theorem [34], the eigenstates of the Hamiltonian and the position eigenstates form two *unitarily inequivalent* basis. We will use both in the following of the paper, and write a generic state $|f\rangle$ as

$$|f\rangle = \int_0^a \mathrm{d}x f(x)|x\rangle, \tag{4}$$

$$= \sum_{n=1}^{\infty} f_n\,|\psi_n\rangle, \tag{5}$$

where $f(x) = \langle x|f\rangle$, $f_n = \langle\psi_n|f\rangle$ and

$$f(x) = \sum_{n=1}^{\infty} c_n\,\psi_n(x) \tag{6}$$

$$c_n = \int_0^a \mathrm{d}x\,\psi_n(x) f(x). \tag{7}$$

Position basis, being independent on the value of the potential width, is suitable for the evaluation of the Fisher information and the signal-to-noise ratio (see the following section), whereas the Hamiltonian basis is of course the privileged one for time evolution. If we prepare a particle in an initial state $|f_0\rangle = \sum_n f_n\,|\psi_n\rangle$, the evolved state at time t is given by

$$\begin{aligned} |f\rangle &= U_t|f_0\rangle \equiv \exp\{-\mathrm{i}Ht\}|f_0\rangle \\ &= \sum_n \mathrm{e}^{-\mathrm{i}E_n t} f_n\,|\psi_n\rangle. \end{aligned} \tag{8}$$

2.1. Quantum estimation theory

It often happens in science that a quantity of interest is not accessible directly. Perhaps, the most prominent example in physics is that of a field, either gravitational, magnetic, or electric. As a matter of fact, no device is actually measuring, e.g. the magnetic field. Rather, one measures the effect of the field on a moving charge, say measuring its acceleration, deflection or displacement, and then *estimate* the field by suitably processing the data observed for the measured quantity.

The chosen measurement and the data processing are together referred to as the *inference strategy* for the parameter of interest ξ [35–38]. After a certain observable X has been chosen, the available data $\mathbf{x} = (x_1, x_2, ..., x_M)$ is a set of outcomes from M repeated measurements of X, i.e. a sample from the distribution $p(\mathbf{x}|\xi) = \Pi_{k=1}^{M} p(x_k|\xi)$, which itself depends on the parameter that has to be estimated. The estimated value for ξ is the average value of an estimator

$$\bar{\xi} = \int \mathrm{d}\mathbf{x}\,p(\mathbf{x}|\xi)\,\hat{\xi}(\mathbf{x}), \tag{9}$$

i.e. a map $\hat{\xi} \equiv \hat{\xi}(\mathbf{x})$ from the space of observations to the space of the parameters. The overall precision of the estimation procedure is quantified by the variance of $\hat{\xi}$, i.e.

$$\mathrm{Var}\,\hat{\xi} = \int \mathrm{d}\mathbf{x}\, p(\mathbf{x}|\xi)\,[\xi(\mathbf{x}) - \bar{\xi}]^2. \tag{10}$$

The variance of any unbiased estimator (i.e. an estimator for which $\bar{\xi} \to T$ in the asymptotic limit $M \gg 1$) for the parameter T is bounded by Cramer–Rao theorem [39–41], stating that

$$\mathrm{Var}\,\hat{\xi} \geqslant \frac{1}{MF(\xi)} \tag{11}$$

where $F(\xi)$ is the Fisher information (FI)

$$F(\xi) = \int \mathrm{d}x\, p(x|\xi) \left[\frac{\partial \log p(x|\xi)}{\partial \xi}\right]^2, \tag{12}$$

$p(x|\xi)$ being the single outcome probability, i.e. the probability of measuring x when the true value of the parameter is ξ. The FI quantifies the amount of information about the parameter ξ that we may extract from the measurement of X.

In a quantum mechanical setting, the conditional probability $p(x|\xi)$ is given by the Born rule $p(x|\xi) = \mathrm{Tr}[P_x \rho_\xi]$, where ρ_ξ is the density operator describing the (parameter-dependent) state of the system and P_x is the projector over the eigenstate of a selfadjoint operator X corresponding to the eigenvalue x.

In order to write the Fisher information in a convenient form, and to maximise its value over the possible observables, we introduce the symmetric logarithmic derivative (SLD) L_ξ, i.e. a selfadjoint operator satisfying the equation

$$\frac{L_\xi \rho_\xi + \rho_\xi L_\xi}{2} = \frac{\partial \rho_\xi}{\partial \xi}. \tag{13}$$

Upon inserting equations (13) in (12) we may find an upper bound for the FI of any quantum measurement

$$F(\xi) \leqslant \mathrm{Tr}[\rho_\xi L_\xi^2] = H(\xi), \tag{14}$$

which is usually referred to as the quantum Fisher information (QFI) [42–44], and coincides with the least monotone quantum Riemannian metric [45]. An optimal estimation strategy should employs measurement with $F(\xi) = H(\xi)$ and then use an optimal estimator which saturates the quantum Cramer–Rao bound $\mathrm{Var}\,\hat{\xi} \geqslant 1/MH(\xi)$. An optimal measurement with $F(\xi) = H(\xi)$ is provided by SLD itself [46], though other problem-specific measurements may achieve similar precision.

