Invariance of the Kohn center-of-mass mode in a conserving theory

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The center-of-mass (c.m.) oscillation of a many-body system in a harmonic trap is known to be independent of the interparticle interaction. However, this is not necessarily the case if the interactions are treated approximately. Here, we prove a simple general criterion for preservation of the c.m. mode: the approximation has to preserve density and momentum. The result equally applies to zero and finite temperatures, as well as to nonequilibrium situations, and to the linear and nonlinear response regimes.

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I. INTRODUCTION

Interacting many-body systems in confinement potentials are of growing interest in many fields, including ions in Penning or Paul traps,1–3 dusty plasmas,4,5 electrons and excitons in quantum wells and dots (see, e.g., Refs. 7–9), or ultracold atoms and molecules forming Bose condensates (see, e.g., Refs. 10–13 for an overview). In all these systems, the problem of collective modes is of high interest since they determine the optical and transport properties, (see, e.g., Refs. 3, 7, and 14). For example, for classical plasmas in traps the spectrum of normal modes, including correlation effects, has been analyzed in detail in Refs. 3 and 4. Further, the normal mode spectrum has turned out to be an important test of the experimental trap profile and of theoretical models as well. In particular, the center-of-mass (c.m.) oscillation of the trapped particles is a sensitive test for many-body theories: possible deviations of its frequency from the trap frequency indicate that the used approximation is inconsistent or not appropriate or that the numerical solution of the model is incorrect. The behavior of the c.m. or sloshing mode has been studied for trapped quantum systems originally by Kohn14 and Brey et al.1 This issue has more recently regained interest in the context of trapped Bose condensates. In particular, the invariance of the Kohn mode by certain approximate theories has been discussed in application to various approximations, mostly mean-field-type models (see, e.g., Refs. 10–12).

The validity of the Kohn theorem for approximate theories will be discussed in detail in this paper. We start in Sec. II with a brief reminder of the Kohn theorem for the case of an exact treatment of the pair interactions. Then, in Sec. III, we introduce approximations for the interactions in a completely general form using nonequilibrium Green’s functions. We then derive the conditions these approximations have to fulfill in order not to violate the Kohn theorem. We conclude with a discussion of the results and of their scope of applicability in Sec. IV.

II. KOHN THEOREM

Let us briefly recall the contents of the Kohn theorem. Consider a quantum N-body system in a three-dimensional harmonic trap. A very general description for identical particles with mass $m$ is provided by the Hamiltonian

$$\hat{H} = \sum_k \hat{H}_k + \sum_{i<k} \hat{w}(\mathbf{r}_i - \mathbf{r}_k),$$

(1)

$$\hat{H}_i = \frac{\hat{p}_i^2}{2m} + \frac{m}{2} \left( \Omega_{x}^2 \xi_{x}^2 + \Omega_{y}^2 \xi_{y}^2 + \Omega_{z}^2 \xi_{z}^2 \right) - e \mathbf{E}(t) \mathbf{r}_i,$$

where, in addition, a homogeneous time-dependent dipole field $\mathbf{E}$ is included. Introducing c.m. and relative coordinates $\mathbf{R} = N^{-1} \sum \mathbf{r}_i$ and $\xi_i$ (e.g., for two particles, $\xi = \mathbf{r}_1 - \mathbf{r}_2$) and masses $M = Nm$, $\mu = m/N$, the Hamiltonian (1) can be written as sum of a c.m. and a relative contribution, $\hat{H} = \hat{H}_{c.m.} + \hat{H}_{rel}$, with

$$\hat{H}_{c.m.} = \frac{\hat{\mathbf{p}}^2}{2M} + \frac{M}{2} \left( \Omega_{x}^2 \xi_{x}^2 + \Omega_{y}^2 \xi_{y}^2 + \Omega_{z}^2 \xi_{z}^2 \right) - e \mathbf{E}(t) \mathbf{R},$$

(2)

$$\hat{H}_{rel} = \sum_{i} \left\{ \frac{\hat{p}_i^2}{2\mu} + \frac{\mu}{2} \left( \Omega_{x}^2 \xi_{i,x}^2 + \Omega_{y}^2 \xi_{i,y}^2 + \Omega_{z}^2 \xi_{i,z}^2 \right) \right\} + \sum_{i<k} \hat{w}(\xi_i - \xi_k),$$

