Phase space localization of antisymmetric functions

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Upper and lower bounds are written down for the minimum information entropy in phase space of an antisymmetric wave function in any number of dimensions. Similar bounds are given when the wave function is restricted to belong to any of the proper subspaces of the Fourier transform operator.

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1. Heisenberg uncertainty relations between position and momentum can be viewed as a constraint on the maximum allowable localization of quantum states in phase space, thereby displaying a basic principle of Quantum Mechanics. In this approach the localization is based on the size of the state. An alternative approach is to introduce an entropy in phase space as a measure of its localization. To be specific, if \( \psi(x) \) is a normalized wave function, the information entropy of the corresponding state in position space is defined as

\[
S_x(\psi) = - \int d^d x |\psi(x)|^2 \log(|\psi(x)|^2),
\]

(where \( d \) denotes the dimension of the space). The more localized the state the lower the entropy. For instance, for a one-dimensional Gaussian \( \psi(x) = (\pi a^2)^{-1/4} \exp(-x^2/2a^2) \) with \( a > 0 \), the behavior of the entropy \( S_x = (1 + \log(\pi a^2))/2 \) is qualitatively similar to that of the dispersion \( \Delta x = a/\sqrt{2} \). However, for a state composed of two well separated Gaussian functions of given widths, the dispersion would increase with the separation whereas the entropy would not. This illustrates the different concept of localization in both approaches.

The entropy in momentum space is defined similarly as

\[
S_k(\psi) = - \int d^d k |\tilde{\psi}(k)|^2 \log(|\tilde{\psi}(k)|^2),
\]

where

\[
\tilde{\psi}(k) = \int d^d x e^{-ikx/\hbar} \psi(x).
\]

For the one-dimensional Gaussian this gives \( \tilde{\psi}(k) = (4\pi a^2)^{-1/4} \exp(-a^2 k^2/2\hbar^2) \) and \( S_k = (1 - \log(4\pi a^2))/2 \), once again displaying a relation between localization in momentum space and entropy in that space. It is then natural to introduce an entropy in phase space as

\[
S(\psi) = S_x(\psi) + S_k(\psi).
\]

This definition respects invariance under dilatations (as also does \( \Delta x \Delta p \)). In the entropic approach the uncertainty principle is expressed by the fact that \( S_x \) and \( S_k \) cannot both be lowered simultaneously without limit. More precisely, the entropy in phase space satisfies the lower bound

\[
S(\psi) \geq d(1 - \log 2).
\]

This bound is sharp and is attained by the Gaussian functions (with non complex width). These are the unique minimizers \([17]\). In the one dimensional case this bound implies Heisenberg’s relation \( \Delta x \Delta p \geq h/2 \) \([13,14]\). We note that, in the literature, the name phase space entropy is used with various meanings, and frequently refers to entropies of matrix densities defined on phase space by means of a Wigner or a Husimi transformation (Wehrl entropy) \([9]\). \( S \) can also be viewed as the information entropy of a probability density in phase space, namely, \( \rho(x,k) = |\psi(x)|^2 |\tilde{\psi}(k)|^2 \).

2. Consider now two particles constrained to have a symmetric or an antisymmetric relative wave function (say, two electrons in a singlet or triplet spin state, respectively). One can ask which is the most localized state in phase space in both cases. In the symmetric case the answer is just a Gaussian function since this is the absolute minimum of \( S(\psi) \) and it is symmetric. In the antisymmetric case the solution is not known but certainly there exists a sharp lower bound, which will be denoted \( C_d \)

\[
S(\psi) \geq C_d \geq d(1 - \log 2), \quad \psi(x) = -\psi(-x).
\]

That the bound \( C_d \) is sharp implies that there exists a (minimizing) sequence of antisymmetric functions \( \psi_n \) such that \( \lim_{n \to \infty} S(\psi_n) = C_d \). It is not guaranteed, however, that \( S(\psi) = C_d \) is fulfilled for any function \( \psi(x) \) in \( L^2(\mathbb{R}^d) \).

