

Force and pressure in many-particle quantum dynamics

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Abstract

The Newtonian concept of force may be useful in some aspects of the dynamics of many-particle quantum systems such as fissioning nuclei. Following Ehrenfest's method, we show that the quantum kinetic force between parts of an extended quantum system can be described by an operator acting on the boundary between the two subsystems. The contribution to the force due to a short-ranged particle interaction can also be treated in the same way. This includes interaction effects treated in density functional theory by local functionals. The force operators are applied to several simple models to demonstrate the method.

I. INTRODUCTION

Ehrenfest's celebrated theorem showed that the classical Newton concept of force applies equally well to the acceleration of isolated quantum systems, but what about forces between parts of extended quantum systems? The question is relevant to the description of the dynamics of nuclear fission. At some point the nucleus is elongated into a shape resembling the nascent fission fragments joined by a small neck. The Coulomb force between the two nascent fragments is counterbalanced by an attractive nuclear force transmitted through the neck region; scission only occurs when neck force is sufficiently weakened.

In this work, we show that in an extended system the quantum force of one part on the rest can be consistently defined. In general, the interaction has long-range components such as the Coulomb and short-range ones such as the exchange-correlation energy in density-functional theory. Except for the long-range components of the interaction, the force reduces to an operator acting at the interface between the two subsystems. The operator contains derivatives of the wave function at the interface due to the kinetic term in the Hamiltonian.

We first consider the Schrödinger equation for a particle in one dimension. We then generalize the operator scope to many-particle systems in three dimensions.

II. PARTICLE IN ONE DIMENSION

A. Kinetic force

Consider a particle in one dimension and governed by the Schrödinger Hamiltonian $H = K + V$. Here K is the kinetic Hamiltonian

$$K = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2}. \quad (1)$$

where M is the mass of the particle. V in the Hamiltonian is a potential depending on x . We divide the space into two subsystems at some point x_0 . The particle number $n_{R,L}$ on each side and the positions of their centers of mass $x_{cm(R,L)}$ are evaluated by restricting the integrations over the wave function to one side or the other of the point x_0 . For the right hand side, this is achieved by the operators

$$\hat{\mathbb{1}}_R = \Theta(x - x_0) \quad (2)$$

$$\hat{x}_R = x\Theta(x - x_0) \quad (3)$$

where Θ is the Heaviside step function. We write the expectation values in the wave function $\phi(x)$ as

$$\langle \phi | \hat{\mathbb{1}}_R | \phi \rangle = n_R \quad (4)$$

$$\langle \phi | \hat{x}_R | \phi \rangle = n_R x_{cm(R)}. \quad (5)$$

Depending on the wave function, both of these quantities can vary with time under the Schrödinger dynamics. However, it is not useful to call the effect on a subsystem a force if the particle number is changing. We therefore restrict the definition to wave functions for which dn_R/dt and d^2n_R/dt^2 are zero at the time when the force is computed. Then the time dependence of Eq. (5) will provide the acceleration a_R of the right-hand side computed as

$$a_R = \frac{1}{n_R} \frac{d^2}{dt^2} \langle \phi | \hat{x}_R | \phi \rangle. \quad (6)$$

Given the acceleration, the Newtonian force can be defined as

$$F_R = M \frac{d^2}{dt^2} \langle \phi | \hat{x}_R | \phi \rangle. \quad (7)$$

We can now carry the derivatives in the Heisenberg representation by twice applying the usual commutator formula

$$\frac{d}{dt} \langle \hat{\mathcal{O}} \rangle = \frac{1}{i\hbar} \langle [\mathcal{O}, H] \rangle. \quad (8)$$

The resulting operator for the kinetic energy term in H is

$$\hat{F}_k(x_0) = -M[K, [K, \hat{x}_R]] = -\frac{\hbar^2}{4M} \left(2 \frac{\overleftarrow{\partial}}{\partial x} \delta(x - x_0) \frac{\overrightarrow{\partial}}{\partial x} - \frac{\overleftarrow{\partial}^2}{\partial x^2} \delta(x - x_0) - \delta(x - x_0) \frac{\overrightarrow{\partial}^2}{\partial x^2} \right) \quad (9)$$