(3)

where we introduced the center of mass and relative momenta $\hat{\mathbf{p}} = \frac{\hat{\mathbf{p}}}{\hat{N}} \hat{\mathbf{R}}$ and $\hat{\mathbf{p}}_{\xi_i} = \frac{\hat{\mathbf{p}}}{\hat{N}} \hat{\xi}_i$. Since the particle interaction appears only in the relative Hamiltonian and $[\hat{H}_{c.m.}, \hat{H}_{rel}] = 0$, the c.m. dynamics of the system (1) coincides with that of a noninteracting system, i.e., $\mathbf{R}(t)$ performs the motion of a forced three-dimensional harmonic oscillator. This is a generalization of the free c.m. oscillation (commonly called Kohn or sloshing mode) to the case of an additional external field. This well-known result was first obtained by Kohn for the case where the electric field and the trap potential are replaced by a homogeneous magnetic field14 and is now commonly called Kohn theorem. The analogous result for the system (1) was proven by Brey et al.7

The Kohn theorem is fairly obvious due to the fact that the exact pair interaction Hamiltonian $\hat{V}_{12} = \sum_{i<j} \hat{w}(\xi_i - \xi_j)$ contains only relative coordinates and thus does not contribute to $\hat{H}_{c.m.}$. However, an exact treatment of the system (1) is, in many cases, not possible and one has to resort to approximations of many-body theory. As a result, the interaction
The expectation value of the interaction energy is readily computed using the coordinate representation of $\hat{\rho}_{12}$ and $\hat{W}_{12}$.

$$\langle \hat{V}_{12}^{\text{ap}} \rangle = \frac{1}{2} \int \text{d}r_1 \text{d}r_2 \hat{W}(r_1 - r_2) \rho_{12}(r_1, r_2; 1; t)$$

Equation (4) shows that the density matrix has no simple dependence on relative and c.m. coordinates; in general, contributions of both do not separate. Even in the simplest approximation, the Hartree approximation, $\rho^H_{12}(r_1, r_2; 1; t) = n(r_1) n(r_2, t)$, depends on both coordinates and not just the distance $r_1 - r_2$. Therefore, it has been concluded that $\hat{\rho}^H_{12}$ violates the Kohn theorem. The situation is similarly complex in the Hartree-Fock (HF) approximation and even more complicated if correlations are being included. Moreover, as we indicated explicitly by the arguments of $\rho$ in Eq. (4), in nonequilibrium, the density matrix may also depend on the trap potential, applied fields, and time, which further complicates the analysis.

Therefore, whether some many-body approximation for $\hat{\rho}_{12}$ correctly obeys the invariance of the c.m. mode of the exact system is a nontrivial question which has been actively studied over the past decade, in particular, for trapped atomic condensates (see e.g., Refs. 10–12 and 16) and electrons in quantum dots. Besides the Hartree approximation, several other variants of collisionless approximations have been studied, including the HF approximation, the HF-Bogolyubov approximation, and the HF-Bogolyubov generalized random phase approximation, which were shown to obey the Kohn theorem. Further, the time-dependent local density approximation and a Tomonaga-Luttinger-type model have been investigated. For the numerous other models, we refer to the papers cited in the above references. However, no general criterion for the fulfillment of the Kohn theorem has been presented so far, which would allow one to avoid the often involved proof for any specific new approximation. This is particularly important for the treatment of strong correlation effects in classical and quantum trapped systems which have come into the focus of research in many fields.

The goal of this paper is to present such a general criterion. We prove that the Kohn theorem is obeyed by any approximation of many-body theory which conserves particle number and total momentum. We further demonstrate that the result holds independently of whether the system was initially in the ground state, equilibrium, or nonequilibrium. Finally, the result equally holds for linear response and for the case of arbitrary strong excitation.