The overall precision of a parameter estimation strategy is determined on the variance of the estimator. In order to compare different strategies, we should assess the variance in terms of the mean value, e.g. by means of the signal-to-noise ratio (SNR)

$$R_\xi = \frac{\xi^2}{\mathrm{Var}(\xi)} \tag{15}$$

that is larger for good strategies. The Cramer–Rao inequality bounds this quantity with the quantum signal-to-noise ratio (QSNR), defined as follows

$$R_\xi \leqslant Q(\xi) = \xi^2 H(\xi). \tag{16}$$

The larger is $Q(\xi)$ the more *estimable* is in principle the parameter. Overall, quantum estimation theory says that in order to optimally estimate a parameter, we should find a state preparation with the largest QSNR and then measure the SLD, or any other observable with a FI as close as possible to the QFI. When the information about the parameter is encoded onto pure states $\rho_\xi = |\psi_\xi\rangle\langle\psi_\xi|$, one has $\rho_\xi^2 = \rho_\xi$, and the SLD may be easily found as

$$L_\xi = 2\,\partial_\xi \rho_\xi = 2\left[|\psi_\xi\rangle\langle\partial_\xi\psi_\xi| + |\partial_\xi\psi_\xi\rangle\langle\psi_\xi|\right]. \tag{17}$$

The corresponding QFI is given by $H(\xi) = \langle\psi_\xi|L_\xi^2|\psi_\xi\rangle$, i.e. [47]

$$H(\xi) = 4\Big[\langle\partial_\xi\psi_\xi||\partial_\xi\psi_\xi\rangle + |\langle\partial_\xi\psi_\xi||\psi_\xi\rangle|^2 + \langle\partial_\xi\psi_\xi||\psi_\xi\rangle^2 + \langle\psi_\xi||\partial_\xi\psi_\xi\rangle^2\Big] \tag{18}$$

$$= 4\Big[\langle\partial_\xi\psi_\xi||\partial_\xi\psi_\xi\rangle - |\langle\partial_\xi\psi_\xi||\psi_\xi\rangle|^2\Big], \tag{19}$$

where the last equality follows from the fact $\langle\psi_\xi||\psi_\xi\rangle = 1,\ \forall\xi$ and thus $\partial_\xi\langle\psi_\xi||\psi_\xi\rangle = \langle\partial_\xi\psi_\xi||\psi_\xi\rangle + \langle\psi_\xi||\partial_\xi\psi_\xi\rangle = 0$, i.e. $\langle\psi_\xi||\partial_\xi\psi_\xi\rangle$ is a purely imaginary quantity.

2.2. Single-particle quantum probes

Using results from the previous section, we now evaluate the information about a contained in the state of a particle in the well, prepared in a given quantum state. In other words, we evaluate the QFI of equation (19) for a generic pure state at time t, as in equation (8). In order to simplify notation, we will use the following shorthands

$$\frac{\partial}{\partial a} \to \partial, \quad \int_0^a \mathrm{d}x \to \int \mathrm{d}x, \quad \sum_{n=1}^{\infty} \to \sum_n. \tag{20}$$

At first, we need the derivative of the state with respect to the parameter a, i.e.

$$|\partial f\rangle = \int \mathrm{d}x \sum_n \partial\left[f_n(x)\mathrm{e}^{-\mathrm{i}E_n t}\psi_n(x)\right]|x\rangle \tag{21}$$

where $g(x,a,t) \equiv \partial\left[f_n\,\mathrm{e}^{-\mathrm{i}E_n t}\psi_n(x)\right]$ is given by

$$g(x,a,t) = \psi_n\partial f_n + f_n\partial\psi_n - \mathrm{i}t f_n\psi_n\partial E_n. \tag{22}$$

In equation (22) we have removed the explicit dependence on a, x and t. The derivatives of the eigenvalues and eigenfunctions in (22) are given by

$$\partial E_n = -\frac{n^2\pi^2}{a^3} \tag{23}$$

$$\partial\psi_n = -\frac{1}{2}\sqrt{\frac{2}{a^3}}\left[\sin\frac{n\pi x}{a} + \frac{2n\pi x}{a}\cos\frac{n\pi x}{a}\right]. \tag{24}$$

In order to proceed we need few scalar products. The first is just the orthonormality of the Hamiltonian basis $\langle\psi_m||\psi_n\rangle = \int \mathrm{d}x\,\psi_n(x)\,\psi_m^*(x) = \delta_{mn}$ and the others are

$$\langle\psi_m||\partial\psi_n\rangle = \frac{2}{a}\,(1-\delta_{mn})\,(-1)^{m+n}\frac{mn}{n^2-m^2} \tag{25}$$

$$\langle \partial\psi_m || \partial\psi_n \rangle = (1-\delta_{mn}) \frac{(-1)^{m+n}}{a^2} \frac{4\,n\,m\,(m^2+n^2)}{(m^2-n^2)^2} + \delta_{mn} \frac{1}{a^2} \left(\frac{n^2\pi^2}{3} + \frac{1}{4} \right). \tag{26}$$