In view of the fact that in the symmetric case the minimizer is a Gaussian, the ground state of a quantum harmonic oscillator, a natural guess would be to take the first excited state for the minimizer in the antisymmetric case. In one dimension this gives

\[
S = -1 + \log 2 + 2\gamma \geq C_1
\]
where $\gamma$ is Euler’s Gamma. Numerically $S = 0.847579$. This is not, however, the true minimizer, since in [18] a better guess $\psi_0$ was proposed which yields
\[ S(\psi_0) = 2(1 - \log 2) \geq C_1 \]  
(8)
(numerically $S = 0.613706$). In fact, based on strong numerical evidence, this was conjectured in [18] to be the true sharp bound in one dimension. (We note that $\psi_0$ represents actually a minimizing sequence and not a truly acceptable state.)

3. Whether this conjecture is true or not, one can now put an upper bound on $C_d$ for arbitrary $d$. Let $\psi_0(x)$ be the one-dimensional best guess for the antisymmetric case found in [18] and let $g(x)$ be a $(d-1)$-dimensional Gaussian function, then for the antisymmetric $d$-dimensional function
\[ \psi(x) = \psi_0(x_1)g(x_2, \ldots, x_d) \]  
(9)
we can immediately evaluate the entropy noting that this quantity is additive for separable functions
\[ S(\psi) = S(\psi_0) + S(g). \]  
(10)
This implies the bounds
\[ (d + 1)(1 - \log 2) \geq C_d \geq d(1 - \log 2). \]  
(11)

The Fourier transform can be regarded as an operator from $L^p(\mathbb{R}^d)$ into $L^q(\mathbb{R}^d)$, where $p^{-1} + q^{-1} = 1$ and $1 < p \leq 2 \leq q$. As already noted in [14] the minimization of the functional $S$ in $\mathbb{R}^d$ is directly related to the norm of the Fourier transform operator, defined as the supremum of $||\hat{\psi}||_q/||\psi||_p$ on $\mathbb{R}^d$. This is because derivating $\int d^d x |\hat{\psi}|^q$ or $(2\pi\hbar)^{-d} \int d^d k |\hat{\psi}|^q$ with respect $q$ at $q = 2$ generates $S_x(\psi)$ and $S_k(\psi)$ respectively. The relation between norm and entropy extends immediately for the subspace of antisymmetric functions $\mathbb{R}^d$. Let $K_{d,q}$ be the norm of the Fourier operator on the antisymmetric subspace of $\mathbb{R}^d$. For this quantity, using the same separable function introduced in [14], we find the bounds
\[ (p^{1/p}q^{-1/q})(d+1)/2 \leq K_{d,q} \leq (p^{1/p}q^{-1/q})d/2. \]  
(12)

4. The form of $\psi_0(x)$ is quite remarkable. It is an antisymmetric array of very narrow Gaussian functions located at equally spaced points and with amplitudes modulated by a very wide Gaussian function. Namely,
\[ \psi_0(x) = e^{-\pi a^2 x^2} \sum_{n \in \mathbb{Z}} (-1)^n e^{-\pi (x-n-\frac{1}{2})^2/a^2}, \quad a \to 0^+. \]  
(13)
As indicated, $a$ is a vanishingly small positive parameter. (We will implicitly assume this in what follows.) Alternatively one can use
\[ \psi_0(x) = \sum_{n \in \mathbb{Z}} (-1)^n e^{-\pi a^2 (n+\frac{1}{2})^2} e^{-\pi (x-n-\frac{1}{2})^2/a^2}, \quad a \to 0^+. \]  
(14)
Both expressions coincide for small $a$. This function is normalized. In the sense of distributions, $\psi_0(x)/a$ is equivalent to
\[ d_0(x) = \sum_{n \in \mathbb{Z}} (-1)^n \delta(x - n - \frac{1}{2}). \]  
(15)

However $d_0$ does not have a well defined entropy: the localization at any particular $x = n + \frac{1}{2}$ contributes with $-\infty$ to the entropy (an ultraviolet divergence) but the freedom to choose any $n$ adds a $+\infty$ (an infrared divergence). This refers both to the position and the momentum space entropies since they are equal for $d_0$ ($d_0$ is essentially equal to its Fourier transform).