### III. VALIDITY OF THE KOHN THEOREM IN A CONSERVING THEORY

Our proof proceeds in three steps. First, we reformulate the Kohn theorem in terms of ladder operators $\hat{C}^\pm$ [Eqs. (5) and (6)]. Second, we introduce the representation of these operators in second quantization [Eq. (9)] which are denoted $\hat{c}^\pm$. Third, we compute the dynamics of the expectation values $c^\pm = \langle \hat{c}^\pm \rangle$ [Eq. (11)] in a given many-body approximation and derive under what conditions it coincides with the dynamics $\hat{C}^\pm(t)$ of the noninteracting system. To classify these approximations, we use the powerful tools of nonequilibrium Green’s functions (see, e.g., Refs. 18, 20, and 21). Use of the equations of motion (14) allows for a very compact proof of the Kohn theorem for many-body approximations.

#### A. Ladder operators

The dynamics of the c.m. mode in an $N$-particle system can be efficiently analyzed using the collective ladder operators $\hat{C}^\pm$,

$$\hat{C}^\pm = \sum_{k=1}^N m \Omega \hat{x}_k \mp i \hat{p}_k,$$

where $\hat{x}_k$ and $\hat{p}_k$ denote coordinate and momentum operators of particle $k$ and, to simplify the notation, we restrict ourselves to the one-dimensional case (the extension to three dimensions is straightforward). Application of $\hat{C}^+$ to the ground state creates an excited state with excess energy $\hbar \Omega$. If the interactions are treated exactly, i.e., by the operator $\hat{V}_{12}$, one verifies by direct calculation that $[\hat{V}_{12}, \hat{C}^\pm] = 0$. As a consequence, the dynamics of $\hat{C}^\pm$, which is given by the Heisenberg equation of motion with the full Hamiltonian [one-dimensional version of Eq. (1)],

$$\frac{d}{dt} \hat{C}^\pm = i \hbar [\hat{H}, \hat{C}^\pm] = \pm i \Omega \hat{C}^\mp \mp i N eE(t),$$

is independent of the interaction terms. Identifying the c.m. as

$$\hat{R} = (2M \Omega)^{-1} (\hat{C}^+ + \hat{C}^-),$$

Eq. (6) immediately confirms that $\hat{R}$ performs a driven oscillation in the harmonic potential,

$$\dot{\hat{R}} + \Omega^2 \hat{R} = NeE(t)/M.$$

Thus, Eq. (6) is a convenient mathematical formulation of the Kohn theorem.

We have now to replace the exact interaction $\hat{V}_{12}$ by an approximation $\hat{V}_{12}^{\text{ap}}$ and to find the conditions under which $[\hat{V}_{12}^{\text{ap}}, \hat{C}^\pm] = 0$ or, equivalently, the conditions under which the time derivative $\dot{\hat{C}}^\pm$ coincides with the right hand side of Eq. (6).

#### B. Second quantization representation of the ladder operators

To introduce many-body approximations, we use the representation of the $N$-body system in terms of field operators $\Psi^\dagger(x_1, t_1)$ and $\Psi(x_1, t_1)$, where the first (second) creates (annihilates) a particle at position $x_1$ and time $t_1$. Further, as usual,
where \([\cdots]\) denotes the commutator and \([\cdots]\) the anticommutator corresponding to the case of bosons and fermions, respectively. We now define the second quantization representation of the ladder operators \(\hat{c}^\pm\),

\[
\hat{c}^\pm(X, T) = \{\hat{p}^\pm(x_1, x'_1)\Psi^\dagger(x'_1, t_1)\Psi(x_1, t_1)\}\,_{1=1^*},
\]

with

\[
\hat{p}^\pm(x_1, x'_1) = m\Omega x_1 + x'_1 \pm \hbar \frac{\partial_{x_1} - \partial_{x'_1}}{2}.
\]

After action of \(\hat{p}\), the result of Eq. (9) is taken at equal arguments \(1 = (x_1, t_1) = 1' = (x'_1, t'_1)\) which equal the macroscopic (c.m.) coordinate and time, \(X = (x_1 + x'_1)/2\) and \(T = (t_1 + t'_1)/2\).

