From single-particle physical distributions to probabilistic measures of two-particle entanglement

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Abstract

An inversion method is formulated for extracting entanglement-related information on two-particle interactions in a one-dimensional system from measurable one-particle position-and momentum- distribution functions. The method is based on a shell-like expansion of these norm-1 measured quantities in terms of product states taken from a parametric orthonormal complete set. The mathematical constraints deduced from these point-wise expansions are restricted by the underlying physics of our harmonically confined and interacting Heisenberg model. Based on these exact results, we introduce an approximate optimization scheme for different inter-particle interactions and discuss it from the point of view of entropic correlation measures.

I. MOTIVATION

Let us take the Hamiltonian, in atomic units, of a *single* harmonic oscillator

$$\hat{H}_0(x) = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega_0^2 x^2. \tag{1}$$

, the ground-state normalized solution to the Schrödinger equation is $\phi_0(x,\omega_0) = (\omega_0/\pi)^{1/4}\exp(-\omega_0 x^2/2)$. Its square gives the normalized density distribution function, $n(x) = [\phi_0(x)]^2$, whose Fourier transform is

$$n(k) = \frac{1}{\sqrt{2\pi}}\, e^{-k^2/(4\omega_0)}. \tag{2}$$

This function can be sampled by X-ray scattering, and by Fourier inversion, one may say that $n(x)$ is accessible experimentally. The normalized one-particle momentum density distribution, $f(k)$, is, on the other hand, connected to Compton scattering. The relation between these real- and momentum-space distributions, i.e., between the two sets of experimental data, is one-to-one because $\phi_0(x) = \sqrt{n(x)}$ and $f(k)$ are given by

$$f(k) = [\phi_0(k,\omega_0)]^2 = \left[\left(\frac{1}{\pi\omega_0}\right)^{1/4} e^{-k^2/(2\omega_0)}\right]^2. \tag{3}$$

From $\phi_0(x,\omega)$ and $\phi_0(k,\Omega)$ we can determine the corresponding kinetic energies

$$<K_1> = \frac{1}{2}\int_{-\infty}^{\infty} dx\left|\frac{d\phi_o(x,\omega)}{dx}\right|^2 = \frac{1}{4}\omega \tag{4}$$

$$<K_2> = \int_{-\infty}^{\infty}\frac{1}{2}k^2 f(k,\Omega)\,dk = \frac{1}{4}\Omega \tag{5}$$

In the noninteracting case, $\omega = \omega_0$ and $\Omega = \omega_0$, these are equal, but in the interacting case below, $(\omega_0 \Rightarrow \Omega_s)$ only Eq.(5) gives the exact result. The definition in Eq.(4), even with the exact density $(\omega_0 \Rightarrow \omega_s)$ [1] gives $[<K_1>/<K_2>] < 1$.

When the Gaussian function $f(k)$ is characterized by $\Omega_s \neq \omega_0$, instead of ω_s used for the density distribution, the one-to-one mapping is lost. In case of harmonic external confinement, one should conclude from this observation that we have at least two similar particles in the ground-state under confinement and, moreover, these particles are dynamically correlated. Is there, in the physically most important interacting case, still something useful which one can extract from the above two observables? How could a proper mathematical recipe be formulated? These are the questions motivating this note on the application of *reduced* information. We feel that examining the weakly interacting two-particle case is a conservative first step having general information-theoretic relevance.

II. DECOMPOSITIONS, CONSTRAINTS, AND OPTIMIZATION

Four our interacting system, there is no simple connection between the normalized position-space density $n(x)$ and the normalized momentum-space density $f(k)$, despite the fact that they are related by the Fourier transformation between the wave functions, and associated density matrices, in these spaces [1]. Furthermore, the reduced one-particle density matrices, the sources of $N(x)$ and $F(k)$ are two-variable functions. They contain more information than the corresponding one-variable probability densities, i.e., their diagonals. Besides, since correlation is encoded differently [2] in the observables discussed above, a successful recipe for extracting information must rest on both densities. Such *chameleon*-like behavior in the observables requires care in their mathematical treatment. One can not simply follow the Duke of Gloucester who, in Shakespeare's play Henry VI, stated: 'I can add colors to the chameleon'.