We also notice that $\langle \psi_m || \partial\psi_n \rangle$ is anti-symmetric for the exchange of n and m whereas $\langle \partial\psi_m || \partial\psi_n \rangle$ is symmetric. Using this symmetry it is easy to prove that $\langle f || \partial f \rangle$ is a purely imaginary quantity at any time, and for any choice of the initial state, whereas $\langle \partial f || \partial f \rangle$ is a real quantity. Overall, we have that the QFI in equation (19) may be rewritten as

$$H(a) = 4\Big[\langle \partial f || \partial f \rangle + \langle f || \partial f \rangle^2 \Big], \tag{27}$$

$$= 4\Big[\langle \partial f || \partial f \rangle - |\langle f || \partial f \rangle|^2 \Big]. \tag{28}$$

2.3. FI for some relevant measures

Let us focus on the static case, i.e. we assume that a particle in the well is prepared in a given quantum state $|f\rangle$, e.g. by a suitable interaction with an external field, possibly assisted by quantum control [48–50]. After state preparation, an observable is measured, without leaving the particle *time to move* within the well, i.e. its quantum state to evolve. We also assume without loss of generality (see below) that the wave function $f(x) = \langle x|f\rangle$ is real. In this conditions $\langle \partial f || f \rangle = 0$ and $H(a) = 4 \int \mathrm{d}x\, (\partial f)^2$. On the other hand, the probability distribution in a position measurement is given by $p(x|a) = |f(x)|^2$ and thus its Fisher information is

$$F(a) = \int \mathrm{d}x\, \frac{1}{|f(x)|^2} \left[\partial |f(x)|^2 \right]^2 \tag{29}$$

$$= 4 \int \mathrm{d}x\, \left[\partial f(x) \right]^2, \tag{30}$$

which is equal to the QFI for any choice of (real) $f(x)$. If $f(x)$ is complex the line of reasoning is the same, though a rotation should be made to the state before measuring position.

Another relevant measurement is that of energy. The possible outcome are the eigenvalues of the Hamiltonian, and the probability distribution is given by

$$p(E_n|a) = |\langle \psi_n || f \rangle|^2 = |f_n|^2. \tag{31}$$

The FI for the energy measurement is thus given by

$$F(a) = \sum_n \frac{1}{|\langle \psi_n | f \rangle|^2} \Big[\partial |\langle \psi_n || f \rangle|^2 \Big]^2 = 4 \sum_n \Big[\partial |f_n| \Big]^2. \tag{32}$$

The energy FI is not, in general, equal to the QFI. In particular, it is useless to prepare the particle in an eigenstate of the Hamiltonian, since the only possible result is the correspondent eigenvalue with probability 1 and the measure does not give any information about the parameter a. On a generic state, we gain some information from an energy measurement if the expansion coefficients does depend on the parameter a.

3. Static probes

Let us start our analysis with different possible single-particle preparations and by focussing on the static case, i.e. we assume that a particle in the well is prepared in a given quantum state $|f\rangle$, possibly by the interaction with an externally controlled field (thus making state preparation independent on the width a itself). An observable is measured immediately after the state preparation, without leaving the particle the time to evolve.

We start considering an eigenstate of the Hamiltonian and calculate the QFI and the QSNR. Since the eigenfunctions are reals, $\langle f||\partial_a f\rangle = 0$ and the Q-quantities reads as follows

$$H_n(a) = 4\langle\partial\psi_n||\partial\psi_n\rangle = \frac{3+4n^2\pi^2}{3a^2} \tag{33}$$

$$Q_n = 1 + \frac{4}{3}n^2\pi^2 = 1 + \frac{8}{3}a^2E_n. \tag{34}$$

The QSNR does not depend on a and increases with n, which means that in principle we should prepare the particle in an eigenstate with large n in order to gain information about the parameter a.

We next consider a superposition of two generic eigenstates

$$|f_{nm}\rangle = \cos\alpha|\psi_n\rangle + \sin\alpha|\psi_m\rangle. \tag{35}$$

Upon straightforward calculations we have

$$Q_{nm}(\alpha) = \cos^2\alpha\, Q_n + \sin^2\alpha\, Q_m + a^2\sin 2\alpha\,\langle\partial\psi_n|\partial\psi_m\rangle, \tag{36}$$

where $\langle\partial\psi_n|\partial\psi_m\rangle$ is given in equation (26). Also in this case the QSNR does not depend on a. We also notice that $Q_{nm}(\alpha) = Q_{mn}(\pi/2-\alpha)$ and thus in the following we consider $m = n+d > n$ and $0 \leqslant \alpha \leqslant \pi/4$.

