Quantum information entropy for one-dimensional system undergoing quantum phase transition*

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Calculations of the quantum information entropy have been extended to a non-analytically solvable situation. Specifically, we have investigated the information entropy for a one-dimensional system with a schematic "Landau" potential in a numerical way. Particularly, it is found that the phase transitional behavior of the system can be well expressed by the evolution of quantum information entropy. The calculated results also indicate that the position entropy S_x and the momentum entropy S_p at the critical point of phase transition may vary with the mass parameter M but their sum remains as a constant independent of M for a given excited state. In addition, the entropy uncertainty relation is proven to be robust during the whole process of the phase transition.

Keywords: quantum information entropy, quantum phase transition, entropy uncertainty relation

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1. Introduction

Recently, there has been a growing interest in dealing with information theoretical measures for quantum-mechanical systems. As an alternative to the Heisenberg uncertainty relation, entropic uncertainty has been particularly examined.[1–3] Among the measures of information entropy, Shannon entropy[4–6] plays a very important role in the measure of uncertainty, which has been tested for various forms of potentials. The entropic uncertainty relation, which is related to the position and momentum spaces, was given by[7–9]

$$S_x + S_p \geq D(1+\ln\pi), \tag{1}$$

where D represents the spatial dimension. In the one-dimensional system, the position-space (S_x) and momentum-space (S_p) information entropies are defined, respectively, by

$$S_x = -\int_{-\infty}^{\infty} |\psi(x)|^2 \ln|\psi(x)|^2 \mathrm{d}x, \tag{2}$$

$$S_p = -\int_{-\infty}^{\infty} |\phi(p)|^2 \ln|\phi(p)|^2 \mathrm{d}p, \tag{3}$$

where $\psi(x)$ is a normalized eigenfunction in spatial coordinates and $\phi(p)$ is its normalized Fourier transform.

Apart from their intrinsic interest, the entropic uncertainty relations have been used widely in atomic and molecular physics.[10–14] For example, the Shannon information entropies for a few molecular potentials have been analytically obtained, i.e., the harmonic oscillator,[15] the Pöschl–Teller (PT),[16,17] the Morse,[16,18] the Coulomb,[19] the potential isospectral to the PT potential,[20] the classical orthogonal polynomials[21–23] and other studies.[24–26] In addition, investigation of the quantum information entropies was also carried for other analytically solved potentials such as the symmetrically and asymmetrically trigonometric Rosen–Morse,[27,28] the PT-like potential,[29] a squared tangent potential,[30] the position-dependent mass Schröinger equation with the null potential,[31] the hyperbolic potential,[32] the infinite circular well[33] and the Fisher entropy for the position-dependent mass Schrödinger equation,[34,35] due to their applications in physics. Notably, the previous discussions related to shannon entropy were mostly focusing on analytically solvable potentials, but not all the interesting quantum systems have the corresponding analytically solvable modes. Then an efficient numerical method would be particularly important. In this work, we will extend the calculations of shannon entropy to the one-dimensional system with a schematic "Landau" potential,[36,37] which may be formally derived in the mean-field level from the vibron model for molecular structures[38,39] and can be only solved in a numerical way. Particularly, there exists a quantum phase transitional behavior in the system as varying the control parameter in this type of potential.[36,37]

2. Schematic "Landau" potential and its numerical solution

One way of addressing quantum phase transitions[40] is to use the potential energy approach. A schematic "Landau" potential is often considered to indicate quantum phase

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transition,[36,37] which is written as

$$V(x) = \frac{M}{2}[x^2 + \beta(x^4 - 2x^2)], \tag{4}$$

with M being the mass parameter and $\beta \in [0,1]$ being the control parameter. One can prove that the minimum of $V(x)$ with $\beta \leq 0.5$ may locate at $x = 0$, while $V(x)$ with $\beta > 0.5$ may have two degenerated minimums at $x \neq 0$, which indicates that quantum phase transition may occur at the critical point $\beta = 0.5$. More specifically, it can be derived that the minimum of $V(\beta)$, $V_{\min}$, and $\partial V_{\min}/\partial x$ at the critical point $\beta = 0.5$ are continuous, but $\partial^2 V_{\min}/\partial x^2$ is discontinuous, which confirms that there indeed exists a second-order quantum phase transition occurring at the critical point $\beta = 0.5$. As we know, quantum phase transition may be reflected not only by the potential surface evolution of the system but also by the low-lying dynamics properties. It is thus expected that quantum phase transition is also indicated by the information entropies. To calculate the information entropy, one has to solve the eigenfunctions $\psi(x)$ from the differential equation

$$\hat{H}\psi(x) = E\psi(x), \tag{5}$$

where the Hamiltonian is presently written as

$$\hat{H} = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{M}{2}[x^2 + \beta(x^4 - 2x^2)]. \tag{6}$$