Below, the central quantity of interest, which takes over the role of \(\hat{c}^\pm(t)\) in Eq. (6), is the ensemble average of Eq. (9) integrated over the coordinates

\[
c^\pm(T) = \int dX [\hat{c}^\pm(X, T) = \int dX \{\hat{p}^\pm(x_1, x'_1)\ih \tilde{G}(1, 1')\}\,_{1=1^*},
\]

where \(1^*\) denotes the limit from above for the time argument, \(t_1^* = t_1 + 0\). In the right hand side of Eq. (11), we expressed the ensemble average of the field operator product by the one-particle nonequilibrium Green’s function (NGF), defined as

\[
\ih \tilde{G}(1, 1') = \pm \langle \hat{T}_c, \Psi(1)\Psi^\dagger(1')\rangle,
\]

where the plus (minus) sign refers to bosons (fermions). Note that \(\tilde{G}\) is defined on the Schwinger/Keldysh contour \(\hat{C}\), and \(\hat{T}_c\) denotes time ordering on \(\hat{C}\) (see, e.g., Refs. 15 and 21).

The use of the NGF technique has the advantage that equilibrium and nonequilibrium averages can be treated on equal footing, and approximations \(G_{12}\) can be systematically derived using Feynman diagrams. Further, as we will see below, this formalism allows for a compact and simple analysis of the validity of the Kohn theorem for many-particle approximations. This is due to the two-time structure of the NGF. Single time quantities, such as the density matrix, follow immediately from the equal time limit of the NGF. Details of this formalism are not important for the derivations below, and the interested reader is referred to the text books.15,18

**C. Time dependence of the ladder operators \(c^\pm(T)\)**

To verify under what conditions the c.m. mode of an approximate theory obeys the noninteracting dynamics [Eq. (6)], we need to compute the derivative of the space integrated expectation value [Eq. (11)] with respect to the c.m. time \(T\),

\[
c^\pm(T) = \int dX [\hat{p}^\pm(x_1, x'_1)\ih \tilde{G}(1, 1')\]\n
\[
\times [w(x_1 - x_2) - w(x_1 - x_2)]G_{12}(1, 2; 1', 2^*)\,_{1=1^*},
\]

where the terms \(\delta_c\) cancel and, in the interaction term, the

\[
\delta_c(T) = \int dX [\hat{p}^\pm(x_1, x'_1)\partial_{x_1} + \partial_{x'_1} + ih \tilde{G}(1, 1')\]\n
\[
\partial_{x_1} + \partial_{x'_1} - [V(1) - V(1')]\,_{1=1^*} + ih \int dX dx_2 [\hat{p}^\pm(x_1, x'_1)\]

The two time derivatives of \(\tilde{G}\) follow directly from the equation of motion of \(\tilde{G}\) and the adjoint equation (first equations of the Martin-Schwinger hierarchy22),

\[
\{\ih \partial_{t_1} - H_1(1')\} \tilde{G}(1, 1') = \ih \int \,_{1} d2W (1 - 2) G_{12}(1, 2; 1', 2^*, 1') \pm \delta_c (1 - 1'),
\]

where \(H_1\) is the single-particle part of the Hamiltonian \(W(1 - 2) = w(x_1 - x_2)\delta_{t_1 - t_2}\), with \(\delta_c\) being the delta function defined on \(\hat{C}\).18 Equations (14) and (15) have a clear content: while the left hand sides describe the single-particle dynamics, interaction effects (mean field plus correlations) are contained in the right hand sides. Here, the central quantity is the two-particle Green’s function defined as

\[
(\ih)^2 G_{12}(1, 2; 1', 2'^*) = \langle \hat{T}_c, \Psi(1)\Psi^\dagger(1')\Psi^\dagger(2')\Psi(2)\rangle,
\]

which is a generalization of the two-particle density matrix \(\rho_{12}(t)\) which is recovered from \(G_{12}\) by taking all time arguments to be equal \(t\) (see, e.g., Refs. 15 and 18). Practically, all relevant many-body approximations can be formulated in terms of \(G_{12}\). For example, the Hartree-Fock approximation follows simply by substituting \(G_{12}(1, 2; 1', 2') \rightarrow G(1, 1')G(2, 2') \pm G(1, 2')G(2, 1')\), whereas the Hartree approximation is just the first term. Finally, the advantage of the formalism of Eqs. (14) and (15) is that it allows us to generalize all approximations known from ground state many-body theory, including diagram expansions, to arbitrary nonequilibrium situations.