In order to properly assess the effects of superpositions we fix the overall energy of the state and compare the QSNR of $|f_{nm}\rangle$ with $Q_{[[\bar n]]}$, where $E_{\bar n}$ is the mean energy of the superposition state $|f_{nm}\rangle$, i.e. $E_{\bar n} = E_n\cos^2\alpha + E_{n+d}\sin^2\alpha$, and $[[x]]$ denotes the round function, i.e. the closest integer to x. We have $n \leqslant \bar n \leqslant n+d$ where

$$\bar n = \sqrt{n^2\cos^2\alpha + (n+d)^2\sin^2\alpha}. \tag{37}$$

A remarkable result may be obtained by considering unbalanced superposition corresponding to small values of α. In this case, upon defining

$$\gamma_{nd}(\alpha) = \frac{Q_{n,n+d}(\alpha)}{Q_{[[\bar n]]}},$$

we have

$$\bar n \overset{\alpha\ll 1}{\simeq} n + O(\alpha^2) \tag{38}$$

$$\begin{aligned}\gamma_{nd}(\alpha) &\overset{\alpha\ll 1}{\simeq} 1 + (-1)^d\, g_{nd}\,\alpha + O(\alpha^2)\\ g_{nd} &= \frac{24n(n+d)(d^2+2nd+2n^2)}{d^2(d+2n)^2(3+4n^2\pi^2)} > 0.\end{aligned} \tag{39}$$

Equations (38) and (39) say that with a negligible increase of energy, and preparing the particle in a superposition with even d, one may increase the QSNR by a non-negligible amount.

Notice that at fixed n, g_{nd} decreases with d, and thus the most convenient superposition is the state $|f_{n,n+2}\rangle$.

The examples above suggest that the delocalisation of the particle inside the well may play a role in increasing the QSNR. This agrees with intuitive arguments based on the fact that position measurement is optimal, and thus the more delocalised is the particle, the more information may be gained from a position measurement. In order to make this reasoning more quantitative, let us consider the family of states $|f_p\rangle$ where the wave function is given by

$$f_p(x;a) = N[-(2x-a)^{2p} + a^{2p}] \tag{40}$$

where $p \in \mathbb{N}^+$, $p > 1$, and the normalization factor is given by

$$N = \sqrt{\frac{1+6p+8p^2}{8p^2 a^{1+4p}}}. \tag{41}$$

The wavefunction in equation (40) becomes more and more flat for increasing p, approaching a box function for large p. In figure 2, we show the behaviour of $f_p(x;a)$ for different values of p and for $a = 1$. Upon exploiting the scaling $f_p(x;a) = 1/\sqrt{a} f_p(x/a;1)$ the behaviour for a generic value of the width may be recovered. Concerning the QSNR, after straightforward calculations we have

$$Q_p = \frac{(1+4p)(1+8p)}{(4p-1)}, \tag{42}$$

which is independent on a and it is an increasing function of p. We have $Q_1 = 15$ and $Q_p \simeq 8p$ for large p ($p \gtrsim 10$ is already enough).

The average energy E_p of a p-state is given by

$$E_p \equiv \langle f_p|H|f_p\rangle = \frac{1}{a^2}\frac{1+6p+8p^2}{4p-1}, \tag{43}$$

and thus, using equations (43) and (3), we have that $E_p = E_n$, i.e. $|f_p\rangle$ and $|\psi_n\rangle$ have the same energy if

$$\frac{1+6p+8p^2}{4p-1} = \frac{n^2\pi^2}{2}.$$

In turn, this means that at fixed energy, the delocalised states $|f_p\rangle$ provide more information than the Hamiltonian eigenstates. This is illustrated in figure 3, where we show the QSRN as a function of energy (in unit of $1/a^2$) for both families of states. Similar conclusions may be obtained by considering some specific measure of delocalisation, e.g. the differential entropy of the position distribution $p(x) = |f(x)|^2$ for different classes of states.

4. Dynamical probes

In practice, it is not possible to prepare a system and perform a measurement instantaneously. As a consequence, a question arises on how the information about the width of the well changes with time. In this section, we will introduce time evolution and analyze whether this degree of freedom may be exploited to increase the QFI. Intuitively, one may expect evolution to be beneficial, since, roughly speaking, the wavefunction does not have the possibility to get out of the well and thus should interact with the walls of the well many times, accumulating more information about the structure of the potential.

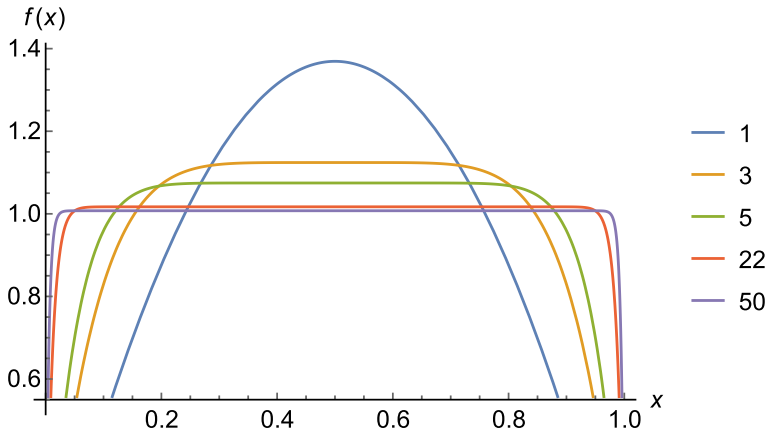

Figure 2. The wave-function in equation (40) for different values of the parameter p. The function becomes more and more flat for increasing p, approaching a box function for large p.