The function $\psi_0(x)$ is a regularized version of $d_0$ in the infrared sector (by using $e^{-\pi a^2 x^2}$ instead of 1) and in the ultraviolet sector (by using $e^{-\pi a^2 /a^2}$ instead of $\delta(x)$). Remarkably the actual value of the entropy depends on the concrete choice of the regularization, i.e. there is no natural value to be assigned to the entropy of $d_0$.

In order to analyze this let us consider a more general regularization
\[ \psi(x) = \varphi(ax) \sum_{n \in \mathbb{Z}} (-1)^n \xi((x-n-\frac{1}{2})/a) \]
\[ = \sum_{n \in \mathbb{Z}} (-1)^n \varphi(a(n+\frac{1}{2}))\xi((x-n-\frac{1}{2})/a). \]  
(16)
(As always, the equality refers to $a \to 0^+$.) Here $\varphi(x)$ and $\xi(x)$ are two even smooth functions of rapid fall at infinity which we assume to be normalized. In this case $\psi(x)$ is also normalized and it will be instructive to show this explicitly. Because the $\xi(x)$ falls rapidly at infinity the regularized deltas do not overlap for small $a$, thus
\[ \int dx |\psi(x)|^2 = \int dx \sum_{n \in \mathbb{Z}} |\varphi(a(n+\frac{1}{2}))|^2 |\xi((x-n-\frac{1}{2})/a)|^2 \]
\[ = \sum_{n \in \mathbb{Z}} |\varphi(a(n+\frac{1}{2}))|^2 \int dx |\xi((x-n-\frac{1}{2})/a)|^2 \]
\[ = a \sum_{n \in \mathbb{Z}} |\varphi(a(n+\frac{1}{2}))|^2 \int dx |\xi(x)|^2 \]
\[ = \int dy |\varphi(y)|^2 \int dx |\xi(x)|^2 \]
\[ = 1. \]  
(17)
A similar calculation for the entropy in position space gives
\[ S_x(\psi) = S_x(\varphi) + S_x(\xi). \]  
(18)
In order to compute the momentum space entropy, we will use from now units $2\pi\hbar = 1$ which give simpler formulas (in particular $S_k(\psi) = S_k(\hat{\psi})$). Note that $S_k(\psi)$ has been defined so that it is numerically independent of
\(\hbar\) (for fixed \(\psi(x)\)). Using Poisson’s summation formula
\[ \sum_n \phi(n) = \sum_n \tilde{\phi}(n)\), one easily obtains
\[
\psi(k) = -i\xi(ak) \sum_{n \in \mathbb{Z}} (-1)^n \tilde{\varphi}((k - n - \frac{1}{2})/a)
= -i \sum_{n \in \mathbb{Z}} (-1)^n \xi(a(n + \frac{1}{2})) \tilde{\varphi}((k - n - \frac{1}{2})/a).
\]
(19)
This expression is formally identical to \(\psi(x)\) in replacing \(\varphi\) and \(\xi\) by \(\xi\) and \(\tilde{\varphi}\) and so
\[ S_k(\psi) = S_x(\tilde{\varphi}) + S_x(\tilde{\xi}) = S_k(\varphi) + S_k(\xi). \]
(20)
This implies for the phase space entropy
\[ S(\psi) = S(\varphi) + S(\xi). \]
(21)
The minimum is then obtained by choosing Gaussians as the regularizing functions \(\varphi\) and \(\xi\), as in \(\psi(x)\).

