Local energy and power in many-particle quantum systems driven by an external electrical field

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Abstract. We derive expressions for the expectation values of the local energy and the local power for a many-particle system of (scalar) charged particles interacting with an external electrical field. In analogy with the definition of the (local) current probability density, we construct a local energy operator such that the time-rate of change of its expectation value provides information on the spatial distribution of power. Results are presented as functions of an arbitrarily small volume $\Omega$, and physical insights are discussed by means of the quantum hydrodynamical representation of the wavefunction, which is proven to allow for a clear-cut separation into contributions with and without classical correspondence. Quantum features of the local power are mainly manifested through the presence of non-local sources/sinks of power and through the action of forces with no classical counterpart. Many-particle classical-like effects arise in the form of current-force correlations and through the inflow/outflow of energy across the boundaries of the volume $\Omega$. Interestingly, all these intriguing features are only reflected in the expression of the local power when the volume $\Omega$ is finite. Otherwise, for closed systems with $\Omega \rightarrow \infty$, we recover a classical-like single-particle expression.

Keywords: mesoscopic systems (theory), quantum transport, local power, local energy, local operators
1. Introduction

Conservation laws are extraordinarily useful mathematical tools for determining the time-evolution of complex systems. Among them, energy conservation is perhaps the most conspicuous one. Different types of energies (kinetic, potential, chemical, etc.) are commonly defined in order to identify a global property of the system which does not change in time, and hence used to impose restrictions on the equations of motion of complex systems.

For open (non-isolated) systems interacting with an out-of-equilibrium environment, energy is no longer a constant of motion but remains a valid and useful concept. The notion of power is introduced in this context as a measure of the rhythm at which systems gain or lose energy through the interaction with the environment. From a theoretical point of view, the concept of power has been used to explore the extension of thermodynamic laws to the realm of quantum mechanics [1–5]. From an operational viewpoint, power plays a central role, e.g. in evaluating the performance of emergent electronic and nanomechanical devices [6–10], for which low-power consumption is a prevailing requirement.

For quantum systems preserving the number of particles, the power supplied by an external (driving or dissipative) force is defined as the time-rate of change of the
expectation value of the energy [11]. For quantum systems which are open to the flow of particles, however, energy can turn into a fuzzy concept unless it is carefully redefined. As will be shown here, the evaluation of the spatial distribution of energy and power (defined for small regions of the physical space) requires a careful theoretical approach.

Access to spatially resolved energy and power can be relevant in the context of local control of particle heating or cooling through the action of laser fields [12]. But more importantly, this information can be used to assess the performance of electronic devices, for which determining the spatial distribution of energy and power along the source, gate or drain regions is of paramount importance [13–15]. In classical mechanics, access to local energy and power information does not pose any mathematical or conceptual difficulty [16]. However, in quantum mechanics, although not far from being measurable [17], the evaluation of such spatially resolved information is accompanied by some conceptual and mathematical intricacies.

In this work we address the specific question of what are the spatial distributions of energy and power transferred by an external electrical field to an ensemble of (scalar) charged particles. In particular, we want to provide an answer to this question without resorting to any kind of thermodynamical argument. To this end, we first define a local energy operator whose expectation value provides a measure of the energy enclosed in an arbitrarily small volume $\Omega$ of the physical space. Local power will be then defined as the time-rate of change of this expectation value. Significantly, we will show that the exact expression for the local power depends on intriguing many-particle current-force correlations and non-local quantum terms that are not present in the standard equation for the total (spatially integrated) power [18].

After this introduction, in section 2 we describe the system under study and motivate the use of local operators. Then, in section 3, we define the local energy operator and evaluate its expectation value. In section 4, we identify the local power as the time derivative of the local energy and discuss its physical soundness. We conclude in section 5.

2. Preliminary discussion

Before deriving expressions for the local energy and power, we provide here a comprehensive description of the system (and environment) that will be approached in this work. We also introduce the concept of local operator, which will be used later in our derivations.

We consider first a quantum system which is kept out of equilibrium by the action of an external (effective) electric field. This system can exchange energy but not particles with its environment. Later we will define a smaller volume $\Omega$, enclosed in the first one, which can exchange both energy and particles with its surroundings. This new volume $\Omega$ can be made as small as required, and thus we will call any observable associated to it local. Our main goal in this work is to find an expression for the power and energy associated to this second volume $\Omega$.
2.1. Energy and power for many-particles driven by an external electrical field

Consider an ensemble of interacting (scalar) charged particles under the action of an external electrical field and defined by the \( N \)-particles state \( |\psi(t)\rangle \). This state can be written in the position representation as the many-particle (scalar) wavefunction \( \psi(r,t) \), where the ket \( |r\rangle = |r_1\rangle \otimes \ldots \otimes |r_N\rangle \) collectively denotes the position of the particles in the \( 3N \)-dimensional configuration space (and \( \otimes \) represents the direct product). We consider here all particles to be spinless. The generalization of our results for multi-component (vector) spinors does not add any conceptual complexity but it certainly complicates our mathematical derivation. Throughout this work we use atomic units (\( m_e = 1, e = 1, \hbar = 1 \) and Coulomb’s constant \( k_e = 1 \)) and bold letters indicate vectors defined in the three-dimensional Cartesian space, i.e. \( |r_k\rangle = |x_k\rangle \otimes |y_k\rangle \otimes |z_k\rangle \).

We assume that the state \( |\psi(t)\rangle \) is effectively governed by the following time-dependent Schrödinger equation:

\[
i \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle = (\hat{K} + \hat{U}(t))|\psi(t)\rangle,
\]

(1)

where \( \hat{K} = \frac{1}{2} \sum_{k=1}^{N} \mathbf{p}_k \cdot \mathbf{p}_k \) is the many-body kinetic energy operator, with \( \mathbf{p}_k \) the linear momentum operator. The term \( \hat{U}(t) = \hat{U}_{\text{con}}(t) + \hat{U}_{\text{ext}}(t) \) represents a (scalar) potential energy operator that accounts for the Coulomb interaction \( \hat{U}_{\text{con}} \) among the \( N \) particles and also for their interaction with an external electrical field through \( \hat{U}_{\text{ext}}(t) \). In the position representation it reads:

\[
U(r, t) = U_{\text{con}}(r) + \sum_k U_{\text{ext}}(r_k, t).
\]

(2)

The Coulomb interaction among particles can be written in terms of the two-particle potential \( U_{k,j} \equiv U_{k,j}(r_k - r_j) \) as:

\[
U_{\text{con}}(r) = \sum_{k} \sum_{j>k} U_{k,j}(r_k - r_j).
\]

(3)

Contrarily, the external potential \( U_{\text{ext}}(r_k, t) \) represents a single-particle (effective) potential that accounts for, e.g. the bias generated by an external battery [30], the effect of an external laser field (in the dipole approximation) [31], or the time-dependent potential generated by quasi-static nuclei (in the Born–Oppenheimer approximation) [32]. In the separation of the potential energy into Coulombic and external components, it is implicitly assumed that there are particles (other than the other particles) whose effect on the evolution of the state \( |\psi(t)\rangle \) can be effectively modeled through a single-particle potential \( U_{\text{ext}}(r_k, t) \). As will be discussed below, this separation plays a crucial role in the proper definition of the concepts of energy and power for open systems.