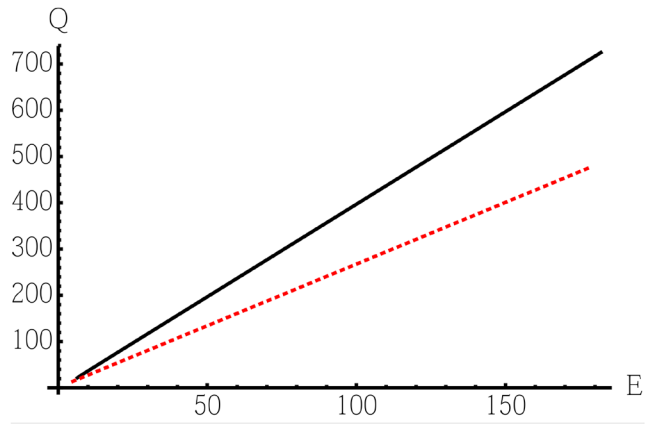

Figure 3. The QSNR as a function of energy (expressed in unit of $1/a^2$) for the Hamiltonian eigenstates (red dotted line) and for the delocalised states $|f_p\rangle$ (black solid line). The plot illustrates that, at any fixed value of the energy, delocalised states provide more information than the Hamiltonian eigenstates.

At first, let us check whether for eigenstate of the Hamiltonian information is left unchanged. If we prepare the particle in an eigenstate $|\psi_n\rangle$ at time t the state of the system is given by

$$\psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\mathrm{e}^{-\mathrm{i}E_n t}, \tag{44}$$

so that

$$|\partial_a\psi_n(t)\rangle = \mathrm{e}^{-\mathrm{i}E_n t}\Big[|\partial_a\psi_n\rangle - \mathrm{i}\,t\,(\partial_a E_n)|\psi_n\rangle\Big], \tag{45}$$

(notice that in this case, the wave function is not real anymore and thus, in general, $\langle\psi||\partial\psi\rangle \neq 0$). The QFI is given

$$H(a) = 4\Big[\langle\partial\psi_n(t)||\partial\psi_n(t)\rangle + \langle\psi_n(t)||\partial\psi_n(t)\rangle^2\Big] \tag{46}$$

$$= \frac{3+4n^2\pi^2}{3a^2}, \tag{47}$$

which is indeed unchanged, compared to the static case.

Let us now consider a generic initial preparation, which evolves as

$$|f(t)\rangle = \sum_n f_n|\psi_n\rangle e^{-iE_nt} \quad f_n = \langle\psi_n||f\rangle \in \mathbb{R}. \tag{48}$$

We do not report the full expression of the QFI and rather assume that the amplitudes f_n do not depends on a, i.e. are determined by external operations. In this case the QFI rewrites as

$$\begin{aligned} H(a,t) =& 4\Bigg\{t^2\sum_n f_n^2\,(\partial E_n)^2 - \left(\sum_n t f_n^2\,\partial_a E_n + \sum_{nm}\sin(\Delta_{nm}t) f_n f_m\langle\psi_m|\partial\psi_n\rangle\right)^2 \\ &+ \sum_{nm}\cos(\Delta_{nm}t) f_n f_m\langle\partial\psi_m|\partial\psi_n\rangle \\ &+ f_n f_m t\sin(\Delta_{nm}t)\,(\partial E_m + \partial E_n)\langle\psi_m|\partial\psi_n\rangle\Bigg\}, \end{aligned} \tag{49}$$

where $\Delta_{nm} = E_n - E_m$. In turn, equation (49) suggests a t^2 dependence of the QFI.

In order to see these feature in a quantitative way, let us consider a simple initial state $|f\rangle$ with wave function of the form $f(x) = \sqrt{30/a^5}x(a-x)$, corresponding to amplitudes $f_n = 0$ when n is even and $f_n = 8\sqrt{15}/n^3\pi^3$ if n is odd. Inserting this expression in the QFI of equation (49) we have

$$\begin{aligned} H(a,t) =& 4\Bigg\{120\,\frac{t^2}{a^6} \\ &+ 1920\sum_{nm}(-1)^{m+n}\frac{(m^2+n^2)}{a^2\pi^4\,n^2\,m^2}\left[\frac{2\,\cos(\Delta_{nm}t)}{\pi^2\,(m^2-n^2)^2} - \frac{t\,\sin(\Delta_{nm}t)}{a^2(m^2-n^2)}\right] \\ &- \left(1920\sum_{nm}(-1)^{n+m}\frac{\sin(\Delta_{nm}t)}{a\,n^2\,m^2\,\pi^6(m^2-n^2)} - 10\,\frac{t}{a^3}\right)^2\Bigg\} \end{aligned} \tag{50}$$