It is clear that the differential equation (6) can be analytically solved in the $\beta = 0$ case, in which the potential form regains the harmonic oscillator one. The eigenfunction in the $\beta = 0$ case can be analytically written as

$$W_m(x) = N_m \mathrm{e}^{-\frac{1}{2}a^2x^2}\mathrm{H}_m(ax), \tag{7}$$

where $\mathrm{H}_m(z)$ is the Hermite polynomial and the normalized factor is given as

$$N_m = \left[\frac{a}{\sqrt{\pi}2^m m!}\right]^{1/2}, \quad a = \sqrt{\frac{M}{\hbar}}. \tag{8}$$

The corresponding eigenvalues are given as

$$E_m = \left(m + \frac{1}{2}\right)\hbar. \tag{9}$$

Although the differential Eq. (6) in the $\beta > 0$ cases cannot be analytically solved, the numerical solutions can be achieved in a systematic scheme as shown below. One can formally expand the eigenfunctions of the n-th excited state $\psi_n(x)$ in terms of the eigenfunctions of the harmonic oscillator given in Eq. (7) as

$$\psi_n(x) = \sum_{m=0}^{t} C_m^n W_m(x), \tag{10}$$

where C_m^n are the expansion coefficients. Therefore, one has to get the coefficients C_m^n at first in order to obtain the eigenfunctions $\psi_n(x)$. For $\beta = 0$, the coefficient is just given as $C_m^n = \delta_{nm}$. For $\beta > 0$, one can diagonalize[41] the Hamiltonian (5) under the harmonic oscillator basis to get coefficients C_m^n. The matrix element of the Hamiltonian under the harmonic oscillator basis is defined as

$$\langle i|\hat{H}|j\rangle = \int_{-\infty}^{\infty} W_i(x)\hat{H}W_j(x)\mathrm{d}x, \tag{11}$$

with $i,\ j = 0,\ 1,\ 2, ..., t$. The number t should, in principle, be taken as infinite since the dimension of the Hilbert space for the infinite well $V(x)$ given in Eq. (4) is infinite. However, one can diagonalize the Hamiltonian with $\beta \in (0,1]$ within a finite subspace with sufficient large-t truncation to get the coefficients accurate enough for the low-lying states.[37] Once one obtains the coefficients C_m^n involved in the eigenfunction $\psi_n(x)$, one can further get the following wave functions in momentum space using the Fourier transform

$$\phi_n(p) = \sum_{m=0}^{t} C_m^n F_m(p), \tag{12}$$

where $F_m(p)$ is the Fourier transform of the harmonic oscillator eigenfunction $W_m(x)$. It is given as

$$\begin{aligned} F_m(p) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} W_m(x)\mathrm{e}^{-\mathrm{i}px}\mathrm{d}x \\ &= N'_m \mathrm{i}^m \mathrm{e}^{-\frac{p^2}{2a^2}}\mathrm{H}_m\left(-\frac{p}{a}\right), \end{aligned} \tag{13}$$

where

$$N'_m = \left[\frac{1}{a\sqrt{\pi}2^m m!}\right]^{1/2}. \tag{14}$$

Within the same numerical scheme, one can also calculate all the other quantities in the position or momentum space.

To check the validity of this method, we calculate the probability density distributions of the eigenfunctions in both the position and momentum spaces, which are defined as

$$\rho(x) = |\psi(x)|^2, \quad \rho(p) = |\phi(p)|^2. \tag{15}$$

The calculated results for the ground state corresponding to $n = 0$ are shown in Fig. 1 for three typical β values. In calculations, the mass parameter in the Hamiltonian (5) is set as $M = 50$ since a relatively large M value may make the phase transitional features more evident according to the analysis given in Ref. [37]. It can be found from panel (a) of Fig. 1 that the position probability density functions $\rho(x)$ for three β values mainly distribute within the range of $x \in [-1,1]$. Specifically, $\rho(x)$ in the $\beta = 0$ and $\beta = 0.5$ cases may develop a peak around $x = 0$ except for that the peak for $\beta = 0.5$ is wider but lower than that for $\beta = 0$. In contrast, $\rho(x)$ in the $\beta = 1$ case may develop the double-peaks structure around $x = \pm 0.7$. As further seen from Fig. 1(b), the momentum probability density function $\rho(p)$ may converge within $p \in [-20,20]$. Similar to $\rho(x)$, $\rho(p)$ in $\beta = 0$ and $\beta = 0.5$ cases also develop a single-peak but around $p = 0$, while $\rho(p)$ in $\beta = 1$ case presents an evidently fluctuating behavior. In short, the different potential structure may lead to the different probability density distribution in both position and momentum spaces.