Let us now address the question of what is the energy associated with the system described by the state \( |\psi(t)\rangle \) (and obeying the effective Hamiltonian \( \hat{H}(t) \) in equation (1)). To correctly answer this question we must guarantee the following three requirements [16]:

\[
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\]
• For an isolated (conservative) system the energy must be conserved, i.e. \\
\langle \hat{E}_{\text{isolated}} \rangle = \text{constant}.

• If the system is not isolated, however, but is in an external time-dependent field which supplies power \( P(t) \), the definition of the energy and the power of the system must satisfy \\
d(\langle \hat{E}(t) \rangle)/dt = P(t).

• When the power supplied by the external field is zero, \( P(t) = 0 \), then \\
\langle \hat{E}(t) \rangle = \langle \hat{E}_{\text{isolated}} \rangle.

Such very simple arguments allow us to unequivocally define the energy associated to the \( N \) particles described by equation (1) as:

\[
\langle \hat{E}(t) \rangle = \langle \psi | (\hat{H} - \hat{U}_{\text{ext}}(t)) | \psi \rangle = \sum_k^N \int_{-\infty}^{+\infty} \mathbf{dr} \ \psi^* \mathbf{r}, t \left( \frac{1}{2} \sum_k^N \nabla_k^2 + U_{\text{cou}}(\mathbf{r}) \right) \psi(\mathbf{r}, t). \tag{4}
\]

The term \( \frac{1}{2} \sum_k^N \nabla_k^2 \) is the many-particle kinetic energy operator in the position representation, with \( \nabla_k^2 = \nabla k \cdot \nabla_k \) and \( \nabla_k = \mathbf{u}_x \frac{\partial}{\partial x_k} + \mathbf{u}_y \frac{\partial}{\partial y_k} + \mathbf{u}_z \frac{\partial}{\partial z_k} \) respectively the Laplacian and nabla operators in the position representation, and \( \{ \mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z \} \) are unitary vectors pointing respectively in the three directions of the physical space. In the language of thermodynamics of small quantum systems, equation (4) is commonly refereed to as the exclusive energy (to differentiate it from the inclusive energy defined through \\
\langle \psi | \hat{H} | \psi \rangle). For commodity, in the following we will simply refer to the exclusive energy \( \langle \psi | (\hat{H} - \hat{U}_{\text{ext}}(t)) | \psi \rangle \) defined in equation (4) as the local energy. Hereafter, we also use the definition \\
\mathbf{dr} = dx_1 \otimes dy_1 \otimes dz_1 \otimes .... \otimes dx_N \otimes dy_N \otimes dz_N.

To see that equation (4) represents the energy of the system, we only need to realize that the electrical power \( P(t) \) provided by the external field, \( U_{\text{ext}}(t) \), can be identified with the time-rate of change of the expectation value of the energy defined in equation (4), i.e.:

\[
P(t) = \frac{d}{dt} \langle \hat{E}(t) \rangle = i \langle [\hat{H}, \hat{K}] \rangle + i \langle [\hat{H}, \hat{U}_{\text{cou}}] \rangle = i \langle [\hat{U}(t), \hat{K}] \rangle + i \langle [\hat{K}, \hat{U}_{\text{cou}}] \rangle + i \langle [\hat{U}(t), \hat{U}_{\text{cou}}] \rangle = i \langle [\hat{U}_{\text{ext}}(t), \hat{K}] \rangle, \tag{5}
\]

where in the last equality we have used that the operators \( \hat{U}(t) \) and \( \hat{U}_{\text{cou}} \) commute. The commutator in the last equality of equation (5) (in the position representation) gives:

\[
P(t) = \frac{1}{2} \sum_k^N \int_{-\infty}^{+\infty} \mathbf{dr} (|\Psi|^2 \nabla_k^2 U_{\text{ext}} + 2\Psi^* (\nabla_k U_{\text{ext}})(\nabla_k \Psi)) = \frac{1}{2} \sum_k^N \int_{-\infty}^{+\infty} \mathbf{dr} (\nabla_k (|\Psi|^2 \nabla_k U_{\text{ext}}) - (\Psi^* \nabla_k \Psi)(\nabla_k U_{\text{ext}}) + (\Psi^* \nabla_k \Psi)(\nabla_k U_{\text{ext}})) = \sum_k^N \int_{-\infty}^{+\infty} \mathbf{dr} \mathbf{J}_k \cdot \mathbf{F}_{\text{ext}}. \tag{6}
\]
where in the last equality we used the Gauss theorem and we have defined the external force \( \mathbf{F}^{\text{ext}}(\mathbf{r}_k, t) = -\nabla U_{\text{ext}}(\mathbf{r}_k, t) \) and the \( k \)th component of the standard probability current density \( \mathbf{J}_k = \langle \hat{J}_k \rangle = \frac{-i}{\hbar} \langle \Psi^* \nabla_k \Psi - \Psi \nabla_k \Psi^* \rangle \) [19]. Notice that equation (6) corresponds to the standard definition of electrical power (see equation (3.6) in [18]).

The above discussion brings us to the main question of this work: what is the spatial distribution of the electrical energy \( \langle \hat{E}(t) \rangle \) and power \( P(t) \) found in equations (4) and (6)? As we will show in the remaining part of this section, answering this questions requires the use of local operators.

2.2. On the physical meaning of local operators

Consider an (arbitrarily) small volume \( \Omega \) (depicted in figure 1), which, for simplicity, has only two surfaces, \( S_4 \) and \( S_1 \), open to the transit of particles. We note that making all surfaces open to the flux of particles would make the notation very tedious without providing any additional insight. Given this volume \( \Omega \), we address now three very simple problems that will be proved to be helpful later in the derivation of our main results.