where all the sums include odd values only. Upon expanding the QSNR $Q(a,t) = a^2H(a,t)$ for short times, one obtains the leading term $Q(a,t) \sim t^2/a^4$, showing that when the state particle evolves within the well the QSNR increases as t^2. On the other hand, a dependence on the width itself appears, making dynamical probes convenient if the well is not too large, compared to the available interaction time. In figure 4 we show the QSNR $Q(a,t)$ as a function of time for different values of the width a. Results are obtained by numerically performing the sums of equation (50) up to $n,m = 50$, corresponding to a residual error $\epsilon \lesssim 10^{-6}$. As it is apparent from the plot, the expansion $Q(a,t) \sim t^2/a^4$ describes rather all the behaviour of $Q(a,t)$ also when the interaction time is not so small. It should be noticed, however, that when the interaction t increases, it becomes more and more difficult to avoid the interaction of the QW with its environment and, in turn, to consider the dynamics purely Hamiltonian. The same behaviour may be observed with different preparation of the particle. Overall, we found that, in general, the amount of information about the parameter a increases quadratically for short

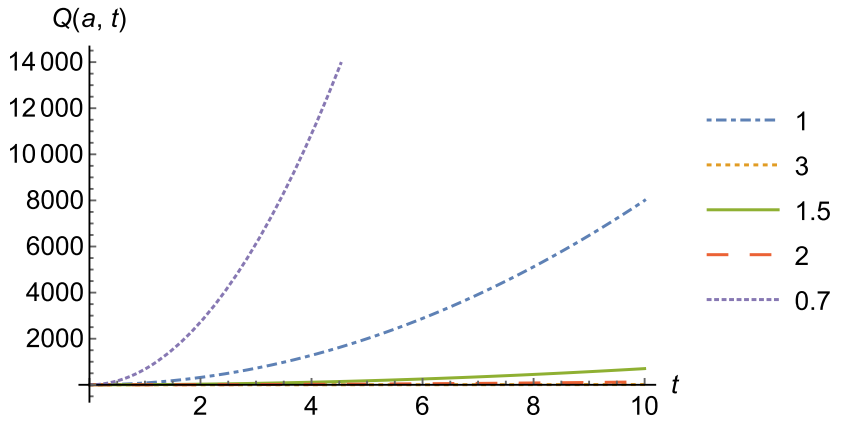

Figure 4. The QSNR $Q(a,t) = a^2 H(a,t)$ see equation (50) as function of time for different values of the parameter a. Numerical results are obtained by truncating the sum in equation (50) at $n, m = 50$, corresponding to a residual error $\epsilon \lesssim 10^{-6}$. The plot shows that the QSNR increases with time an decreases with the width a.

time at any fixed value of a. At the same time, evolution brings a dependence on the width itself, making more and more difficult to estimate its value as it increases.

5. Entangled probes

In the previous sections, we have considered a single particle as in the well as a quantum probe for its width. In this section we address the use of more than one particle, and, in particular, of N particles prepared in an entangled state. For the sake of simplicity, we take the particles identical, but distinguishable, and non interacting. We will start from two-particle probes, and then generalise the analysis to N particles.

5.1. Two-particle entangled probes

In the case of two particles, the total Hamiltonian is given by $H_{tot} = H_1 + H_2 + V$, where H_i the kinetic term $p_i^2/2m_i$ and the potential is that of equation (1). The eigenstates are the tensor products $|\psi_i\rangle \otimes |\psi_j\rangle$ of the single-particle eigenstates of equation (2), and the eigenvalues E_{tot} are the sum $E_i + E_j$ of the eigenvalues in equation (3).

For any two-particle state

$$|f\rangle\rangle = \int\int \mathrm{d}x_1 \mathrm{d}x_2 f(x_1, x_2)\, |x_1\rangle \otimes |x_2\rangle, \tag{51}$$

and assuming a real wave-function $f(x_1, x_2)$ the QFI is given by $H(a) = 4 \iint \mathrm{d}x_1 \mathrm{d}x_2\, [\partial f(x_1, x_2)]^2$, thus confirming that also for two particles the (joint) measurement of position is an optimal measurement. Notice that the measurement of the position of only one of the particles is not optimal.

Let us now consider the two particles prepared in an energy-particle entangled state, i.e. in a superposition state where we do not know which particle is in which (Hamiltonian) eigenstate. The wave-function is given by

$$\Psi(x_1, x_2) = \frac{\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)}{\sqrt{2}}. \tag{52}$$

Following the procedure outlined in the previous sections, we may easily evaluate the QSNR, which may be expressed as

$$\mathcal{Q}^{(2)}_{n_1 n_2} = \mathcal{Q}_{n_1} + \mathcal{Q}_{n_2} + 32\,\frac{n_1^2\, n_2^2}{(n_1^2 - n_2^2)^2}, \tag{53}$$

where $\mathcal{Q}_{n_1}$ and $\mathcal{Q}_{n_2}$ are the single particle QSNRs given in equation (34). Equation (53) contains a remarkable result: the QSNR obtained using two particles in an entangled state is always greater that the QSNR obtained using the two particles in two successive experiments.