5. We will now study maximally localized (minimum uncertainty) states in other subspaces of \(L^2(\mathbb{R})\). To this end let us consider generalizations of the distribution \(d_0(x)\). These more general distributions \(u(x)\) will be composed of a set of well-separated Dirac deltas with different amplitudes and enjoying some periodicity properties. After suitable infrared and ultraviolet regularization we can then use the same procedure described above to compute the entropy. Specifically, we assume
\[
u(x) = \sum_{k=1}^N b_k \delta(x - x_k) \quad \text{for} \quad 0 \leq x < r,
0 \leq x_1 < \cdots < x_N < r,
|u(x + r)| = |u(x)|.
\]
(22)
Assuming that no \(b_k\) vanishes, \(u(x)\) is the superposition of \(N\) series, each series \(k = 1, \ldots, N\) being composed of equidistant deltas of strength \(|b_k|^2\). The period \(r\) is common to the \(N\) series. In principle one could consider a larger family of distributions by taking linear combinations of \(u_0, \sum_i u(x)\) with different periods \(r_i\), however, in order to guarantee that the deltas are well-separated (and this is essential for being able to compute the norm and the entropy) the ratios \(r_i/r_j\) must be rational numbers. In this case we are back within the class of distributions defined in \(\{\phi\}\) with \(r\) equal to a common multiple of the \(r_i\).

Next we regularize \(u(x)\) with normalized functions \(\varphi(x)\) and \(\xi(x)\) as in \(\{\tilde{\phi}\}\). This amounts to make a convolution of \(u(x)\) with \(\xi(x/a)\) and multiply by \(\varphi(ax)\) (in any order). The norm of the resulting function \(\psi(x)\) can be computed along the lines of \(\{\tilde{\phi}\}\) (working with each series of deltas separately). This gives
\[
\int dx |\psi(x)|^2 = r^{-1} \sum_{k=1}^N |b_k|^2.
\]
(23)
The norm decreases for increasing \(r\) (for fixed \(b_k\)) since less strength falls under the profile \(\varphi(ax)\). The entropy in position space can also be computed (exploiting again that the deltas are well-separated as \(a\) goes to zero) and this gives
\[ S_x(\psi) = S_x(\varphi) + S_x(\xi) + S(b) - \log(r), \]
(24)
where
\[ S(b) = - \sum_{k=1}^N \rho_k \log \rho_k, \quad \rho_k = |b_k|^2 / \sum_{j=1}^N |b_j|^2. \]
(25)
Eq. (24) nicely shows how the various structures combined in \(\psi(x)\) contribute additively to the entropy. \(S(b)\) corresponds to an entropy for the mixing of the various series in \(u(x)\). If the number of series is small, or more precisely if the strength is concentrated in a few series, this mixing entropy will decrease. However, the term \(- \log(r)\) indicates that what really matters for the entropy of \(\psi(x)\) is the effective number of series per unit length. This is sensible since any \(u(x)\) with \(N\) series and period \(r\) can also be regarded as having \(nN\) series and period \(nr\) for \(n = 2, 3, \ldots\).

Assuming that \(\tilde{u}(x)\) belongs to the same class \(\{\tilde{\phi}\}\) for some \(\tilde{b}_k, \tilde{N}\) and \(\tilde{r}\), the total phase space entropy becomes
\[ S(\psi) = S(\varphi) + S(\xi) + S(b) + S(\tilde{b}) - \log(r\tilde{r}). \]
(26)
As a consequence the optimum small and large scale profiles \(\xi\) and \(\varphi\) are Gaussians, and we will assume that in what follows.

