

Thus, in principle, almost all the excitation energies ($E_n - E_0$) of the system can be obtained by Fourier-analyzing the displacement field – the only exception being those excitations that are not connected to the ground-state by a finite matrix element of the current-density operator.

In this paper we will introduce an approximate expression for the force density

$$F_{\mu,1}(\mathbf{r}, t) \equiv -n_1(\mathbf{r}, t) \partial_\mu V_0(\mathbf{r}) - \partial_\nu P_{\mu\nu,1}(\mathbf{r}, t), \quad (13)$$

which appears on the right hand side of Eq. (10), as a linear functional of $\mathbf{u}(\mathbf{r}, t)$. The expression will be presented in terms of the functional

$$E[\mathbf{u}] \equiv \langle \psi_0[\mathbf{u}] | \hat{H}_0 | \psi_0[\mathbf{u}] \rangle, \quad (14)$$

which is the energy of the distorted ground-state $|\psi_0[\mathbf{u}]\rangle$, obtained from the undistorted ground-state $|\psi_0\rangle$ by virtually displacing the volume element located at \mathbf{r} to a new position $\mathbf{r} + \mathbf{u}(\mathbf{r}, t)$. More precisely, we will show that the equation of motion for \mathbf{u} takes the form:

$$mn_0(\mathbf{r}) \partial_t^2 \mathbf{u}(\mathbf{r}, t) = -n_0(\mathbf{r}) \nabla V_1(\mathbf{r}, t) - \frac{\delta E_2[\mathbf{u}]}{\delta \mathbf{u}(\mathbf{r}, t)}, \quad (15)$$

where $E_2[\mathbf{u}]$ is the second order term in the expansion of $E[\mathbf{u}]$ in powers of \mathbf{u} . The functional $E_2[\mathbf{u}]$ has an exact expression in terms of the one-particle density matrix and the pair correlation function of the *ground-state*, which is a major simplification, since ground-state properties, unlike time-dependent properties, are accessible to computation by a variety of numerical and analytical methods.

Furthermore, we will show that the kinetic part of the force density functional $\delta E_2[\mathbf{u}]/\delta \mathbf{u}$ is local, in the sense that it depends only on a finite number of spatial derivatives (up to the fourth) of the displacement field at a given position. Thus, our equation of motion reduces to a fourth-order differential equation for \mathbf{u} when interaction effects are neglected. The inclusion of interaction effects leads to the appearance of nonlocal contributions to the energy, and the equation of motion becomes a fourth-order *integro-differential* equation for the displacement field. However, the complexity of this equation remains essentially unchanged as the number of particles increases.

Our equation of motion has two especially appealing features: (i) it is exact for one-electron systems at all frequencies and (ii) it can be physically justified for generic many-electron systems at high frequency or, more generally, at all frequencies for which a collective description of the motion is plausible. Thus the range of frequencies for which our approximation makes sense is expected to be wider in strongly correlated systems than in weakly correlated ones.

We discuss several qualitative features of our equation (uniform electron gas limit, harmonic potential theorem)

and present its solution in simple one- and two-electron models, where the results can be checked against exact calculations. The results are encouraging. Although we are not able to resolve all the different excitation energies of the models under study, we find that groups of excitation characterized by similar displacement fields are represented by a single mode of an average frequency, in such a way that the spectral strength of this mode equals the sum of the spectral strengths of all the excitations in the group. In this sense our approximation can be viewed as a (considerable) refinement and extension of the traditional single-mode approximation for the homogeneous electron gas to strongly inhomogeneous quantum systems. In spite of the somewhat limited range of validity of the present treatment (the linear response regime), we feel that this is an important first step in a direction that might eventually lead to the construction of useful force density functionals for far-from-equilibrium processes.

This paper is organized as follows. In Section II we present a complete derivation of the linearized equation of motion for the displacement field. We begin by deriving a formally exact expression for the force density (Section II A), on which we perform the “elastic approximation” (Section II B). The expression for the force density in the elastic approximation is worked out in sections II C (kinetic part) and II D (potential part). A simplified form of the equation of motion, valid for one-dimensional systems, is presented in Section II E. Appendixes A through C provide supporting material for this part. In Section III we discuss the relation between quantum continuum mechanics and time-dependent current density functional theory. In section IV we show how the linear equation of motion derived in Section II leads to an eigenvalue problem for the excitation energies. In Section IV A we demonstrate the hermiticity of this eigenvalue problem and the positive-definiteness of the eigenvalues. In Section IV B we connect the eigenvalue problem to the high-frequency limit of the linear response theory. In Section IV C we prove that the first moment of the current excitation spectrum obtained from the solution of our eigenvalue problem is exact. Appendixes D and E contain supporting material for this part. In Section V we present a few simple applications of our theory for the excitations of (i) a homogeneous electron gas (Section V A) (ii) the linear harmonic oscillator and the hydrogen atom (Section V B), and (iii) a system of two-electrons in a one-dimensional parabolic potential interacting via a soft Coulomb potential. The analytic solution of the last model in the strong correlation regime is featured in Appendix F. Finally, Section VI contains our summary and a few speculations about future applications of the theory.