To show how Eq. (9) works, we apply it to some very simple Hamiltonians. The first is a particle in a box. The n -th stationary state in the box has the wave function

$$\phi = \sqrt{\frac{2}{L}} \sin(k_n x) \quad (10)$$

where L is the length of the box and $k_n = n\pi/L$. Its energy is

$$E_n = \frac{\hbar^2 k_n^2}{2M}. \quad (11)$$

The force exerted by the particle on the boundary can be calculated by the usual relation between force, energy, and displacement

$$F = -\frac{dE_n(L)}{dL} = \frac{\hbar^2 \pi^2 n^2}{ML^3}. \quad (12)$$

This force must be sustained throughout the interior of the box. If we arbitrarily divide the space in two the same force must act between the two sides. Applying Eq. (9) we find

$$F_R = \frac{\hbar^2}{ML} \left(\left(\frac{d \sin(k_n x)}{dx} \Big|_{x_0} \right)^2 - \sin(x_0) \frac{d^2 \sin(k_n x)}{dx^2} \Big|_{x_0} \right) = \frac{\hbar^2 \pi^2 n^2}{ML^3} \quad (13)$$

in agreement with Eq. (12).

Another simple example is the expansion of a Gaussian wave packet. The initial wave function may be written

$$\phi(x) = \frac{1}{b^{1/2} \pi^{1/4}} e^{-x^2/2b^2}. \quad (14)$$

Here b is a parameter controlling the width of the Gaussian. The time-dependent Schrödinger equation has the exact solution

$$\phi(x, t) = \frac{1}{b^{1/2} \pi^{1/4}} (1 + i\hbar t/Mb^2)^{-1/2} \exp(-\frac{1}{2}x^2/b^2(1 + i\hbar t/M)). \quad (15)$$

There is no particle transfer at $x_0 = 0$ so we can calculate the force at that point. The center-of-mass position of the right-hand side particle density is

$$\langle x_R \rangle = \int_{x_0}^{\infty} dx x |\phi(x, t)|^2 = \frac{b}{2} \pi^{1/2} (1 + (\hbar t/Mb^2)^2)^{1/2} \quad (16)$$

By explicit differentiation of Eq. (16), the acceleration of right-hand density distribution is

$$\frac{d^2}{dt^2} \langle \hat{x}_R \rangle = \frac{1}{2\pi^{1/2} M^2 b^3} (1 + (\hbar t/Mb^2)^2)^{-3/2}. \quad (17)$$

The force calculated from this acceleration together with Eq. (7) agrees with that obtained by the expectation value of Eq. (9) in the wave function $\phi(x, 0)$. The important point is that Eq. (9) only requires information about the wave function around the point $x_0 = 0$, and yet it perfectly describes the cm acceleration of all the matter to the right of that point.

1. Potential contribution

Now we add an external potential field V to the Hamiltonian and treat the associated force F_V acting on a region in the same way. The operator requires the double commutator

$$\hat{a}_R = -\frac{1}{\hbar^2} [V, [K, \hat{x}_R]] \quad (18)$$

and is evaluated as

$$\langle \hat{a}_R \rangle = \int_{x_0}^{\infty} dx \rho(x) \frac{\partial V}{\partial x}; \quad (19)$$

Not surprisingly, this formula is very similar to Ehrenfest's second equation, $d\langle p \rangle/dt = -\langle dV/dx \rangle$. To illustrate the application of Eq. (19), consider a particle in the ground state of the harmonic oscillator Hamiltonian. It is convenient to express the potential in the form

$$V(x) = \frac{\hbar^2}{2Mb^4}x^2. \quad (20)$$

Its ground state is the wave function of Eq. (14). Since it is stationary, the acceleration is zero everywhere and there should be an exact force balance at all points:

$$F_K + F_V = 0 \quad \text{for all } x_0. \quad (21)$$

It is an easy exercise to verify that

$$F_K = \frac{\hbar^2\nu^{3/2}}{2M\pi^{1/2}}e^{-\frac{1}{2}\nu x_0^2}. \quad (22)$$

Carrying out the integration in Eq. (19), one obtains the negative of Eq. (22). This verifies the force balance for the ground state, but in fact it must be true for excited states as well.

B. Beyond the one-particle Hamiltonian

The formulas of the last subsections are easily generalized to multiparticle systems when particles interact through mean-field potentials. For the kinetic quantum force, all the physics is governed by one-body operators and so all of the forces are additive. The summation can be carried out at the level of the wave function to obtain the the single-particle density matrix $\rho(x, x')$. The corresponding kinetic force is then given by the compact expression

$$F_K = -\frac{\hbar^2}{2M} \left. \frac{d^2}{ds^2} \rho(x_0 + s/2, x_0 - s/2) \right|_{s=0}. \quad (23)$$

An even more compact expression makes use of the Wigner representation of the density matrix, $f(x, p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \exp(ips) \rho(x + s/2, x - s/2)$. Then Eq. (23) becomes

$$F_K = \frac{\hbar^2}{M} \int_{-\infty}^{\infty} dp p^2 f(x_0, p) \quad (24)$$

To introduce particle-particle interactions, we first note that the instantaneous force can be derived by expanding the Hamiltonian evolution operator to second order in time. In mean-field theory the single-particle potential can be expanded as well. However, the time-dependent corrections to the instantaneous potential start with terms beyond second order

in time and so can be dropped. All that is required to treat interaction effects is determine their contribution with an instantaneous single-particle potential.