We note that similar relations are obtained for the \(p\)-norms, namely
\[ \int dx |\psi(x)|^p = r^{-1} \sum_{k=1}^N |b_k|^p \int dy |\varphi(y)|^p \int dx |\xi(x)|^p. \]
(27)
6. The Fourier transform operator naturally decomposes \(L^2(\mathbb{R})\) into the four invariant subspaces corresponding to its four eigenvalues \(\lambda = \pm 1, \pm i\). We want to find maximally localized states in each such subspace. The Gaussians belong to the subspace \(\lambda = 1\) so they are also the minimizer in this subspace. Our best guess for antisymmetric functions \(\psi_0(x)\) belongs to the subspace \(\lambda = -1\), so this is also our best guess in this subspace. It remains to consider the cases \(\lambda = -i\) and \(\lambda = i\). Brute force numerical minimization suggests that the minimizers in these two cases belong to the class \(\{\tilde{\phi}\}\) with Gaussian regularization. In order to study this further let us introduce the set of distributions
\[ \phi(x, r, \alpha, \beta) = \sum_{n \in \mathbb{Z}} e^{-2\pi i \beta n} \delta(x - r(n + \alpha)), \]
(28)
for non vanishing real \(r\) and real \(\alpha\) and \(\beta\). Not all these functions are independent since
\[ \phi(x, r, \alpha, \beta) = \phi(x, -r, -\alpha, -\beta) = \phi(x, r, \alpha, \beta + 1) \]
\[ = e^{-2\pi i \beta} \phi(x, r, \alpha + 1, \beta) \]
(29)
and all different results are covered by $0 < r$, $0 \leq \alpha, \beta < 1$. Under Fourier transform one finds
\begin{equation}
\tilde{\phi}(x, r, \alpha, \beta) = r^{-1} e^{2\pi i \alpha \beta} \phi(x, r^{-1}, -\alpha, \beta).
\end{equation}

Therefore, the distributions $\phi(x, r, \alpha, \beta)$ and their Fourier transform belong to the class in (22) with $N = 1$.

In order to minimize the mixing entropy $S(b)$ we start by looking for solutions of the form $\tilde{\phi} = \lambda \phi$. The unique solutions are $\phi(x, 1, 0, 0)$ with $\lambda = 1$ and $\phi(x, 1, \frac{1}{2}, \frac{1}{2})$ with $\lambda = -1$ both with entropy $1 - \log 2$ after Gaussian regularization (the latter solution is just $\delta_0$).

The simplest guess is to project a single distribution $\phi$ on the subspaces $\lambda = -1$ or $\lambda = i$. If $F$ denotes the Fourier transform operator, the projector on the subspace $\lambda$ is $P_\lambda = (1 + \lambda^{-1} F + \lambda^{-2} F^2 + \lambda^{-3} F^3)/4$. Thus a combination of no more than four $\phi$'s is sufficient to yield a distribution of the type $\tilde{u}(x) = \lambda u(x)$. A further simplification can be achieved as follows. All functions with $\lambda = -1$ are necessarily even (symmetric), so for these functions $P_{\lambda=-1} = (1 - F)/2$ and only two $\phi$'s are involved after projection. Similarly, the functions $\lambda = i$ are odd and for these functions $P_{\lambda=i} = (1 - iF)/2$. In both cases we will seek a minimum of this form, i.e. projections of a single even or odd $\phi$. Of course it is not guaranteed that the true minimum is obtained in this way.

Two remarks should be made. First, the projection $\nodegree \lambda \phi$ involves periods $r$ and $r^{-1}$. This combination is acceptable only if $r/r^{-1} = r^2$ is a rational number. We will take $r = \sqrt{q/p}$, where the positive integers $q$ and $p$ have no common divisor. Second, although each $\phi$ contains a single series of deltas, the combination of two $\phi$'s may have many more than two series of deltas. For instance $u(x) = \phi(x, 1/2, 0, 0) + \phi(x, 2, 0, 0)$ has period $r = 2$ and $N = 4$ with $x_k = 0, 1/2, 1, 3/2$ and $b_k = 2, 1, 1, 1$. In practice $u(x)$ will be composed of two $\phi$'s with periods $r = \sqrt{q/p}$ and $r^{-1}$. In order to disentangle the different series contained in $u(x)$ it will be necessary to bring all the $\phi$'s to a common period. To this end the following identity is useful
\begin{equation}
\phi(x, r, \alpha, \beta) = \sum_{k=0}^{n-1} e^{-2\pi i \beta k} \phi(x, nr, \frac{k + \alpha}{n}, n\beta),
\end{equation}
where $n$ is any positive integer. In our case the smallest common period is $r' = p/r = qr^{-1} = \sqrt{pq}$.