The details of the one-to-one correspondence outlined above for the one-particle case suggest that decompositions of $N(x)$ and $F(k)$, when properly normalized, into *products* of one-variable functions belonging to complete sets, and the Fourier-transformation ($\mathcal{F}$) link between these sets, could form the mathematical basis of the recipe. In the extraction of information, one requires spatially-independent decomposition weights. Since these weights are eigenvalues of the underlying one-body matrices they allow a detailed analysis of entanglement entropies. However, the two-variable eigenfunctions, i.e., the natural orbitals, are not directly accessible experimentally. Thus, physically important information, say the energy scales behind extensions of these optimal orbitals in real space, remains intact.

In this note we consider a *weakly* interacting two-particle system under common harmonic confinement $(1/2)\omega_0^2(x_1^2 + x_2^2)$. This is the standard condition, e.g.in recent experiments on optically trapped systems with controllable number of constituents [3]. For this system we introduce, assuming $\omega_s \neq \Omega_s$, the two Gaussians

$$\phi_1(x, \omega_s) = \left(\frac{\omega_s}{\pi}\right)^{1/4} e^{-\frac{1}{2}\omega_s x^2} \tag{6}$$

$$\phi_2(k, \Omega_s) = \left(\frac{1}{\pi\Omega_s}\right)^{1/4} e^{-\frac{1}{2}\frac{k^2}{\Omega_s}}. \tag{7}$$

in order to *model* the correlated density distribution function, $N(x) = [\phi_1(x)]^2$, and the correlated momentum distribution function, $F(k) = [\phi_2(k)]^2$. The case $\omega_0 = \omega_s = \Omega_s$ obviously corresponds to the noninteracting situation where, of course, $\phi_2(k) = \mathcal{F}[\phi_1(x)]$.

The desired product-representations of the experimental data-functions, $N(x) = [\phi_1(x)]^2$ and $F(k) = [\phi_2(k)]^2$, with common spatially-independent weighting coefficients necessary for a linear mapping, such as Fourier transformation, are given by

$$N(x, \omega_s) = \sum_{m=0}^{\infty} (1 - Z) Z^m \left[\phi_m(\sqrt{\bar{\omega}}x)\right]^2 \tag{8}$$

$$F(k, \Omega_s) = \sum_{m=0}^{\infty} (1 - Z) Z^m \left[\phi_m(k/\sqrt{\bar{\omega}})\right]^2 \tag{9}$$

$$\phi_m(\sqrt{\alpha}u) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^m m!}} e^{-\frac{1}{2}\alpha u^2} H_m(\sqrt{\alpha}u). \tag{10}$$

Here $\bar{\omega}$ is an orbit-parameter. For Gaussian densities these Mehler's [4] representations are point-wise [5], and $\sum_{m=0}^{\infty}(1 - Z)Z^m = 1$. The constraints on the expansions are

$$\omega_s = \bar{\omega} \frac{1 - Z}{1 + Z} \tag{11}$$

$$\frac{1}{\Omega_s} = \frac{1}{\bar{\omega}} \frac{1 - Z}{1 + Z}, \tag{12}$$

from which $\bar{\omega} = \sqrt{\omega_s \Omega_s}$ and $Z = [1 - \sqrt{\omega_s/\Omega_s}]/[1 + \sqrt{\omega_s/\Omega_s}] \leq 1$. Since we know from the physics [1] of kinetic energy that $[< K_2(\Omega_s) > / < K_1(\omega_s) >] \geq 1$, we have $(\Omega_s/\omega_s) \geq 1$.

A useful probabilistic measure of correlation is the purity Π. From the properties of our normalized occupation numbers, $P_m \equiv (1 - Z)Z^m$, this measure is given by

$$\Pi = \sum_{m=0}^{\infty} (P_m)^2 = \frac{1 - Z}{1 + Z} = \sqrt{\frac{\omega_s}{\Omega_s}} \leq 1, \tag{13}$$

in terms of the ratio of ω_s and Ω_s, which characterize the experimentally accessible distributions in position and momentum spaces, respectively. Related, commonly applied information-theoretic quantities are [6] the Rényi's (R) and von Neumann's (N) entropies

$$S_R(q) = \frac{1}{1 - q} \ln \frac{(1 - Z)^q}{1 - Z^q} \tag{14}$$

$$S_N = -\left[q^2 \frac{d}{dq}\left(\frac{1 - q}{q} S_R(q)\right)\right]_{q=1} = -\ln(1 - Z) - \frac{Z}{1 - Z} \ln Z. \tag{15}$$

Von Neumann's S_N is the entropy of thermodynamics. But, in agreement with an earlier remark [7], the above measures depend solely on a ratio of physical parameters. For entropies, taken at arbitrary q values, the orbit-extension parameter, $\bar{\omega}$, is not needed. Therefore, pure information-theoretic measures alone are not applicable directly to determine scale-dependent physical quantities. Determining the *sign* of the inter-particle interaction (see, below) could be a nontrivial problem for reverse engineering, due to duality [8–10].

