

Many-body excitation spectra of trapped bosons with general interaction by linear response

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Abstract. The linear-response theory of the multiconfigurational time-dependent Hartree for bosons method (LR-MCTDHB) for computing many-body excitations of trapped Bose-Einstein condensates [Phys. Rev. A **88**, 023606 (2013); J. Chem. Phys. **140**, 034108 (2014)] is implemented, for the first time, for systems with general interparticle interaction. This allows us to investigate the many-body excitation spectrum of interacting bosons with, for instance, a long-range interaction. Illustrative numerical examples for repulsive and attractive bosons are provided. The LR-MCTDHB theory is capable of identifying all excitations, including the excitations which are not unraveled within Bogoliubov-de Gennes equations. The theory is herewith benchmarked against the exactly-solvable one-dimensional harmonic-interaction model. As a complementary result, using a complex transformation, we represent LR-MCTDHB in a compact block-diagonal form, opening up thereby an avenue for treating larger many-body systems. We expect the LR-MCTDHB theory and its implementation for general interparticle interaction to provide a proved probe into the many-body excitations involved in the out-of-equilibrium dynamics of trapped interacting bosons.

1. Introduction

The standard and most popular avenue to compute the dynamics (and excitations) of a Bose-Einstein condensate (BEC) is the Gross-Pitaevskii equation, which assumes all bosons to occupy a single one-particle state [1-4]. Clearly, whenever the system under investigation is not fully condensed one has to go beyond Gross-Pitaevskii theory in order to faithfully account for the system's dynamics, a matter which is well documented in the literature, see, e.g., the recent book [5] and references therein.

The usual way to account for excitations in a BEC is to build them atop the Gross-Pitaevskii ground state, taking a particle out from the condensate to an excited one-particle state. Formally, this leads to the Bogoliubov-de Gennes equations which often are also referred to as linear response of the Gross-Pitaevskii equation [1-10]. It turns out, as we have recently shown for contact interaction [11], that even if the ground state is well described by the fully-condensed Gross-Pitaevskii wavefunction, many excitations are missing by this standard treatment. For fully-fragmented ground states [12], more excitations appear [13]. Thus, to describe systems whose ground states are not fully condensed and, importantly, to identify new classes of excitations which cannot be resolved by the standard tools, suitable methods are in need.

Consider N trapped bosons, interacting by a generic interparticle interaction. The many-



particle Hamiltonian is written as follows

$$\hat{H}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{j=1}^N \hat{h}(\mathbf{r}_j) + \sum_{k>j=1}^N \hat{W}(\mathbf{r}_j, \mathbf{r}_k). \quad (1)$$

Here $\hat{h}(\mathbf{r})$ is the one-body Hamiltonian which consists of kinetic and potential (trap) terms and $\hat{W}(\mathbf{r}, \mathbf{r}')$ is a generic interparticle interaction which is symmetric to permutation of the particles' coordinates. In the familiar case for ultracold bosonic atoms it takes the form $\hat{W}(\mathbf{r}, \mathbf{r}') = \lambda_0 \delta(\mathbf{r} - \mathbf{r}')$ where the interaction parameter λ_0 is proportional to the s-wave scattering length.

We recall that by approximating the system's time-dependent wavefunction by the product state

$$\Psi_{\text{GP}}(\mathbf{r}_1, \dots, \mathbf{r}_N; t) = \phi(\mathbf{r}_1, t) \cdots \phi(\mathbf{r}_N, t) \equiv |N; t\rangle \quad (2)$$

and utilizing the Dirac-Frenkel variational principle, the Gross-Pitaevskii equation, $i\dot{\phi}(\mathbf{r}, t) = [\hat{h}(\mathbf{r}) + \lambda|\phi(\mathbf{r}, t)|^2]\phi(\mathbf{r}, t)$, where $\lambda = \lambda_0(N-1)$, is obtained.

The linear-response theory atop the Gross-Pitaevskii mean-field wavefunction (2) is formally obtained by linearizing the Gross-Pitaevskii equation around the ground-state solution. It results in the Bogoliubov–de Gennes equations which take on the matrix form

$$\mathcal{L}_{\text{BdG}} \begin{pmatrix} u^k \\ v^k \end{pmatrix} = \omega_k \begin{pmatrix} u^k \\ v^k \end{pmatrix}, \quad \mathcal{L}_{\text{BdG}} = \begin{pmatrix} \hat{h} + 2\lambda|\phi_0|^2 - \mu & \lambda(\phi_0)^2 \\ -\lambda(\phi_0^*)^2 & -(\hat{h}^* + 2\lambda|\phi_0|^2 - \mu) \end{pmatrix}. \quad (3)$$

The linear-response matrix \mathcal{L}_{BdG} depends explicitly on the ground-state orbital ϕ_0 . μ is the chemical potential. The excitation spectrum ω_k of the BEC as well as the so-called response amplitudes u^k and v^k are obtained by solving the eigenvalue system (3).