Let us first compute the probability of finding a particle \( k \) inside the volume \( \Omega \) (irrespective of where the rest of \( N - 1 \) particles are). According to Born’s rule, the probability of finding the \( N \) particles at positions \( \mathbf{r} = (\mathbf{r}_1, ..., \mathbf{r}_N) \) in the configuration space is \( \langle \psi | \hat{N}(\mathbf{r}) | \psi \rangle = |\psi(\mathbf{r}, t)|^2 \), where \( \hat{N}(\mathbf{r}) = |\mathbf{r}| \) is the position operator. Therefore, we can try to answer the question above about the particle \( k \) inside the volume \( \Omega \) by introducing a similar (position-like) operator:

\[
\hat{N}_k, \Omega = \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k |\mathbf{r}_k\rangle \langle \mathbf{r}_k| \otimes |\mathbf{r}_k\rangle \langle \mathbf{r}_k| = \mathbb{I}_k \otimes \int_{\Omega} d\mathbf{r}_k |\mathbf{r}_k\rangle \langle \mathbf{r}_k|,
\]

where we have defined \( \tilde{\mathbf{r}}_k = (\mathbf{r}_1, ..., \mathbf{r}_{k-1}, \mathbf{r}_{k+1}, ..., \mathbf{r}_N) \), \( |\tilde{\mathbf{r}}_k\rangle \langle \tilde{\mathbf{r}}_k| = |\mathbf{r}_1\rangle \langle \mathbf{r}_1| \otimes ... \otimes |\mathbf{r}_{k-1}\rangle \langle \mathbf{r}_{k-1}| \otimes |\mathbf{r}_{k+1}\rangle \langle \mathbf{r}_{k+1}| \otimes ... \otimes |\mathbf{r}_N\rangle \langle \mathbf{r}_N| \), and \( \tilde{\mathbf{r}}_k = \int_{\Omega} d\mathbf{r}_k |\mathbf{r}_k\rangle \langle \mathbf{r}_k| \). Notice that strictly speaking the order of the operators in the Kronecker product cannot be changed without changing its meaning. Nevertheless, changing the notation accordingly would make the presentation of the results cumbersome, and hence we assume from now on that the practical product ordering corresponds to the lexicographic ordering of subindices (i.e. the operator \( |\mathbf{r}_k\rangle \langle \mathbf{r}_k| \) acts on the \( k \)th degree of freedom independently of its order).

The expectation value of the operator in (7) provides the required information:

\[
\langle \hat{N}_k, \Omega(t) \rangle = \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k |\psi(\mathbf{r}, t)|^2.
\]

Notice that the above expectation value is valid either for fermions or bosons. For identical particles, the shape of the wavefunction imposes that \( \langle \hat{N}_k, \Omega(t) \rangle = \langle \hat{N}_j, \Omega(t) \rangle \) for any \( j \neq k \), and thus particles cannot be distinguished one from each other.

We now move to a second illustrative example. We want to compute the expectation value of the \( k \)th component of the probability current density given that the \( k \)th particle is sitting inside the volume \( \Omega \) (independently of the location of the rest of particles). We know that the current density operator can be written
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Figure 1. Schematic representation of the open volume Ω in which the local energy and power are calculated. The volume Ω interchanges energy and particles with the outside. For simplicity, we consider the surfaces S1 and S4 open to the transit of particles, while in the rest of the surfaces a vanishing wavefunction is considered. The total number of particles inside and outside Ω is N, but only some of them contribute to the energy and power inside Ω.

as \( \hat{J}_k(r) = \frac{1}{2}( |r_k\rangle \langle r_k| \otimes |r_k\rangle \langle r_k| \hat{P}_k + |r_k\rangle \langle r_k| \hat{P}_k^\dagger |r_k\rangle \langle r_k| ) \) and its expectation value simply reads \( \langle \hat{J}_k(r, t) \rangle = \frac{1}{2}( \psi^\dagger \nabla_k \psi - \psi \nabla_k \psi^\dagger ) \) [19]. Similarly, we can define the following local current operator:

\[
\hat{J}_{k,\Omega} = \frac{1}{2} \int_\Omega d\mathbf{r}_k \int_\Omega d\mathbf{r}_k |r_k\rangle \langle r_k| \otimes ( |r_k\rangle \langle r_k| \hat{P}_k + \hat{P}_k^\dagger |r_k\rangle \langle r_k| )
\]

\[
= \mathbf{i}_k \otimes \frac{1}{2} \int_\Omega d\mathbf{r}_k ( |r_k\rangle \langle r_k| \hat{P}_k + \hat{P}_k^\dagger |r_k\rangle \langle r_k| )
\]

(9)

whose expectation value provides the requested information, i.e.:

\[
\langle \hat{J}_{k,\Omega} \rangle = \frac{-i}{2} \int_\infty \int_\Omega d\mathbf{r}_k d\mathbf{r}_k ( \psi^\dagger (\mathbf{r}, t) \nabla_k \psi (\mathbf{r}, t) - \psi (\mathbf{r}, t) \nabla_k \psi^\dagger (\mathbf{r}, t) )
\]

(10)

Finally, in a third example, we discuss the operator that provides the probability of finding two particles, say the \( k \)th and \( j \)th particles, inside the volume \( \Omega \) no matter where the other particles are. We define such operator to be:

\[
\hat{I}_{k,j,\Omega} = \int_\infty \int_\Omega d\mathbf{r}_k, d\mathbf{r}_k |\mathbf{r}_k, \mathbf{r}_k\rangle \langle \mathbf{r}_k, \mathbf{r}_k| \otimes |r_k\rangle \langle r_k| \otimes |r_j\rangle \langle r_j|
\]

\[
= \mathbf{i}_{k,j} \otimes \int_\Omega d\mathbf{r}_k, d\mathbf{r}_k |\mathbf{r}_k, \mathbf{r}_k\rangle \langle \mathbf{r}_k, \mathbf{r}_k| \otimes |r_k\rangle \langle r_k| \otimes |r_j\rangle \langle r_j|
\]

(11)

where we have now defined \( \bar{\mathbf{r}}_{k,j} = (\mathbf{r}_1, \ldots, \mathbf{r}_{k-1}, \mathbf{r}_{k+1}, \ldots, \mathbf{r}_{j-1}, \mathbf{r}_{j+1}, \ldots, \mathbf{r}_N) \), \( |\bar{\mathbf{r}}_{k,j}\rangle = \cdots \otimes |\mathbf{r}_{k-1}\rangle \otimes |\mathbf{r}_{k+1}\rangle \otimes \cdots \otimes |\mathbf{r}_{j-1}\rangle \otimes |\mathbf{r}_{j+1}\rangle \otimes \cdots \) and \( \mathbf{i}_{k,j} = \int_\infty d\mathbf{r}_{k,j} |\bar{\mathbf{r}}_{k,j}\rangle \langle \bar{\mathbf{r}}_{k,j}| \). The expectation value of the operator in equation (11) provides the desired information, i.e.:
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\[ \langle \hat{\Pi}_{k,\Omega}(t) \rangle = \int_{\infty}^{t} d\tau_k \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j \psi(\mathbf{r}, t)^2. \] (12)

The above three examples will be very helpful in our definition of the local energy. In particular, the last example above will be relevant in the definition of the internal (two-particle) Coulombic operator.

