Continuum Mechanics for Quantum Many-Body Systems: The Linear Response Regime

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We derive a closed equation of motion for the current density of an inhomogeneous quantum many-body system under the assumption that the time-dependent wave function can be described as a geometric deformation of the ground-state wave function. By describing the many-body system in terms of a single collective field we provide an alternative to traditional approaches, which emphasize one-particle orbitals. We refer to our approach as continuum mechanics for quantum many-body systems. In the linear response regime, the equation of motion for the displacement field becomes a linear fourth-order integro-differential equation, whose only inputs are the one-particle density matrix and the pair correlation function of the ground-state. The complexity of this equation remains essentially unchanged as the number of particles increases. We show that our equation of motion is a hermitian eigenvalue problem, which admits a complete set of orthonormal eigenfunctions under a scalar product that involves the ground-state density. Further, we show that the excitation energies derived from this approach satisfy a sum rule which guarantees the exactness of the integrated spectral strength. Our formulation becomes exact for systems consisting of a single particle, and for any many-body system in the high-frequency limit. The theory is illustrated by explicit calculations for simple one- and two-particle systems.

I. INTRODUCTION

The dynamics of quantum many-particle systems poses a major challenge to computational physicists and chemists. In the study of ground-state properties one can rely on a variational principle, which enables a variety of powerful statistical methods (in addition to exact diagonalization) such as the quantum variational Monte Carlo method and the diffusion Monte Carlo method.[1] In time-dependent situations, the absence of a practical variational principle has greatly hindered the development of equally powerful methods. Yet it is hard to overestimate the importance of developing effective techniques to tackle the quantum dynamical problem. Such a technique could allow, for example, to follow in real time the evolution of chemical reactions, ionization and collision processes.

One of the most successful computational methods developed to date is the time-dependent density functional theory (TDDFT), or its more recent version – time-dependent current density functional theory (TDCDFT).[2] In this approach, the interacting electronic system is treated as a noninteracting electronic system subjected to an effective scalar potential (a vector potential in TDCDFT) which is self-consistently determined by the electronic density (or by the current density).[3,4] Thus, one avoids the formidable problem of solving the time-dependent Schrödinger equation for the many-body wave function. Even this simplified problem, however, is quite complex, since it involves the determination of N time-dependent single particle orbitals – one for each particle. Furthermore, there are features such as multiparticle excitations[5] and dispersion forces[6] that are very difficult to treat within the conventional approximation schemes.

An alternative approach, which actually dates back to the early days of the quantum theory, attempts to calculate the collective variables of interest, density and current, without appealing to the underlying wave function.[7–9] This approach we call "quantum continuum mechanics" (QCM), because in analogy with classical theories of continuous media (elasticity and hydrodynamics), it attempts to describe the quantum many-body system without explicit reference to the individual particles