2. Many-body theory

In many situations as mentioned above the ground state of the BEC cannot be described well by the wavefunction Eq. (2). Importantly, even when the ground state is well approximated by the Gross-Pitaevskii wavefunction (2), the standard linear-response atop misses many excitations [11], also see the benchmarks in Sec. 3 below. The natural idea was to use a more extended ansatz for the system's wavefunction, and then to perform linear response atop [11, 14]. We recall that linear response atop the exact ground state gives rise to the exact many-body excitation spectrum, see, e.g., [15, 16].

Let us briefly describe the underlying many-body theory for BECs used in the present work before we proceed to its linear response. In the multiconfigurational time-dependent Hartree for bosons (MCTDHB) method [17, 18] the bosons are allowed to occupy not one but $j = 1, \dots, M$ one-particle functions (modes) ϕ_j . The many-body wavefunction is assembled by distributing the N bosons over the M one-particle functions

$$\Psi(t) = \sum_{\vec{n}} C_{\vec{n}}(t) |\vec{n}; t\rangle, \quad (4)$$

where $C_{\vec{n}}(t)$ are the expansion coefficients and $|\vec{n}; t\rangle$ are permanents (Fock states) with $\vec{n} \equiv (n_1, \dots, n_M)$, $n_1 + \dots + n_M = N$. Utilizing the Dirac-Frenkel variational principle, the one-particle functions ϕ_j as well as the expansion coefficients $C_{\vec{n}}$ are determined self-consistently. This leads to a system of coupled equations which has been coined in the literature the MCTDHB method [17, 18]. The MCTDHB method has been used for unveiling many-body phenomena with repulsive and attractive BECs in one-dimensional setups, see, e.g., [19–26], and benchmarked

against an exactly-solvable model [27]. Most recently, MCTDHB was extended to two and three spatial dimensions, and employed to establish the mechanism of fragmentation and generic regimes of dynamics in repulsive BECs with strong, finite-range interparticle interactions [28, 29].

The successes of the MCTDHB method to accurately compute many-body out-of-equilibrium dynamics of BECs stem from the employment of the self-consistent (time-adaptive) multiconfigurational wavefunction (4). The wavefunction (4) contains a substantially larger number of variational parameters (i.e., modes, and Fock states and their expansion coefficients) in comparison with the standard Gross-Pitaevskii wavefunction (2). Clearly, if the obtained many-body dynamics is accurate then MCTDHB manages to resolve the excitation spectra of BECs. This has motivated us to pursue its linear response, as a venue to research on the many-body level excitations of trapped BECs directly, i.e., without propagation.

The derivation of the linear-response (LR) theory atop the wavefunction (4) is rather lengthy but otherwise straightforward [11, 14]. We will not repeat it here and begin from the final result for the resulting LR-MCTDHB theory, which takes on the form of the eigenvalue equation [11, 14]

$$\mathcal{L} \begin{pmatrix} \mathbf{u}^k \\ \mathbf{v}^k \\ \mathbf{C}_u^k \\ \mathbf{C}_v^k \end{pmatrix} = \omega_k \begin{pmatrix} \mathbf{u}^k \\ \mathbf{v}^k \\ \mathbf{C}_u^k \\ \mathbf{C}_v^k \end{pmatrix}. \quad (5)$$

The linear-response matrix \mathcal{L} of the many-boson wavefunction Ψ is more involved than the Bogoliubov–de Gennes linear-response matrix (3). We will discuss its structure shortly. Physically, the response amplitudes of all modes, \mathbf{u}^k and \mathbf{v}^k , and of all expansion coefficients, \mathbf{C}_u^k and \mathbf{C}_v^k , combine to give the many-body excitation spectrum ω_k . For comparison, in the Bogoliubov–de Gennes linear-response matrix (3) there is only a single block representing the sole one-particle function used to describe the BEC within Gross-Pitaevskii theory. In Ref. [11] we have successfully managed to explicitly construct \mathcal{L} for bosons interacting by contact potential and obtained the many-body excitation spectrum.

There is another way to group the linear-response matrix which we are now going to exploit. Namely, first to list the orbitals' and coefficients' 'u' blocks and then the respective 'v' blocks. In this way each of the new blocks has the same dimension, see below. The spectrum, of course, does not change. Hence, reshuffling the blocks of \mathcal{L} the final result can be written as

$$\mathcal{L} \begin{pmatrix} \mathbf{u}^k \\ \mathbf{C}_u^k \\ \mathbf{v}^k \\ \mathbf{C}_v^k \end{pmatrix} = w_k \begin{pmatrix} \mathbf{u}^k \\ \mathbf{C}_u^k \\ \mathbf{v}^k \\ \mathbf{C}_v^k \end{pmatrix}, \quad \mathcal{L} = \left(\begin{array}{c|c} \mathcal{L}^u & \mathcal{L}^v \\ \hline -(\mathcal{L}^v)^* & -(\mathcal{L}^u)^* \end{array} \right), \quad (6)$$

where details of the blocks of \mathcal{L} are collected in [30].