We now proceed in computing \(c^\pm(T)\) [Eq. (13)] by eliminating the time derivatives of \(\tilde{G}\) with the help of Eqs. (14) and (15),

\[
\hat{c}^\pm(T) = \int dX \{\hat{p}^\pm(x_1, x'_1)\}[\hbar^2 (\partial_{x_1} - \partial_{x'_1})^2 + V(1) - V(1')]\,_{1=1^*} + \ih \int dX dx_2 [\hat{p}^\pm(x_1, x'_1)\]

\[
\times [w(x_1 - x_2) - w(x_1 - x_2)]G_{12}(1, 2; 1', 2^*)\,_{1=1^*},
\]
time integration has been carried out. Further, we introduced the total single-particle potential $V(1)=m\Omega^2 x_1^2/2-eE(t_1)x_1$. Applying the operator $\hat{Y}$ under the integrals, we obtain the single-particle contribution to Eq. (17):

$$\hat{c}_{12}^+(T) = \int dX \left\{ \left[ m\Omega^2 \mp \hbar \frac{\partial_{x_1} - \partial_{x_2}}{2} \right] \hat{\hbar} \frac{\partial_{x_1} - \partial_{x_2}}{2m} \partial_{x_1} \right\}
- [V(1) - V(1')] \tilde{G}(1,1') \right\}_{t_1 = t_1^+}
= - \int dX \left\{ \left[ \pm \frac{V'(1) + V'(1')}{2} \right] \hbar \frac{\partial_{x_1} - \partial_{x_2}}{2} \right\} \tilde{G}(1,1') \right\}_{t_1 = t_1^+},
$$

(18)

where a partial integration over $X$ has been performed taking into account that $\tilde{G}$ vanishes for $|X| \rightarrow \infty$, and we denoted $V'(1) = dV(x_1, t_1)/dx_1$. For a harmonic confinement potential, the derivative of $V$ yields $m\Omega^2 x_1$ and we obtain $\hat{c}_{12}^+ = \pm i\Omega \epsilon^z \mp ieNE$. Thus, the single-particle contributions to the dynamics of the center of mass yield exactly the result (6) of the noninteracting system, as it should be.

What is left now is to analyze the interaction contributions $\hat{c}_{12}$ to Eq. (17):

$$\hat{c}_{12}^+(T) = i\hbar \int dx dx_2 \left\{ \left[ m\Omega^2 \pm \hbar \frac{\partial_{x_1} - \partial_{x_2}}{2} \right] w(x_1 - x_2)
- w(x_1' - x_2') \tilde{G}_{12}(1,2;1',2') \right\}_{t_1 = t_1^+}.
$$

Contributions proportional to $\Omega^2$ vanish because the potentials cancel for $x_1=x_1'$. The remaining contribution involves derivatives of the interaction potential, and the integrand can be transformed according to

$$\left\{ \left[ \partial_{x_1} w(x_1 - x_2) + \partial_{x_2} w(x_1 - x_2) \right] \tilde{G}_{12}(1,2;1',2') \right\}_{t_1 = t_1^+}
= \left\{ 2w'(X - x_2) \tilde{G}_{12}(1,2;1',2') \right\}_{t_1 = t_1^+}.
$$

Since the force $-w'(x)$ is an odd function of the argument, the expression in parentheses vanishes under the integral over the coordinates of both particles if $G_{12}$ is even, i.e., if

$$G_{12}(1,2;1',2') = G_{12}(2,1;2',1').
$$

(19)

Thus, symmetry of $G_{12}$ with respect to the arguments of particles 1 and 2 is sufficient for vanishing of the interaction contribution $\hat{c}_{12}^+$. Summarizing the above results for $\hat{c}_1$ and $\hat{c}_{12}$, we obtain for their sum [Eq. (17)]

$$\frac{d}{dt} e^{i\epsilon} = \pm i\Omega \epsilon^z \mp ieNE(t),
$$

(20)
i.e., we exactly recover the noninteracting dynamics of Eq. (6) as was the case for the exact treatment of the interactions. Obviously, condition (19) is fulfilled for the Hartree and HF approximations, and the same holds for all standard many-body approximations including the Born approximation, the random phase (or GW) approximation, the ladder approximation, etc.

## IV. CONCLUSION

Thus, we can formulate the main conclusion of this paper: any many-body approximation specified by $G_{12}$ obeys the Kohn theorem if two conditions are fulfilled.