Case $\lambda = -1$. There are three classes of single distributions $\phi$ which are even under $x \rightarrow -x$, namely $\phi(x, r, 0, 0)$, $\phi(x, r, 0, 1/2)$ and $\phi(x, r, 1/2, 0)$, and arbitrary period $r$. The case $(1/2, 0)$ needs not be considered since it will be generated after projection of the case $(0, 1/2)$.

Projection of $\phi(x, r, 0, 0)$ on the $\lambda = -1$ subspace gives
\begin{equation}
u(x) = \phi(x, r, 0, 0) - r^{-1} \phi(x, r^{-1}, 0, 0).
\end{equation}
In this case we find a total of $N = q + p - 1$ series of period $r' = \sqrt{pq}$. (Actually $\phi(x, r, 0, 0)$ gives $p$ series of period $r'$ and $\phi(x, r^{-1}, 0, 0)$ gives $q$ series of period $r'$ but one of the series is common to both functions.) Of these, $p - 1$ series have amplitude $b_k = 1$, $q - 1$ series have amplitude $b_k = -r^{-1}$ and there is a single series with amplitude $1 - r^{-1}$. A numerical survey shows that the best case corresponds to $q = 1$ and $p = 2$ (or vice versa). This corresponds to a distribution $u(x)$ composed of only two series of period $r' = \sqrt{2}$ and weights $p_1 = (2 - \sqrt{2})/4$ and $p_2 = (2 + \sqrt{2})/4$. The mixing entropy is $S(b) = \log(r') = \log 2 + \frac{1}{\sqrt{2}} \log(\sqrt{2} - 1)$. The total phase space entropy (i.e., adding the Gaussian contribution $1 - \log 2$ and an overall factor of two to account for the momentum space entropy) is thus
\begin{equation}
S_{\lambda=-1} = 2 + \sqrt{2} \log(\sqrt{2} - 1) = 0.753550
\end{equation}
corresponding to the distribution
\begin{equation}
u(x) = (1 - \sqrt{2})\phi(x, \sqrt{2}, 0, 0) + \phi(x, \sqrt{2}, 1/2, 0).
\end{equation}
This is our best guess for the subspace $\lambda = -1$.

The other possibility in this subspace is to project $\phi(x, r, 0, 1/2)$. The analysis is slightly more involved in this case. If $p$ is odd the number of series is $p + q$ and the total entropy is $S = 2$ for any choice of $p$ and $q$. If $p$ is even the number of series is $q + p - 1$ and the entropy depends on the concrete values of $q$ and $p$. The best choice corresponds to $q = 1$, $p = 2$ and yields the same distribution $u(x)$ in (34).

Case $\lambda = +i$. The only possibility of an odd $\phi$ is $\phi(x, r, 1/2, 1/2)$. This gives
\begin{equation}
u(x) = \phi(x, r, 1/2, 1/2) - r^{-1} \phi(x, r^{-1}, 1/2, 1/2).
\end{equation}
If $p$ or $q$ is even the number of series is $q + p$ and for all choices of $q$ and $p$ the total entropy is 2. If $q$ and $p$ are odd the number of series is $q + p - 1$. The best choice corresponds to $q = 3$ and $p = 1$ (or vice versa) with a total phase space entropy
\begin{equation}
S_{\lambda=i} = 2 - \frac{2}{\sqrt{3}} \log(\sqrt{3} + 1) = 0.839465
\end{equation}
This is our best guess for the subspace $\lambda = +i$.

These results are well below the guesses based on the lowest harmonic oscillator states which yield $S = 1.51934$ for $\lambda = -1$ and $S = 1.38155$ for $\lambda = i$.

By using (27) these results extend immediately to relations for the norm of the Fourier transform operator from $L^0(\mathbb{R}^d)$ into $L^0(\mathbb{R}^d)$, restricted to the proper subspaces $\lambda = \pm 1, \pm i$.

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