The simplest case to deal with is a two-body finite-range interaction $v(x - x')$. By Eq. (19) the force F_V may be expressed

$$F_V = M \int_{x_0}^{\infty} dx \rho(x) \int_{-\infty}^{\infty} dx' \rho(x') \frac{d}{dx} v(x - x'). \quad (25)$$

Next split the integral over x' into two at the integration point x . The contribution with x' in the range $x < x' < \infty$) can be shown to vanish; physically the interactions between particles in the same region do not affect the center-of-mass motion in that region. Thus F_V reduces to

$$F_V = M \int_{x_0}^{\infty} dx \rho(x) \int_{-\infty}^x dx' \rho(x') \frac{d}{dx'} v(x'' - x') \quad (26)$$

This form is appropriate as it stands for long-range forces such as the Coulomb interaction. It needs the entire density distribution to calculate it, but at least it doesn't require numerical differentiation of global energies.

As the range of the interaction decreases, it is clear that only the the density near x_0 contributes to the integral. An easy way to derive the force is to follow the spirit of density function theory, where the interaction energy density \mathcal{V} is treated as a local function of position. We start with a simple form for the interaction energy functional, $\mathcal{V} = \frac{1}{2}v_0\rho^2(x)$. The corresponding single-particle potential is

$$V(x) = \frac{d\mathcal{V}(x)}{d\rho} = v_0\rho(x). \quad (27)$$

Inserting this in Eq (26), we have

$$F_V = v_0 \int_{x_0}^{\infty} dx \rho(x) \frac{d\rho}{dx} = \frac{1}{2}v_0 \int_{x_0}^{\infty} dx \frac{d}{dx} \rho^2(x) = -\frac{1}{2}v_0\rho^2(x_0). \quad (28)$$

To obtain the far right-hand equality, we have assumed that $\rho \rightarrow 0$ at large x .

Eqs. (23) and (28) can be easily tested in the one-dimensional Fermi gas model. We first derive the force from the total energy in a box. The total force on the box wall can be calculated as before by taking the derivative of the total energy with respect to box size. The result is

$$E = \frac{\hbar^2 k_F^2}{6M} N + \frac{v_0}{2L} N^2 \quad (29)$$

where N is the number of particles, $k_F \approx \pi N/L$ and $\rho = N/L$. Taking the derivative, the force on the wall is

$$F_b = -\frac{dE}{dL} = \frac{\hbar^2 k_F^2 N}{3M L} + \frac{1}{2} v_0 \frac{N^2}{L^2}. \quad (30)$$

The first term is the kinetic contribution; it may be calculated from Eq. (9) taking $(\rho(x + s/2, x - s/2) = \sin(k_F s)/(\pi s)$. The second is identical to Eq. (28).

The same method can be used to derive the force associated with any energy density functional \mathcal{V} that can be expanded in powers of the local density $\rho(x)$. We write

$$\mathcal{V}(\rho) = \sum_m \frac{1}{m!} v_m \rho^m. \quad (31)$$

Then F_V can be evaluated similarly to Eq. (28) as

$$F_V = \sum_m \frac{1}{m!} (m-1) v_m \rho(x_0)^m. \quad (32)$$

This can also be expressed as [10]

$$F_V = V(x_0)\rho(x_0) - \mathcal{V}(x_0). \quad (33)$$

In the last form, the force is seen to depend only on the density at the interface.

III. THREE DIMENSIONS

The generalization to three dimensions is trivial if the interface between the two subsystems is a plane. Then the kinetic force operator acts perpendicular to the plane and just requires an integration over the transverse coordinates. Formally, one can define a stress tensor Π that transmits momentum from one part of the system to another. In the co-moving frame of the medium, the stress tensor Π associated with density-functional dynamics is given by an expression very similar to the one-dimensional formula,

$$\Pi_{ij}(\vec{r}) = \frac{\hbar^2}{M} \nabla_{s_i} \nabla_{s_j} \rho(\vec{r} - \vec{s}/2, \vec{r} + \vec{s}/2) + (V(\vec{r})\rho(\vec{r}) - \mathcal{V}(\vec{r})) \delta_{ij}. \quad (34)$$

The two terms represent the kinetic and interaction contributions, respectively. The interaction term is isotropic, but that need not be the case for the kinetic term. A perpendicular Newtonian force can be calculated across any plane by the integral

$$\vec{F} \cdot \vec{u} = \int \Pi \cdot d\vec{A} \quad (35)$$

where \vec{u} is a unit vector perpendicular to the plane \vec{A} . In practice, one would choose a plane going through the neck region that joins the two nascent fragments. Note that there is no mechanism here to generate a transverse force between subsystems.