To proceed in our realistic modeling of a confined system [3], we add to the Schrödinger Hamiltonian the tunable (via λ, see below) two-particle interaction

$$\hat{H}(x_1, x_2) = -\frac{1}{2}\left(\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2}\right) + \frac{1}{2}\omega_0^2(x_1^2 + x_2^2) + v_H(|x_1 - x_2|), \tag{16}$$

When $v_H \neq 0$, we get $\Omega_s \neq \omega_0$, $\omega_s \neq \omega_0$, $\Omega_s \neq \omega_s$. In order to have a rigorous foundation for understanding information-extraction from observables, we turn to the specific [11] interaction $v_H(|x_1 - x_2| = \lambda(\omega_0^2/2)(x_1 - x_2)^2$. Based on this interaction, we recently derived closed-form expressions [12] for both two-variable one-matrices

$$\Gamma_1(x_1, x_2) = \phi_s(x_1)\,\phi_s(x_2) \times e^{-D[(x_1-x_2)/\sqrt{2}]^2} \tag{17}$$

$$\Gamma_1(k_1, k_2) = \frac{1}{\sqrt{\pi(\omega_s + 2D)}}\, e^{-\frac{1}{2}(k_1^2+k_2^2)\frac{\omega_s+D}{\omega_s(\omega_s+2D)}}\, e^{+\frac{Dk_1k_2}{\omega_s(\omega_s+2D)}} \tag{18}$$

where, with $\omega_s \equiv 2\omega_1\omega_2/(\omega_1 + \omega_2)$, we introduced the following abbreviations

$$\phi_s(x) = \left[\frac{\omega_s}{\pi}\right]^{1/4} e^{-\frac{1}{2}\omega_s x^2} \tag{19}$$

$$D = \frac{1}{4}\frac{(\omega_1 - \omega_2)^2}{\omega_1 + \omega_2} \geq 0. \tag{20}$$

We derive $\omega_1 = \omega_0$ and $\omega_2 = \omega_0\sqrt{1 + 2\lambda}$ in the underlying [12] normal-mode separation of the Schrödinger equation with Eq.(16). Thus, for the repulsive harmonic inter-particle interaction, the allowed range is $\lambda \in (-0.5, 0]$. Both ω_s and D, and therefore Z, show a dual character [8–10]. This means that to any allowed repulsive coupling there exists a corresponding attractive one with the same value for Zl. Clearly, with Heisenberg's inter-particle interaction model [11] the measurable $N(x) = \Gamma_1(x, x)$ and $F(k) = \Gamma_1(k, k)$ are known theoretically. Therefore, in this case, we get $\Omega_s = \omega_s + 2D$, by which the kinetic energy becomes $< K_2 >= (1/4)(\omega_s + 2D) > (1/4)\omega_s =< K_1 >$. But, and this is crucial to information-extraction, by taking the diagonal of Eq.(17) to get a measurable distribution we have no *separate* access to $D(\omega_1, \omega_2)$ which produces non-idempotency.

Finally, we turn to an optimization procedure which may connect two Schrödinger Hamiltonians. One could replace, following a recent proposal [13], a realistic two-particle Hamiltonian having non-harmonic inter-particle interaction by the Heisenberg Hamiltonian (H). For instance, one could apply total-energy correspondence as a constraint on such replacement. One may argue, of course, that the λ-coupling in Eq.(16) has been chosen qualitatively and it is this mapping correspondence which would allow it to be determined quantitatively. We

expect, based on physical considerations, that such an optimized correspondence between two Hamiltonians can be reasonable only if the harmonically confined particles interact *weakly*. [3]. At that small coupling the non-idempotency driver scales as $D \sim \lambda^2$, i.e., the deviations of ω_s and $\Omega_s > \omega_s$ from ω_0 are small. The associated entropies are small as well. However, at stronger couplings, one may get a serious problem by applying such an optimization scheme to information-theoretic measures.