3. Spatial distribution of energy

We are now in a position to derive an expression for the local energy operator. Let us first define such an operator, generically, as the sum of a local kinetic energy operator and a local potential energy operator, i.e.: \( \hat{\mathcal{E}}_\Omega = \hat{\mathcal{K}}_\Omega + \hat{\mathcal{C}}_\Omega \). Below we discuss separately these two operators \( \hat{\mathcal{K}}_\Omega \) and \( \hat{\mathcal{C}}_\Omega \).

3.1. Local kinetic energy operator

Taking advantage of the example for the local current density operator in equation (9), we here define the (Hermitian) local kinetic energy operator \( \hat{\mathcal{K}}_\Omega \) associated to the volume \( \Omega \) as:

\[ \hat{\mathcal{K}}_\Omega = \frac{1}{4} \sum_k N_k \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k (|\mathbf{r}_k \rangle \langle \mathbf{r}_k | \otimes |\mathbf{r}_k \rangle \langle \mathbf{r}_k | \hat{\mathbf{p}}_k^2 + |\mathbf{r}_k \rangle \langle \mathbf{r}_k | \hat{\mathbf{p}}_k^2 |\mathbf{r}_k \rangle \langle \mathbf{r}_k |) \]

\[ = \mathbf{1}_k \otimes \frac{1}{4} \sum_k N_k \int_{\Omega} d\mathbf{r}_k (|\mathbf{r}_k \rangle \langle \mathbf{r}_k | \hat{\mathbf{p}}_k^2 + \hat{\mathbf{p}}_k^2 |\mathbf{r}_k \rangle \langle \mathbf{r}_k |). \] (13)

The above operator provides the expectation value of the kinetic energy comprised in the (two-terminal) open volume \( \Omega \):

\[ \langle \hat{\mathcal{K}}_\Omega \rangle = \text{Real} \left( \frac{-1}{2} \sum_k N_k \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k \psi^*(\mathbf{r}, t) \nabla_k^2 \psi(\mathbf{r}, t) \right). \] (14)

Equation (14) accounts for any \( k \)th particle contribution to the kinetic energy in the volume \( \Omega \) independently of where the rest of the \( N-1 \) particles reside. Notice that an alternative definition of the local kinetic energy operator could have been: \( \frac{1}{4} \sum_k N_k \int_{\Omega} d\mathbf{r}(\mathbf{r}) \langle \mathbf{r} | \hat{\mathbf{p}}_k^2 + \hat{\mathbf{p}}_k^2 |\mathbf{r} \rangle \). However, such a local operator does not provide the desired information, i.e. its expectation value would be only different from zero in those situations where the support of all one-dimensional reduced probability densities \( \rho_k(\mathbf{r}_k, t) = \int_{\infty}^{t} d\mathbf{r}_k |\Psi|^2 \) simultaneously intersect the volume \( \Omega \).

In view of equation (14), it is worth noting that in classical mechanics the increment of the \( k \)th particle kinetic energy is always reflected into the increase of its associated electrical current. That is not the case in quantum mechanics, where the expectation values of the kinetic energy and current density are not directly related. To better appreciate this important point, following the hydrodynamic formulation of the
wavefunction \cite{20–23}, it is useful to introduce the polar expression of the wavefunction \( \Psi(\mathbf{r}, t) = R(\mathbf{r}, t)e^{iS(\mathbf{r}, t)} \) into equation (14). Then, we find:

\[
\langle \hat{K}_\Omega \rangle = \text{Real} \left( -\frac{1}{2} \sum_k^N \int_\infty^\infty d\mathbf{r}_k \int_\Omega d\mathbf{r}_k \left( R\nabla_k^2 R + i\nabla_k(R^2 \nabla_k S) - R^2(\nabla_k S)^2 \right) \right),
\]

which, by keeping the real part only, can be rewritten as:

\[
\langle \hat{K}_\Omega \rangle = \sum_k^N \int_\infty^\infty d\mathbf{r}_k \int_\Omega d\mathbf{r}_k R^2 \left( Q_k + \frac{(\nabla_k S)^2}{2} \right),
\]

where \( Q_k(\mathbf{r}, t) = -\nabla_k^2 R(2R) \) is the \( k \)th component of the so-called quantum potential \cite{20–23}, which is closely related to the most common concept of quantum pressure that arises in the hydrodynamical formulation of the motion of a quantum fluid \cite{22, 24}. A real time-independent quantum state, i.e. with current density equal to zero, does still contribute to equation (16) in the form of \( Q_k \). This point will be discussed in more detail in section 3.3.

### 3.2. Local Coulombic energy operator

In order to define the operator related with the potential energy associated to the volume \( \Omega \), we now rely on the third example introduced in section 2.2. The operator in equation (11) was designed to provide the probability of finding simultaneously two particles \( k \) and \( j \) at the same time in the volume \( \Omega \), irrespective of the position of the other \( N - 2 \) particles. Because the Coulombic interaction is defined through a two-particle potential energy operator, \( \hat{U}_{j,k} \), we can define the potential energy in the volume \( \Omega \) in terms of the following operator:

\[
\hat{C}_\Omega = \sum_k^N \sum_{j > k} \int_\infty^\infty d\mathbf{r}_{j,k} \int_\Omega d\mathbf{r}_j \int_\Omega d\mathbf{r}_k |\psi(\mathbf{r}, t)|^2 \hat{U}_{j,k}(\mathbf{r}_j, \mathbf{r}_k).
\]

The expectation value of the above operator represents a measure of the internal (Coulombic) energy in the volume \( \Omega \), i.e.:

\[
\langle \hat{C}_\Omega \rangle = \sum_k^N \sum_{j > k} \int_\infty^\infty d\mathbf{r}_{j,k} \int_\Omega d\mathbf{r}_j \int_\Omega d\mathbf{r}_k |\psi(\mathbf{r}, t)|^2 U_{j,k}(\mathbf{r}_j, \mathbf{r}_k),
\]

which can be written in terms of the hydrodynamic form of the wavefunction as:

\[
\langle \hat{C}_\Omega \rangle = \sum_k^N \sum_{j > k} \int_\infty^\infty d\mathbf{r}_{j,k} \int_\Omega d\mathbf{r}_k \int_\Omega d\mathbf{r}_j R^2 U_{j,k}(\mathbf{r}_j, \mathbf{r}_k).
\]