Motivated by the results of section 3, let us now consider two-particle probes prepared in an entangled state of two single-particle delocalised states of equation (40) with different indices, i.e.

$$f_{p_1 p_2}(x_1, x_2) = \frac{1}{\sqrt{2}}\Big[f_{p_1}(x_1; a) f_{p_2}(x_2; a) + f_{p_1}(x_2; a) f_{p_2}(x_1; a)\Big]. \tag{54}$$

The corresponding QSNR is given by

$$\mathcal{Q}^{(2)}_{p_1 p_2} = \mathcal{Q}_{p_1} + \mathcal{Q}_{p_2} + \frac{(1+4p_1)(1+4p_2)(1+4p_1+4p_2)}{2(4p_1^2 + 4p_2^2 + 8p_1 p_2 - 1)}, \tag{55}$$

where $\mathcal{Q}_{p_1}$ and $\mathcal{Q}_{p_2}$ are given in equation (42). The additional term is positive definite also in this case, i.e. entanglement leads to superadditivity of the QFI and the QSNR. In order to evaluate quantitatively the improvement, let us introduce the ratio

$$\gamma_{p_1 p_2} = \frac{\mathcal{Q}^{(2)}_{p_1 p_2}}{\mathcal{Q}_{p_1} + \mathcal{Q}_{p_2}} > 1. \tag{56}$$

In figure 5 we show $\gamma_{p_1 p_2}$ as a function of p_1 and p_2 in the range $p = 2, .., 15$ (γ_{pp} is undefined). Larger values of $\gamma_{p_1 p_2}$ corresponds to light blue regions (smaller values to red regions). The ratio $\gamma_{p_1 p_2}$ achieves its maximum value $\gamma \simeq 5/4$ for $p_2 = p_1 \pm 1$. For increasing values of both the indices, the region in which γ is close to its maximum becomes larger and larger.

5.2. N-particle entangled probes

Given the results of the previous section, a question arises on whether using more particles one may achieve a better precision. The answer is positive, as it may easily be shown upon considering the following three-particle entangled probe, prepared in a *W*-like state with a wave-function of the form

$$\begin{aligned}\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}\Big[&\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) \\ &+ \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3) \\ &+ \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)\Big].\end{aligned} \tag{57}$$

Upon exploiting equation (25) one arrives at

$$H^{(3)}_{n_1 n_2} = \frac{1}{3}\Big[\,6H_{n_1}(a) + \,3H_{n_2}(a) + 48\,\big|\langle\partial\psi_{n_1}|\psi_{n_2}\rangle\big|^2\Big],$$

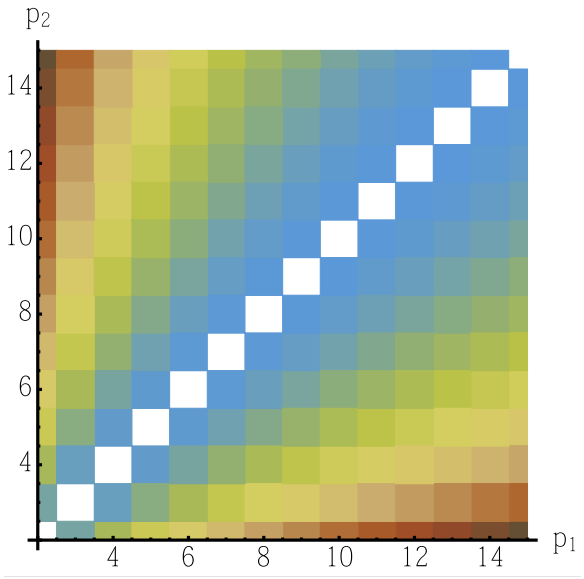

Figure 5. The ratio $\gamma_{p_1p_2}$ as a function of p_1 and p_2 in the range $p = 2, .., 15$ (γ_{pp} is undefined). The plot tells us that the entanglement makes the QSNR super-additive and that the QSNR of a two-particle entangled states is always larger than the sum of the two single-particle QSNRs. Light blue regions correspond to larger values of $\gamma_{p_1p_2}$, which achieves its maximum value $\gamma \simeq 5/4$ for $p_2 = p_1 \pm 1$.

where $H_n(a)$ is given in equation (33). The QSNR is thus given by

$$Q^{(3)}_{n_1n_2} = 2Q_{n_1} + Q_{n_2} + 64\,\frac{n_1^2\,n_2^2}{(n_1^2 - n_2^2)^2}, \tag{58}$$

where we have the sum of the single-particle QSNRs and an additional positive definite term, which is twice the one obtained with two particles, see equation (53). In order to compare the two results in the high-energy regime $n_1, n_2 \gg 1$, let us consider the most convenient choice for both, i.e. $n_1 \to n$, $n_2 \to 1 + n$. In this case, we have

$$\frac{Q^{(3)}_{n,1+n}}{2Q_n + Q_{1+n}} \overset{n\gg 1}{=} 1 + \frac{4}{\pi^2} + O(\frac{1}{E_n}) \tag{59}$$

$$\frac{Q^{(2)}_{n,1+n}}{Q_n + Q_{1+n}} \overset{n\gg 1}{=} 1 + \frac{3}{\pi^2} + O(\frac{1}{E_n}). \tag{60}$$

The argument may be then generalized to more particles, thus confirming that entanglement is a resource in the estimation of the width, and that the enhancement may increase with the number of entangled particles.