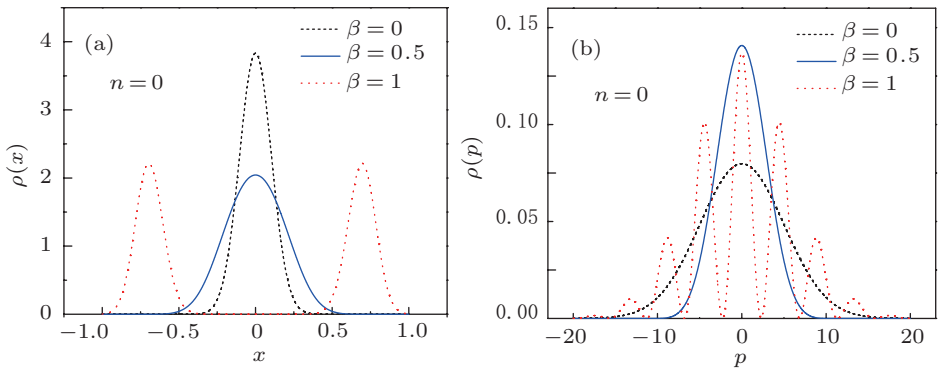


Fig. 1. (color online) Probability density distribution, $\rho(x)$ (a) and $\rho(p)$ (b), for the ground states with three typical β values.

3. Information entropy

3.1. Information entropy at the critical point

Once the probability density functions are obtained, the position and momentum space information entropies for the one-dimensional potential can be calculated by using Eqs. (2) and (3). Here, we will focus on discussing the situation at the critical point $\beta = 0.5$, where the system is undergoing a second-order quantum phase transition as mentioned above. The position and momentum entropy densities can be defined as

$$\rho_s(x) = |\psi(x)|^2 \ln|\psi(x)|^2, \quad \rho_s(p) = |\phi(p)|^2 \ln|\phi(p)|^2. \quad (16)$$

To show the properties of the information entropy densities, we plotted position and momentum entropy densities $\rho_s(x)$ and $\rho_s(p)$ together with the probability density functions $\rho(x)$ and $\rho(p)$ in Fig. 2 for the three lowest-lying states corresponding to $n = 0,\ 1,\ 2$. As seen from Figs. 2(a) and 2(b), $\rho(x)$ and $\rho(p)$ are symmetric with respect to $x = 0$ or $p = 0$ for all excited states and show a multi-peak structure: single-peak for $n = 0$, double-peak for $n = 1$ and triple-peak for $n = 3$. The resulting position information entropy density $\rho_s(x)$ is also symmetric with respect to $x = 0$ for all excited states and also presents a multi-peak structure for different n number as seen in Fig. 2(c). In contrast, the momentum information entropy density $\rho_s(p)$ may give an inverse multi-peak structure for different n number as shown in Fig. 2(d). Besides, the most part of the amplitude of $\rho_s(x)$ is positive for a given n in contrast to $\rho_s(p)$, of which the whole amplitude of $\rho_s(p)$ is negative.