By virtue of equation (19), only the potential energy associated to pairs of particles both lying in the volume \( \Omega \) is taken into account. In other words, the potential energy associated to the (Coulomb) interaction of a pair of particles, one sitting in the volume \( \Omega \) and the other one outside, is considered to be external, and thus, it does not contribute to the sum in equation (19).
This particular way of defining the potential energy operator in equation (17) will be proved correct later. Here, we motivate its definition by discussing a particular example where an electronic device is biased by the action of an external electrical field. Roughly speaking, the battery providing the given bias can be understood as ultimately made of a large number of particles. In fact, it is the action of all particles conforming the battery on the electrons of the electronic device what is regarded in a practical way as the bias. The reason why we commonly call this bias external potential is simply because we are not considering the particles of the battery among the simulated particles, and hence the (exclusive) energy associated to our system (e.g. the conduction electrons) does not include the energy of the battery. Therefore, coming back to our problem, when we look at the volume $\Omega$ as our system of interest (i.e. the local region where we want to compute the energy and power), all particles outside this region play the role of an additional external field that is added up to the external field $U_{\text{ext}}(t)$.

### 3.3. On the physical meaning of the local expectation value of the energy

We can now gather equations (16) and (19) to write an expression for the expectation value of the local energy in the volume $\Omega$, i.e.:

$$
E_{\Omega}(t) = \langle \hat{E}_\Omega \rangle = \sum_k^N \int_{-\infty}^{\infty} d\bar{r}_k \int_{\Omega} d\mathbf{r}_k R_k^2 \left( Q_k + \frac{(\nabla_k S)^2}{2} \right) + \sum_k^N \sum_{j>k}^N \int_{-\infty}^{\infty} d\bar{r}_{j,k} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j R_{j,k}^2 U_{j,k}.
$$

(20)

To gain some physical insight into the meaning of equation (20), we can first consider its classical limit [25] by just eliminating any contribution associated to the quantum potential $Q_k$, and reinterpreting $\nabla_k S$ as the (local) $k$th particle velocity field, i.e.:

$$
E_{\Omega,\text{class}}(t) = \sum_k^N \int_{-\infty}^{\infty} d\bar{r}_k \int_{\Omega} d\mathbf{r}_k R_{\text{class}}^2 \frac{(\nabla_k S_{\text{class}})^2}{2} + \sum_k^N \sum_{j>k}^N \int_{-\infty}^{\infty} d\bar{r}_{j,k} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j R_{\text{class}}^2 U_{j,k}.
$$

(21)

According to classical statistical mechanics [25], an ensemble of (scalar) charged particles can be described by a wavefunction $\Psi_{\text{class}} = R_{\text{class}}e^{iS_{\text{class}}}$, where the phase $S_{\text{class}}(\mathbf{r}, t)$ is nothing but the action defined through the classical Hamilton–Jacobi equation, and $R_{\text{class}}(\mathbf{r}, t)$ obeys a classical continuity equation [21, 25]. The classical expression in equation (21) allows us to regard the term $R^2 Q_k$ in equation (20) as an explicit signature of the quantum nature of our many-body system. In this regard, to better understand the role played by the quantum potential $Q_k$ in equation (20), let us neglect the Coulomb interaction and consider a separable many-particle wavefunction $\psi(\mathbf{r}, t) = \psi_1(x_1)\ldots\psi_N(z_N)e^{i\xi t}$. Then, we can gain some insight into the meaning of the term $R^2 Q_k$ by considering the following two examples:
(i) Let us assume first that each single-particle state can be represented through a plane wave $\psi_{k,x}(x) = e^{i p_{k,x} x}$ with momentum $p_{k,x}$. For a plane wave $R_{k,x} = cte$, and then $Q_{k,x} = 0$. Furthermore, since $S_{k,x} = p_{k,x} x_k$, then $(\nabla_k S)^2 / 2 = (p_{k,x}^2 + p_{k,y}^2 + p_{k,z}^2) / 2$ and $J_k = R^2(p_{k,x} u_x + p_{k,y} u_y + p_{k,z} u_z)$. Therefore, in the limit where $Q_k = 0$ (for any $k$), the expectation value of the kinetic energy is proportional to the current density.

(ii) Alternatively, consider the single-particle states $\psi_{k,x}(x)$ to be eigenfunctions of a (infinite) quantum well. Such states do not carry current density because their associated wavefunctions are real. In this respect, the expectation value of the kinetic energy operator is still different from zero but now equal to the quantized energy levels that the states are occupying. Therefore, as shown in equation (16), it is possible to increase the kinetic energy without modifying the current density. Notice that this very simple example has no classical counterpart.

Therefore, in general, the expectation value of the (local) kinetic energy includes a classical-like contribution directly related to the current density, and a non-classical component associated to the quantum potential. This is a well-known result in the context of a hydrodynamical formulation of quantum mechanics [20–23]. Finally, notice that in the limit $\Omega \to \infty$, equation (20) simply reduces to the expectation value of equation (4).

4. Spatial distribution of power

We finally jump into the question of what is the spatial distribution of power. As already mentioned, such a local quantity must be consistent with the definition of the local energy in equation (20). In particular we must guarantee that:

$$P_{\Omega}(t) = \langle \hat{P} \rangle = \frac{d}{dt} \langle \hat{E}_\Omega \rangle. \quad (22)$$

We can certainly look for an operator $\hat{P}$ that obeys the above equation, but it seems much practical here to directly evaluate the time-derivative of the expectation value of the local energy. This is precisely what we will do in the following section.

4.1. Expectation value of local power

The time-derivative of the expectation value of the local energy in equation (20) reads:

$$P_{\Omega}(t) = \frac{d}{dt} \langle \hat{E}_\Omega \rangle = \frac{d}{dt} \left( \hat{K}_\Omega + \hat{C}_\Omega \right)$$

$$= \sum_{k=1}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k \frac{\partial R^2}{\partial t} \left( Q_k + \frac{(\nabla_k S)^2}{2} \right)$$

$$+ \sum_{k=1}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k R^2 \left( \frac{\partial Q_k}{\partial t} + (\nabla_k S) \cdot (\nabla \nabla S) \right)$$

$$+ \sum_{k=1}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_k \frac{\partial R^2}{\partial t} U_{j,k}. \quad (23)$$

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Equation (23) already contains the information we are looking for. Nonetheless, in order to understand the physical meaning of its main building-blocks, in the following we will manipulate it in order to get a more comprehensive result.