In practice in calculating dynamics in nuclear physics, condensed matter physics and quantum chemistry, one defines the configurations by minimizing an energy functional in the presence of a fixed external field. In such situations the wave function has no currents so the conditions for calculating the force across a plane are satisfied. However, the constrained minimization procedure also permits a third way to calculate force. This is to use the Feynman-Hellman theorem and calculate the energy derivative as an expectation value of the derivative of the constraining field. This is a much easier task than to explicitly calculate total energy derivatives numerically. Still, the quantum force operator might still be useful in some situations and as an independent check on computations carried out by other methods.

IV. APPENDIX

A. Pairing

Pairing is very important in low-frequency nuclear dynamics. At present, the most well-justified models incorporating pairing are based on the Hartree-Fock-Bogoliubov (HFB) extension of mean-field theory. It is now possible to carry out the integration of the HFB equations of motion without uncontrolled approximation [11]. It is also clear from simplified implementations that lifetimes are strongly dependent on the pairing field [12, 13]. The force associated with pairing can be derived in the same way as we treated the ordinary interactions in the Hamiltonian. The dynamics is governed by the HFB equation of motion, also known as the Bogoliubov-de Gennes equation. This is written

$$i\hbar \frac{d}{dt} \begin{pmatrix} \vec{v}_\alpha \\ \vec{u}_\alpha \end{pmatrix} = \begin{pmatrix} H & \Delta \\ -\Delta^* & -H \end{pmatrix} \begin{pmatrix} \vec{v}_\alpha \\ \vec{u}_\alpha \end{pmatrix}, \quad (36)$$

in the usual notation. The pairing energy associated with a two-body interaction \bar{v} can be expressed $E_p = \frac{1}{4} Tr_2 \kappa^* \bar{v} \kappa$ [14] where $\kappa = \sum_\alpha v_\alpha u_\alpha^T$; the Δ field is given by $\Delta = \frac{1}{2} \bar{v} \kappa$. The expressions for the energy and field are very similar to those for the ordinary interaction with the replacement of ρ by κ . We expect that the derived force will come out in a similar way if the interaction \bar{v} is short-ranged. Then the force would be equal to the pairing energy

density at the division point. For most physical systems, the pairing energy density is small compared to other interaction terms, so the pairing force can be neglected in practice.

1. *Adiabaticity*

For the complete dynamics of 3-D media it is essential to understand the time scale of the collective motion with respect to the time scale to establish local equilibrium. For slow collective motion, the presence of interactions beyond mean field keeps the Fermi surface nearly spherical and the resulting stress tensor is nearly isotropic. In the opposite limit, the stress tensor remembers the strain history of the system, and the Fermi surface can have quadrupolar distortion. In terms of the Lamé parameterization of the stress tensor, in the adiabatic case the compressibility is governed by a pressure field

$$P = \lambda + \frac{2}{3}\mu \quad (37)$$

whereas in the diabatic case the longitudinal stress for a strain field in the z direction is given by

$$\Pi_{zz} = \lambda + 2\mu. \quad (38)$$

The kinetic stress tensor for a diabatically deformed Fermi surface has Lamé coefficients

$$\lambda = \mu = \frac{k_f^2}{5M}. \quad (39)$$

A number of Fermionic systems exhibit diabatic dynamics in high-frequency oscillations. We mention zero sound in liquid ^3He [15], the wave-length dependence of plasmons in conductors [16], and the giant quadrupole resonance in large nuclei [17].

These considerations only indirectly affect the forces we have calculated here. As stated earlier, the force or stress tensor depends only on the instantaneous state of the system. If that wave function is obtained by a constrained mean field solution with density constraint operators, it will have no local currents although it may have a deformed Fermi surface as a result of the constraints. If one releases the constraints and allows the system to evolve, the proto-fragments will at first be accelerated away from each other by the force dynamics treated here. But later as the state of system changes, the compressibility will play a role. A stronger restoring force will be present in the diabatic dynamics than in the adiabatic. The considerations discussed here cannot tell us whether the system eventually come apart in fragments.

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