Notice, however, that precision strongly depends on the preparation of the probe, and that entanglement alone is not enough to improve precision. In order to show this explicitly, let us consider the case of N distinguishable particles prepared in a GHZ-like state, i.e. with a wave-function given by

$$\Psi(x_1, x_2, ...) = \frac{1}{\sqrt{2}}\Big[\prod_{i=1}^{N}\psi_{n_i}(x_i) + \prod_{j=1}^{N}\psi_{m_j}(x_j)\Big] \tag{61}$$

where state $\mathbf{m} = \{m_1, ...\}$ is a permutation of $\mathbf{n} = \{n_1, ...\}$ and $\psi_k(x)$ is the kth eigenstate of the Hamiltonian. The wave-function is real and so $H(a) = 4\langle\partial_a\Psi||\partial_a\Psi\rangle = 4(I_1 + I_2)/a^2$ where

$$I_1 = a^2\int\prod_{i=1}^{N}\mathrm{d}x_i\left\{\Big[\sum_{j=1}^{N}\partial\psi_{n_j}(x_j)\prod_{l\neq j}\psi_{n_l}(x_l)\Big]\Big[\sum_{k=1}^{N}\partial\psi_{n_k}(x_k)\prod_{h\neq k}\psi_{n_h}(x_h)\Big]\right\}, \tag{62}$$

$$I_2 = a^2\int\prod_{i=1}^{N}\mathrm{d}x_i\left\{\Big[\sum_{j=1}^{N}\partial\psi_{n_j}(x_j)\prod_{l\neq j}\psi_{n_l}(x_l)\Big]\Big[\sum_{k=1}^{N}\partial\psi_{m_k}(x_k)\prod_{h\neq k}\psi_{m_h}(x_h)\Big]\right\}. \tag{63}$$

Using results from previous sections and after calculations, we have

$$I_1 = \sum_{j=1}^{N}\Big(\frac{n_j^2\pi^2}{3} + \frac{1}{4}\Big), \tag{64}$$

$$I_2 = 4\sum_{k,j=1}^{N}\delta_{m_k n_j}\delta_{m_j n_k}\Big(\frac{n_k n_j}{n_k^2 - n_j^2}\Big)^2\prod_{\substack{l\neq k\\ l\neq j}}\delta_{n_l m_l}. \tag{65}$$

The corresponding QSNR is given by

$$Q^{(N)}_{n_1,n_2,...,n_N} = \sum_{j=1}^{N}Q_{n_j} + 16\sum_{k,j=1}^{N}\delta_{m_k n_j}\delta_{m_j n_k}\Big(\frac{n_k n_j}{n_k^2 - n_j^2}\Big)^2\prod_{\substack{l\neq k\\ l\neq j}}\delta_{n_l m_l}.$$

The presence of 'conflicting deltas' in the expression of $Q^{(N)}_{n_1,n_2,...,n_N}$ make it impossible to surpass the two-particle QSNR $Q^{(2)}_{n_1 n_2}$ of equation (53) using N-particle GHZ-like states.

6. Conclusions

In this paper, we have used quantum estimation theory as the proper framework to address the precise characterization of an infinite potential wells, i.e. the estimation of its width. In particular, we have been looking for the optimal measurement to be performed on the particles in the well, and for their best preparation, in order to obtain the ultimate bound to precision, as imposed by quantum mechanics. In doing this we have evaluated the quantum Fisher information of the corresponding quantum statistical models, and the Fisher information for selected kind of measurements. We have also considered different preparations of the system in order to illustrate the different features of the problem. Finally, we have evaluated the quantum signal-to-noise ratio (QSNR) in order to compare the different working regimes.

Our results show that the best measurement we may perform on a static system, is the position measure, because in that case the FI equals the QFI for any state and any value of the width. On the contrary, performing an energy measurement is useless unless one is able to

prepare suitable superpositions with parameter dependent coefficients. In a static setting, the QSNR is independent of the width, and the best way to initialise the system is to prepare it in a delocalized state, which could be an eigenstate of the Hamiltonian with a large eigenvalue, or a wave-function as the polynomial in equation (40). We have then considered time evolution inside the wells and found that the QSNR increases with time as t^2, at least for short evolving time. Letting the system evolve is thus convenient, since the amount of information increases. On the other hand, the QSNR decreases with a itself, and so time evolution is a resource only if the well is large enough compared to the available interaction time.

Finally, we have considered N-particle probes and found that entanglement enhances precision, since the QSNR is the sum of the single-particle QSNRs plus a positive definite term, which depends on state preparation, and may increase with the number of entangled particles.

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