We now quantify this problem by considering the attractive ($\lambda > 0$) case in Eq. (16). Say we construct a more realistic model by taking for the inter-particle interaction

$$v_C(|x_1 - x_2|) = \frac{\Lambda}{(x_1 - x_2)^2}$$

with $\Lambda > 0$. We focus here on the strong coupling limit [14, 15]. From the prescribed equivalence of ground-state energies $E_H(\lambda \to \infty) \propto \sqrt{1 + 2\lambda}$ and $E_C(\Lambda \to \infty) \propto \sqrt{1 + 4\Lambda}$, with $v_H(\lambda)$ and $v_C(\Lambda)$ respectively, we get the simple correspondence $\lambda = 2\Lambda$. However, with the singular interaction above. one gets, in the associated Wigner-crystal limit at strong coupling, Λ-independent occupation numbers [14, 15]. Thus the purity is approximately $\Pi_C(\Lambda \to \infty) \simeq 0.528$. In the energetically optimized Heisenberg case, i.e., with a harmonic interaction $v_H(\lambda = 2\Lambda)$, we obtain the different behavior, $\Pi_H(\Lambda) \simeq \sqrt{2}/\Lambda^{1/4}$ at $\Lambda \to \infty$.

This, seemingly, moderate numericaldifference in an information-theoretic measure is related, physically, to crucially different behaviors of the underlying wave function as a function of the relative coordinate. Our quantitative observation at strong coupling is not in contradiction with the prediction [13] which relies on perturbation theory. Clearly, one can only get a physically reasonable approximation for the linear entropy, $L_C = 1 - \Pi_C$, at small (i.e., perturbative) coupling within the proposed optimization framework.

III. SUMMARY

An inversion method is formulated for extracting entanglement-related information on two-particle interactions from measurable one-particle distribution functions in position and momentum spaces. The method is based on shell-like expansions of these measurable norm-1 quantities in terms of properly weighted product states taken from a parametric complete orthonormal set. It is found that without further physical details, encoded in the two-variable reduced one-particle density matrices, an unambiguous characterization of the inter-particle interaction is not possible by inverting such information.

We have, therefore, given a concrete answer to Pauli's general question [16] of whether the position and momentum probability densities are sufficient to determine the statistical state operator. These distributions are not sufficient. One method for resolving the dual character in the sign of an inter-particle interaction is to make use of the dynamical evolution [12] of the correlated state. In such evolution, one of the normal-mode frequencies, i.e., $\omega_0\sqrt{1+2\lambda}$ in the Heisenberg model, could be measurable via the corresponding breathing mode [13].

Based on exact results obtained with Heisenberg's Hamiltonian, an optimization procedure for introducing a different inter-particle interaction is formulated and analyzed quantitatively from the point of view of entropic correlation measures. This analysis shows that , as expected,an energy-based optimization scheme could be useful only at weak inter-particle couplings.

[1] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory* (Springer-Verlag, Berlin, 1990).

[2] J. E. Harriman, Z. Naturforsch. **47a**, 203 (1991).

[3] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature (London) **440**, 900 (2006); A. N. Wenz, G. Zürn, S. Murmann, I. Brouzos, T. Lompe, and S. Joachim, Science **342**, 457 (2013).

[4] A. Erdélyi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), p. 194.

[5] F. Riesz and B.-Sz. Nagy, *Functional Analysis* (Ungar, New York, 1955).

[6] A. Rényi, *Probability Theory* (North-Holland, Amsterdam, 1970).

[7] M. Srednicki, Phys. Rev. Lett. **71**, 666 (1993).

[8] J. Pipek and I. Nagy, Phys. Rev. A **79**, 052501 (2009).

[9] M. L. Glasser and I. Nagy, Phys. Lett. A **377**, 2317 (2013).

[10] Ch. Schilling and R. Schilling, J. Phys. A: Math. Theor. **47**, 415305 (2014).

[11] W. Heisenberg, Z. Phys. **38**, 411 (1926).

[12] I. Nagy, J. Pipek, and M. L. Glasser, arXiv: .... [cond-mat.stat-mech].

[13] C. R. McDonald, G. Orlando, J. W. Abraham, D. Hochstul, M. Bonitz, and T. Brabec, Phys. Rev. Lett. **111**, 256801 (2013).

[14] P. Koscik, Phys. Lett. A **379**, 293 (2015).

[15] O. Osenda, F. M. Pont, A. Okopinska, and P. Serra, J. Phys. A: Math. Theor. **48**, 485301 (2015), and references therein.

[16] L. E. Ballentine, *Quantum Mechanics* (World Scientific, Singapore, 1998), pp. 213-215.