By introducing the mentioned hydrodynamic form of the wavefunction $\Psi = R e^{iS}$ into equation (1) and then separating into imaginary and real parts, one gets respectively a continuity equation for the full probability density:

$$\frac{\partial R^2}{\partial t} + \sum_j \nabla_j \cdot J_j = 0,$$

and a quantum Hamilton–Jacobi-like equation for the full phase [20–23]:

$$\frac{\partial S}{\partial t} + U + \sum_j \frac{N}{2} (\nabla_j S)^2 = 0.$$

Let us notice that equation (25) can be written in a more standard way by introducing a further spatial differentiation and defining a stress tensor through the gradient of the quantum potential. This leads to the equation of motion for a quantum fluid [24]. Hereafter, it will be nonetheless convenient to use equation (25) and its definition in terms of the quantum potential. Introducing equations (24) and (25) into equation (23) we find:

$$P_\Omega(t) = -\sum_k \int_{\infty}^t d\bar{r}_k \int_{\Omega} dr_k \nabla_k \left( R^2(\nabla_k S) Q_k + R^2(\nabla_k S) \left( \frac{(\nabla_k S)^2}{2} \right) \right)$$

$$+ \sum_k \int_{\infty}^t d\bar{r}_k \int_{\Omega} dr_k \sum_{\xi} R^2(\nabla_\xi S)(\nabla_\xi Q_k)$$

$$+ \sum_k \int_{\infty}^t d\bar{r}_k \int_{\Omega} dr_k R^2 \frac{dQ}{dt}$$

$$- \sum_k \int_{\infty}^t d\bar{r}_k \int_{\Omega} dr_k R^2(\nabla_k S)(\nabla_k U_{\text{ext}})$$

$$- \sum_k \int_{\infty}^t d\bar{r}_k \int_{\Omega} dr_k R^2(\nabla_\xi S) \left( \nabla_k \sum_j \sum_{\xi>j} U_{j,\xi} \right)$$

$$- \sum_k \int_{\infty}^t d\bar{r}_k \int_{\Omega} dr_k R^2(\nabla_\xi S) \left( \nabla_\xi \sum_j Q_j \right)$$

$$- \sum_k \sum_{j>k} \int_{\infty}^t d\bar{r}_{j,k} \int_{\Omega} dr_k \int_{\Omega} dr_j \sum_{\xi} (\nabla_j J_\xi) U_{k,j}.$$  

The above equation can be greatly simplified if one defines an external force,

$$F_{\text{ext}}(r_k, t) = -\nabla_k U_{\text{ext}}(r_k, t),$$
the \(k\)th component of the Coulomb force,
\[
F_{k}^{\text{cou}}(r) = -\nabla_k \sum_{j=1}^{N} \sum_{\xi>j} U_{j,\xi},
\]
and the \(k\)th component of a quantum force,
\[
F_{k}^{\text{qua}}(r, t) = -\nabla_k Q(r, t),
\]
that arises in the context of a hydrodynamical representation of the wavefunction due to the presence of the (full) quantum potential \(Q(r, t) = \sum_{\xi=1}^{N} Q_{\xi}(r, t)\) [21, 23]. Taking into account these force definitions and rewriting the first term on the rhs of equation (26) by using the Gauss theorem, we can write:
\[
P_\Omega(t) = -\sum_{k}^{N} \int_{\Omega} \text{d}r \left[ u_x \cdot J_k \left( Q_k + \left( \frac{\nabla_k S^2}{2} \right) \right) \right]_{S^4}^{\Omega}
\]
\[
+ \sum_{k}^{N} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} J_k \cdot (\nabla_\xi Q_k)
\]
\[
+ \sum_{k}^{N} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' R^2 \frac{dQ}{dt}
\]
\[
+ \sum_{k}^{N} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \left[ (F^{\text{ext}} + F_{k}^{\text{ext}} + F_{k}^{\text{qua}}) - \sum_{k \neq j}^{N} \sum_{\xi} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} \nabla_\xi (J_k U_{k,j}) \right]
\]
\[
+ \sum_{k \neq j}^{N} \sum_{\xi} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} \nabla_\xi U_{k,j},
\]
where we have used the following definition \([f(r)]_{S^4}^{\Omega} = \int \text{d}y_k \text{d}z_k f(r)|_{y_k=x_{S^4}} - \int \text{d}y_k \text{d}z_k f(r)|_{y_k=x_{S^4}},\]
and \(u_x \cdot J_k\) is the longitudinal component of the \(k\)th component of the current probability density. Furthermore, we can use the following two identities. First,
\[
\sum_{k}^{N} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} J_k \cdot F_{k}^{\text{cou}} = \sum_{k \neq j}^{N} \sum_{\xi} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} \nabla_\xi U_{k,j}
\]
\[
= \sum_{k}^{N} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} J_k \cdot F_{k}^{\text{cou,ext}},
\]
where we have defined the Coulombic force generated by all particles outside the volume \(\Omega\) on the \(k\)th particle as \(F_{k}^{\text{cou,ext}}(r) = -\nabla_k \sum_{j=k}^{N} U_{k,j}^{\text{ext}},\) being \(U_{k,j}^{\text{ext}} = U_{k,j}\theta(x_j - x_{S^4})\theta(x_{S^4} - x_j).\)
And second:
\[
\sum_{k \neq j}^{N} \sum_{\xi} \int_{\Omega} \text{d}r \int_{\Omega} \text{d}r' \sum_{\xi} \nabla_\xi (J_k U_{k,j}) = \sum_{k}^{N} \int_{\Omega} \text{d}r \left[ u_x \cdot J_k \left( \sum_{j \neq k}^{N} U_{j,k}^{\text{int}} \right) \right]_{S^4}^{\Omega},
\]
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where we have defined the internal potential energy $U^\text{int}_{k,j} = U_{k,j} \theta(x_{S1} - x_j) \theta(x_j - x_{S4})$. Using equations (31) and (32) we already attain the second main result of this work:

$$P_{\Omega}(t) = \sum_{k}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j \mathbf{J}_k \cdot (\mathbf{F}^\text{ext} + \mathbf{F}^\text{con,ext} + \mathbf{F}^\text{qua}_k)$$

$$- \sum_{k}^{N} \int_{\Omega} d\mathbf{r}_k \left[ \mathbf{u}_k \cdot \mathbf{J}_k \left( Q_k \frac{(\nabla_k S)^2}{2} + \sum_{j}^{N} U^\text{int}_{k,j} \right) \right]_{S4}^{S1}$$

$$+ \sum_{k}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j R^2 \frac{\partial Q_k}{\partial t}$$

$$+ \sum_{k}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j \left( \sum_{j}^{N} \mathbf{J}_j \cdot \nabla_j Q_k \right),$$  \hspace{1cm} (33)

The power transferred by an external (effective) force to an ensemble of (scalar) charged particles can be locally resolved according to equation (33). In the following section we discuss term by term the physical soundness of the above result.