(A) $\tilde{G}$ simultaneously obeys the first equation of the Martin-Schwinger hierarchy and its adjoint [Eqs. (14) and (15)].

(B) $G_{12}$ obeys the symmetry (19).

Note that our derivation did not involve information on the type of pair interaction $w$ and is thus valid for arbitrary pair potentials. Also, no specific ensemble had to be specified for the average (in the Green’s function); therefore, the derivation is valid for $N$-body systems originally in the ground state, at finite temperature, or in nonequilibrium.

Obviously, our result is trivially generalized to the three-dimensional (two-dimensional) case by using three (two) types of ladder operators, one for each of the independent c.m. modes. Also, while our derivation was performed for a single component system, generalizations to multicomponent systems, including Bose condensates or mixtures of fermions and bosons, are straightforward by using the corresponding matrix (Nambu) Green’s functions (see, e.g., Ref. 10).

Our result can also be directly extended to many-particle systems in a homogeneous magnetic field where, instead of the c.m. oscillation, the cyclotron rotation (CR) is observed. Again, it is known that the CR with $\omega_c = eB/(mc)$ is not altered by pair interactions if they are treated exactly.14 The question of invariance of the CR under an approximation $\chi_{12}^{approx}$ can be analyzed exactly as above: one only has to replace the ladder operators $\hat{C}^\pm$ by the combinations of the total momentum $P_z = P_z + iP_y$, with $P = \{p_x, p_y, \pm \hbar, p_z\}$, for a B field in the $z$ direction.14 The result is again that any many-body approximation obeying conditions (A) and (B) will preserve the CR.

Interestingly, conditions (A) and (B) are exactly the two criteria of Baym and Kadanoff known to be sufficient for conservation of density (continuity equation), momentum, and total energy.18,24 These so-called conserving approximations are, therefore, also the ones which obey the Kohn theorem. Frequently, many-body approximations are classified by the self-energy $\Sigma$, instead of the two-particle Green’s function $G_{12}$. The relation is very simple:15,18 $i\hbar \int d2W(1 \rightarrow 2) G_{12}(1,2;1',2') = \int d2\Sigma(1,2) G(2,1')$. Alternatively, one can show25 that conditions (A) and (B) are equivalent to existence of a functional $\Phi$ such that

$$\delta \Phi [\tilde{G}] / \delta \tilde{G}(1',1) = 0.
$$

Thus, we may conclude that any such “$\Phi$-derivable approximation” for the self-energy fulfills the Kohn theorem.

This result has important implications not only for Green’s functions theory but also for other classes of approximations, such as the ones used in time-dependent density functional theory (TDDFT). It was recently proven26 that any exchange correlation functional of TDDFT which is derived from a $\Phi$-derivable approximation satisfies the so-
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In summary, we have shown that the independence of the c.m. oscillation in a harmonic potential of the particle interaction is fulfilled not only for the exact problem but also for a broad class of approximations of many-body theory. Therefore, for a reasonable theoretical modeling of trapped classical or quantum systems, including ultracold ions, dusty plasmas, nanostructures, or quantum gases, it is crucial to use approximations that conserve density, total momentum, and total energy. These conserving approximations have been shown to obey the Kohn theorem in all situations of practical importance, for weak and strong correlations, for weak or strong time-dependent homogeneous excitation, and for systems initially in the ground state, in equilibrium, and in nonequilibrium. Finally, our result establishes an important test for computer simulations of correlated many-body systems in nonequilibrium (see, e.g., Refs. 19, 20, 27, and 28). Since the center-of-mass motion $\mathbf{R}(t)$ coincides with that of noninteracting particles [Eq. (8)], any initial (ground state or equilibrium) density profile $n_0(\mathbf{r}) = n(\mathbf{r}, t=0)$ should retain its shape over the whole volume once initially only the c.m. mode is excited, i.e., $n(\mathbf{r}, t) = n_0(\mathbf{r} - \mathbf{R}(t))$. This is a very sensitive test for the quality of any numerical code for trapped classical or quantum many-body systems.

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22 This definition is related to the standard definition $\bar{G} = \pm G$ and is used here to simplify the notation in the derivations which apply to fermions and bosons.