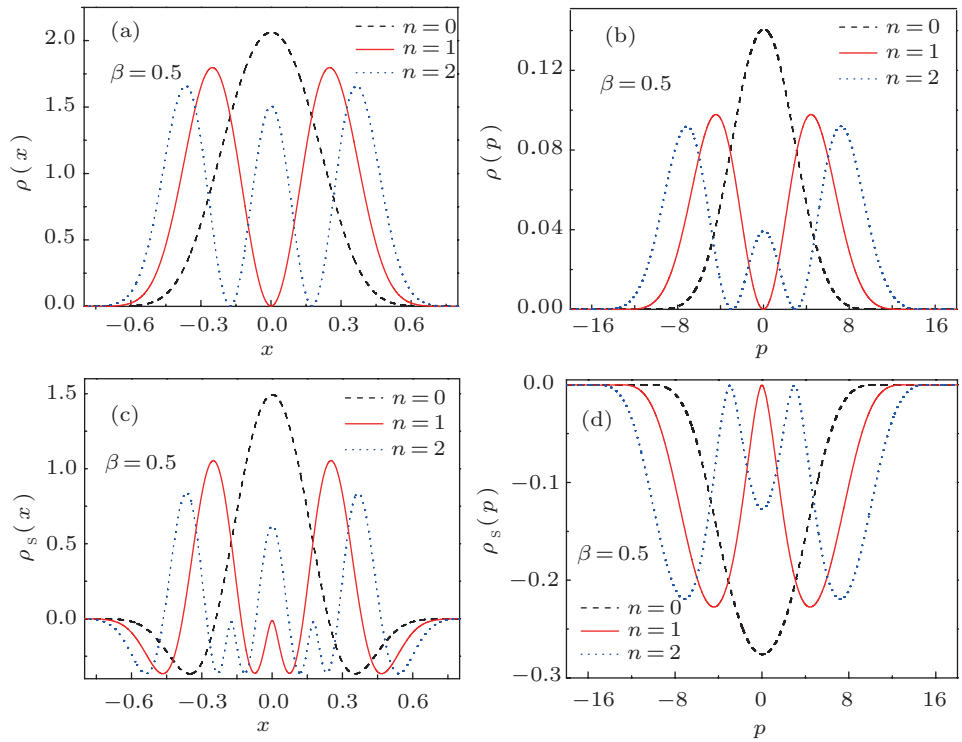


Fig. 2. (color online) Position and momentum probability densities ((a) and (b)) together with the corresponding information entropy densities ((c) and (d)) at the critical point $\beta = 0.5$ for the low-lying states with $n = 0,\ 1,\ 2$. In calculations, the mass parameter has been set as $M = 50$.

By using the information entropy densities, one can calculate the information entropies defined in Eqs. (2) and (3), which can be reexpressed as

$$S_x = -\int_{-\infty}^{\infty} \rho_s(x)\mathrm{d}x, \quad S_p = -\int_{-\infty}^{\infty} \rho_s(p)\mathrm{d}p. \tag{17}$$

Generally speaking, quantum fluctuations in the system around the critical point may be much larger than other situations, since the system undergoing quantum phase transition is relatively unstable. It would be interesting to find out whether the entropic uncertainty relation can be satisfied or not at the critical point. In Table 1, we give the numerical results of information entropies S_x, S_p and their sum S_x+S_p with different n numbers and M values. It is clearly seen from Table 1 that the entropy uncertainty relation is satisfied very well in all cases. Particularly, the values of S_x might be negative in some cases, but the sum of S_x and S_p for a given n may remain as an M-independent constant, of which the value always stays above the stipulated lower bound of the value (1+lnπ).

Table 1. Positive and momentum entropies at the critical point for the low-lying states $n = 0,\ 1,\ 2$ with different mass M.

n	M	S_x	S_p	S_x+S_p	1+lnπ
0	5	0.4874	1.6648	2.1522	2.1447
	20	0.0253	2.1269	2.1522	2.1447
	50	−0.2801	2.4323	2.1522	2.1447
1	5	0.6234	1.9968	2.6202	2.1447
	20	0.1613	2.4589	2.6202	2.1447
	50	−0.1441	2.7643	2.6202	2.1447
2	5	0.7192	2.1548	2.8740	2.1447
	20	0.2570	2.6170	2.8740	2.1447
	50	−0.0484	2.9224	2.8740	2.1447

3.2. Information entropy evolution via quantum phase transition

To test the transitional behavior of the information entropy within $\beta \in [0,1]$, the calculated results of S_x and S_p for $n = 0,\ 1$ are shown in Fig. 3 as a function of the control parameter β. As seen from Fig. 3(a), the position information entropies S_x show a non-monotonically evolution for both $n = 0$ and $n = 1$ as changing of β. Specifically, S_x may rapidly increase from negative values to positive values and then drop to negative values again with the variation of β. In contrast, the momentum information entropy S_p decreases at first and then grows up as the changing of β. More importantly, the results indicate that there is a sharp change in both S_x and S_p around the critical point $\beta_c = 0.5$, which in turn indicates that the absolute value of the derivative $\partial S_x/\partial\beta$ or $\partial S_p/\partial\beta$ may reach its maximum around the critical point β_c. One can thus derive that the system is undergoing a phase transition around the critical point β_c. It should be noted that the turn points of S_x and S_p appearing after the critical point β_c shown in Fig. 3 may rapidly approach the line denoted by β_c as increasing of M, which indicate that the turn points will coincide with the line in the large-M limit.