4.2. On the physical meaning of the expectation value of local power

First of all, and as we did for the local energy in equation (20), we perform a first test of validity for equation (33) by taking the (previously introduced) classical limit [25]. By simply setting the quantum potential $Q_k$ to zero we get:

$$P_{\Omega,\text{class}}(t) = \sum_{k}^{N} \int_{\Omega} d\mathbf{r}_k \int_{\Omega} d\mathbf{r}_j \mathbf{J}_{k,\text{class}} \cdot (\mathbf{F}^\text{ext} + \mathbf{F}^\text{con,ext}_k)$$

$$- \sum_{k}^{N} \int_{\Omega} d\mathbf{r}_k \left[ \mathbf{u}_k \cdot \mathbf{J}_{k,\text{class}} \left( \frac{(\nabla_k S_{\text{class}})^2}{2} + \sum_{j}^{N} U^\text{int}_{k,j} \right) \right]_{S4}^{S1},$$  \hspace{1cm} (34)

where $\mathbf{J}_{k,\text{class}} = R_{\text{class}} \nabla_k S_{\text{class}}$ according to the classical wavefunction $\Psi_{\text{class}} = R_{\text{class}} e^{iS_{\text{class}}}$ [21, 25]. The first term in equation (34) corresponds to the standard definition of power as the product of the current by the external force, $\mathbf{J}_k \cdot \mathbf{F}^\text{ext}$ [18]. Here, however, as already discussed in section 3.2, particles outside $\Omega$ are effectively contributing to the external field in the form of $\mathbf{J}_k \cdot \mathbf{F}^\text{con,ext}_k$. The second term in equation (34) simply arises because the volume $\Omega$ is finite, i.e. energy (both kinetic and Coulombic) can flow across the surfaces $S1$ and $S4$ along with the charged particles.

In our discussion of equation (33), we are now left with all pure quantum contributions to the local power. Let us first focus on the current-force correlation $\mathbf{J}_k \cdot \mathbf{F}^\text{qua}_k$ included in the first term of equation (33). This term accounts for the fact that time variations of the kinetic energy in the volume $\Omega$ can be also due to the work done by a force with no classical counterpart. More specifically, according to our hydrodynamical language [20–23], the quantum force $\mathbf{F}^\text{qua}_k$ is responsible for those changes in
the current density that are not directly associated to the action of an electrical force [28]. Consider, e.g. a electron impinging into a double barrier structure. It can happen that at later times the electron occupies a resonant state of the double barrier, and thus its associated current density decreases significantly. Such a damping effect is due (not to the action of an external or Coulombic force, but) to the quantum force $F_{k}^{\text{qua}}$, which accounts for the confining effects within the double barrier [26, 27, 29]. Notice that, due to the finite nature of the volume $\Omega$, in addition to these quantum current-force correlations, the quantum force is accompanied by the flux of quantum potential energy across the surfaces $x = S4$ and $x = S1$ (which is included in the second term of equation (33)). Finally, the third and fourth terms in equation (33) arise because of the explicit time variations of the quantum potential energy density $R^2Q_k$ in the volume $\Omega$. While the third term accounts for time variations of the quantum potential $Q_k$, the fourth term rates the change on the quantum potential energy due to the rearrangement of all particle positions.

In the remaining part of the manuscript we consider a clarifying limit of our expression in equation (33). We want to take the limit, $\Omega \to \infty$, where we implicitly assume that the extension of the support of the many-particle wavefunction is finite (for $r^2R^2 \to 0$ as $r \to \infty$). In order our local energy definition in equation (20) (and hence our finding in equation (33)) to be correct, in this limit we should recover equation (6). We will mathematically denote this closed-system limit as $\Omega \to \infty$. Equation (33) now reads:

$$P(t) = \sum_{k}^{N} \int_{\infty} \text{d}r J_{k} \cdot (F_{k}^{\text{ext}} + F_{k}^{\text{con,ext}} + F_{k}^{\text{qua}})$$

$$- \sum_{k}^{N} \int_{\infty} \text{d}r \left[ u_{k} \cdot J_{k} \left( Q_{k} + \frac{(\nabla_{k} S)^2}{2} + \sum_{j \neq k}^{N} U_{k,j}^{\text{int}} \right) \right]_{S4}^{S1}$$

$$+ \sum_{k}^{N} \int_{\infty} \text{d}r R^2 \frac{\partial Q_{k}}{\partial t} + \sum_{k,j}^{N} \int_{\infty} \text{d}r (J_{j} \cdot \nabla_{j} Q_{k}).$$

(35)

The second term in equation (35) simply vanishes because $r^2R^2 \to 0$ as $r \to \infty$. In addition, the following three equalities hold:

$$\sum_{k}^{N} \int_{\infty} \text{d}r J_{k} \cdot F_{k}^{\text{qua}} = - \sum_{k,j}^{N} \int_{\infty} \text{d}r J_{k} \cdot \nabla_{k} Q_{j}$$

$$= - \sum_{k,j}^{N} \int_{\infty} \text{d}r J_{j} \cdot \nabla_{j} Q_{k},$$

(36)

and

$$\sum_{k}^{N} \int_{\infty} \text{d}r J_{k} \cdot F_{k}^{\text{con,ext}} = 0,$$

(37)

Note that the closed system limit can be equivalently taken in two different ways: either we place the surfaces $S4$ and $S1$ far enough such that the full wavefunction vanishes there, or we make $x_{S4} = x_{S1}$ (for periodic systems).
and
\[
\int_\infty \! dR^2 \frac{\partial Q_k}{\partial t} = -\frac{1}{2} \int_\infty \! dR^2 \frac{\partial}{\partial t} \left( \frac{\nabla^2 R}{R} \right) = -\frac{1}{2} \int_\infty \! dR \nabla_k \left( R \nabla_k \frac{\partial R}{\partial t} - \frac{\partial R}{\partial t} \nabla_k R \right) = 0.
\]

Introducing the above three equalities into equation (35), the expectation value of the total power finally reduces to:
\[
P(t) = \sum_k N \int_\infty \! dR \textbf{J}_k \cdot \textbf{F}^{ext}.
\]

Therefore, for the (full) closed quantum system we recover the classical-like expression already found in equation (6). Equation (39) does only include the single-particle classical force \( \textbf{F}^{ext} \). Many-body effects are now only implicit in the many-body current components \( \textbf{J}_k \), and non-local effects originating from the time derivative of the quantum potential \( Q_k \) just canceled out. Therefore, the above limit demonstrates that any explicit many-body or quantum signature found in equation (33) originates only because of the openness of the volume \( \Omega \).

5. Conclusions

In this work we derived exact expressions for the spatial distribution of energy and power for quantum systems consisting of \( N \) (interacting) charged particles in an effective (driving or dissipative) electric field. Expectation values of the local energy and the local power, found respectively in equations (20) and (33), are the main results of this work. Our final results were written in terms of an arbitrarily small volume \( \Omega \), and interpreted from the quantum hydrodynamic point of view. Such a representation was proved to be helpful in the understanding of the main building-blocks of equations (20) and (33).

The expectation value of the local (or exclusive energy if preferred) energy in equation (20) comprises two terms: the kinetic and the potential energy contributions, which are respectively represented by the local operators derived in equations (13) and (17). The expectation value of the local kinetic energy in equation (16) can be further decomposed into a classical-like term, which is directly related to the current probability density, and a non-classical term, which is linked to the so-called quantum potential. The expectation value of the local potential energy in equation (19) is the sum of contributions associated to pairs of particles laying (both) in the volume \( \Omega \).

The expectation value of local power in equation (33), was found to consist of four main terms. Classical-like contributions, explicitly written in equation (34), are represented by single-particle and many-body current-force correlations respectively of the form \( \textbf{J}_k \cdot \textbf{F}^{ext} \) and \( \textbf{J}_k \cdot \textbf{F}_{\text{cont.}ext} \), and accompanied by the flow of (classical) energy across the surfaces \( S4 \) and \( S1 \). Explicit quantum contributions to the local power were proved to be directly linked to the quantum potential concept. In this respect, the quantum
potential contributes to the local power not only in the form of purely quantum current-force correlations $\mathbf{J}_k \cdot \mathbf{F}_{\text{qua}}$ and the inflow/outflow of quantum energy across the borders of the volume $\Omega$, but also, non-locally, through time variations of its associated energy density, which lead to the last two terms in equation (33).

The soundness of our results in equations (20) and (33) was first proven in relation to the classical limit $Q \to 0$, which lead to equations (21) and (34) respectively. Might be more intriguing was the closed system limit $\Omega \to \infty$. In particular, this limit greatly simplified the final expression for the total power by reducing it to the well-known expression in equation (6) (or equivalently equation (39)). In this respect, an interesting conclusion of our work is that both quantum and many-body features, explicitly manifested in the expression for the local power in equation (33), cannot be distinguished anymore when power is integrated all over the physical space. Non-locality and many-body correlations arising in equation (33) will be numerically studied in future works for low-dimensional system of interest, targeting low-power and energy harvesting nanoscale devices.

We want to finally stress that neither irreversible processes nor thermodynamical arguments were considered in this work. Nonetheless, local power for a quantum system has been shown to reveal intriguing features that we also expect to occur in irreversible (dissipative) quantum processes.

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References

[1] Solinas P, Averin D V and Pekola J P 2013 Phys. Rev. B 87 060508
[2] Salmilehto J, Solinas P and Möttönen M 2014 Phys. Rev. E 89 052128
[3] Venkatesh B P, Watanabe G and Talkner P 2015 New J. Phys. 17 075018
[4] Talkner P and Hänggi P 2016 Phys. Rev. E 93 022131
[5] Campisi M, Hänggi P and Talkner P 2011 Rev. Mod. Phys. 83 771
[6] Tian B, Zheng X, Kempa T J, Fang Y, Yu N, Yu G, Huang J, Lieber C M 2007 Nature 449 885
[7] Chang H-Y et al 2013 ACS Nano 7 5446
[8] Wang H et al 2012 Nano Lett. 12 4674
[9] Gu L et al 2012 Nano Lett. 13 91
[10] Qin Y, Xudong W and Zhong L W 2008 Nature 451 809
[11] Yang K-H 1983 J. Phys. A: Math. Gen. 16 935
[12] Phillips W D 1998 Rev. Mod. Phys. 70 721
[13] D’Agosta R and Di Ventra M 2008 J. Phys.: Condens. Matter 20 374102
[14] D’Agosta R, Sai N and Di Ventra M 2006 Nano Lett. 6 2935
[15] Tsutsui M, Kawai T and Taniguchi M 2012 Sci. Rep. 2 217
[16] Kobe D H and Yang K-H 1987 Eur. J. Phys. 8 236
[17] Zvi I et al 2008 Nat. Nanotechnol. 3 727
[18] Kobe D H, Wen E C-T and Yang K-H 1982 Phys. Rev. D 26 1927
[19] Cohen-Tannoudji C, Diu B and Laloe F 2009 Quantum Mechanics vol 1 (New York: Wiley)
[20] Holland P R 1995 The Quantum Theory of Motion: An Account of the de Broglie–Bohm Causal Interpretation of Quantum Mechanics (Cambridge: Cambridge University Press)
[21] Oriols X and Mompart J (ed) 2012 Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology (Singapore: Pan Stanford Publishing)
[22] Wyatt R 2005 Quantum Dynamics with Trajectories: Introduction to Quantum Hydrodynamics (New York: Springer)
[23] Benseny A, Albareda G, Sanz A S, Mompart J and Oriols X 2014 Eur. Phys. J. D 68 1
[24] Di Ventra M 2008 Electrical Transport in Nanoscale Systems (Cambridge: Cambridge University Press)
[25] Rosen N 1964 Am. J. Phys. 32 377
[26] Albareda G, Marian D, Benali A, Yaro S, Zanghi N and Oriols X 2013 J. Comput. Electron. 12 405
[27] Albareda G, Suñé J and Oriols X 2009 Phys. Rev. B 79 1
[28] Albareda G, Traversa F L, Benali A and Oriols X 2012 Fluctuation Noise Lett. 11 1242008
[29] Traversa F L et al 2011 IEEE Trans. Electron Devices 58 2104
[30] Albareda G, Benali A and Oriols X 2013 J. Comp. Electron. 12 730
[31] Albareda G, Suñé J and Oriols X 2009 Phys. Rev. B 79 1
[32] Albareda G, Bofill J M, Tavernelli I, Huarte-Larrañaga F, Illas F and Rubio A 2015 J. Phys. Chem. Lett. 6 1529

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