To further check the entropy uncertainty relation in the whole transitional region with $\beta \in [0,1]$, the results of S_x+S_p are shown in Fig. 4 as a function of the control parameter β. It can be seen from Fig. 4 that S_x+S_p may approximately remain unchanged up to the critical point $\beta = \beta_c = 0.5$ especially for the $n = 0$ case, in which the value almost sustains to be equivalent to 1+lnπ before $\beta = \beta_c$. When beyond $\beta = \beta_c$, the results of S_x+S_p in the two cases denoted by $n = 0$ and $n = 1$ may rapidly converge to almost the same constant value as shown in Fig. 4.

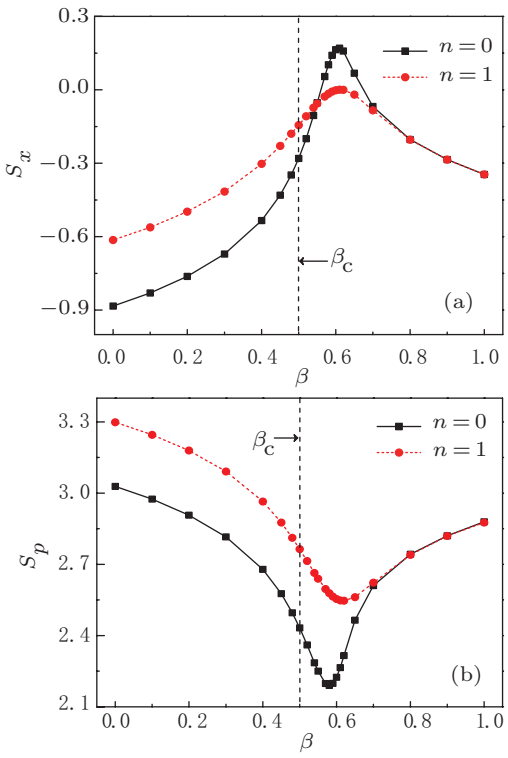


Fig. 3. (color online) The evolutions of position and momentum information entropies, S_x (a) and S_p (b) for $n = 0,\ 1$ as a function of the control parameter β, where the mass parameter is set as $M = 50$.

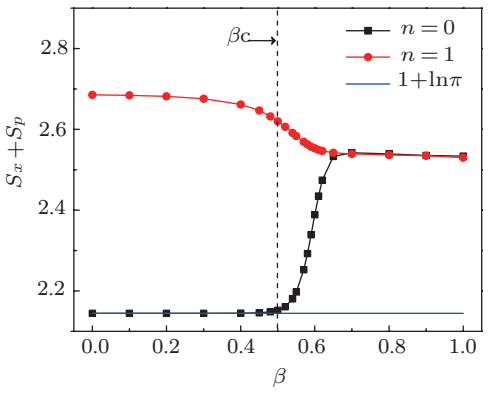


Fig. 4. (color online) The same as those in Fig. 3 but for the sum S_x+S_p.

Anyway, the results in Fig. 4 indicate that the entropic uncertainty relation would be well satisfied during the whole process of quantum phase transition.

4. Conclusion

In this paper, we have studied information entropy for a non-analytically solvable potential by adopting the diagonalization scheme. Concretely, we have investigated the properties of the position and momentum quantum information entropies of the one-dimensional system with a schematic "Landau" potential, in which the variation of the control parameter β may lead to a second-order quantum phase transition. It was found that the entropy density functions $\rho_s(x)$ and $\rho_s(p)$ at the critical point β_c may generally give multi-peak distributions that are symmetric with respect to $x = 0$ or $p = 0$. It was also found that the results of the position and momentum information entropies S_x and S_p may change with the variations of the mass parameter M or the quantum number n but their sum $S_x + S_p$ for a given n number remains as a constant independent of the mass parameter M. The further calculations show that there would be a rapidly non-monotonic change in both S_x and S_p around the critical point β_c, which justifies that the quantum phase transition can indeed be characterized by the evolution of the quantum information entropies. Finally, the results indicate that the entropic uncertainty relation given in Eq. (1) is very robust for the one-dimensional system during the whole process of quantum phase transition. Overall, the present numerical method seems quite valid to discuss the information entropy in this type of potential.

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