The above general relation between the 'u' and 'v' blocks of \mathcal{L} is appealing since we may mix them and eventually block diagonalize \mathcal{L} . For this, consider the transformation

$$\mathbf{Q} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & \mathbf{1}\theta \\ \mathbf{1} & -\mathbf{1}\theta \end{pmatrix}, \quad (7)$$

where θ is the operation of complex conjugation, for example, $\theta\mathbf{v}^k = (\mathbf{v}^k)^*$. It is not difficult to show that \mathbf{Q} block diagonalizes \mathcal{L} ; Consult the appendix for additional details. The final result reads

$$\begin{aligned} \mathcal{L}_f^{(2)} \begin{pmatrix} \mathbf{f}^k \\ \mathbf{C}_f^k \end{pmatrix} &= w_k^2 \begin{pmatrix} \mathbf{f}^k \\ \mathbf{C}_f^k \end{pmatrix}, & \mathcal{L}_f^{(2)} &= (\mathcal{L}^u - \mathcal{L}^v\theta)(\mathcal{L}^u + \mathcal{L}^u\theta), \\ \mathcal{L}_g^{(2)} \begin{pmatrix} \mathbf{g}^k \\ \mathbf{C}_g^k \end{pmatrix} &= w_k^2 \begin{pmatrix} \mathbf{g}^k \\ \mathbf{C}_g^k \end{pmatrix}, & \mathcal{L}_g^{(2)} &= (\mathcal{L}^u + \mathcal{L}^u\theta)(\mathcal{L}^u - \mathcal{L}^v\theta), \end{aligned} \quad (8)$$

with the relations between the eigenvectors' blocks $\mathbf{f}^k, \mathbf{g}^k = \frac{1}{\sqrt{2}}[\mathbf{u}^k \pm (\mathbf{v}^k)^*]$ and $\mathbf{C}_f^k, \mathbf{C}_g^k = \frac{1}{\sqrt{2}}[\mathbf{C}_u^k \pm (\mathbf{C}_v^k)^*]$.

Eq. (8) is the main result of this work on the theory side; We compactly represent the LR-MCTDHB theory in a block-diagonal form. Because the resulting (square of the) excitation spectrum is bound from below, this will open up an avenue for treating larger systems. First, this in particular would allow one to use standard diagonalization techniques for matrices with bound spectra. Here, Eq. (8) defines the basic operation of matrix-to-vector multiplication used in such techniques. Second, it reduces the size of the linear-response matrix to half its size. Furthermore, since \mathbf{Q} in Eq. (7) is a complex transformation, the block diagonalization can be used with complex wavefunctions and with complex hermitian Hamiltonians. This situation is encountered, e.g., when a system is described in the rotating frame. Thus, the block diagonalization derived in the present work for the many-body theory also generalizes the literature block-diagonalization treatment of the Bogoliubov–de Gennes equations, see, e.g., [31–33], which only used a real transformation. This concludes our block diagonalization of the LR-MCTDHB theory.

3. Illustrative numerical examples and benchmarks

In the following section we would like to report, for the first time, the implementation and application of LR-MCTDHB with general interparticle interaction. As an illustrative system we have chosen the harmonic-interaction model [34–37]. This is an analytically-solvable model, yet, it is not at all trivial to be treated numerically. First, because the interaction is non-contact the construction of various matrix elements for computing the ground-state wavefunction and its response matrix are much more involved. We have now successfully coped with this demanding task. Second, the solution of the problem on the computer is done in the laboratory frame, where all the bosons are indistinguishable. This is unlike the analytical solution which exploits the separability of the center-of-mass and relative coordinates' degrees-of-freedom. As mentioned above, the harmonic-interaction model and a time-dependent extension of which have been used to benchmark MCTDHB [27]. Hence, we expect the model to be instrumental in benchmarking the excitation spectrum computed by the many-body linear-response theory.

In Eq. (1) the one-body Hamiltonian is now $\hat{h}(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\Omega^2 x^2$. The two-body interaction reads $W(x-x') = K(x-x')^2$, representing thereby long-range interaction. The parameter $K < 0$ ($K > 0$) indicates repulsion (attraction) between the bosons. In what follows we set without loss of generality $\Omega = 1$. The exact excitation energies of the one-dimensional harmonic-interaction model are known and given by [34, 36]

$$\omega[n_{CM}, n_{rel}] = n_{CM} + n_{rel}\delta_N, \quad \delta_N = \sqrt{1 + 2NK}, \quad (9)$$

with the center-of-mass (CM) and relative coordinates' (rel) quantum numbers $n_{CM} = 1, 2, 3, \dots$ and $n_{rel} = 2, 3, \dots$.

We consider $N = 1000$ weakly-interacting repulsive bosons ($K = -0.0001$) and compare in Table 1 below the LR-MCTDHB results with the analytical formula (9). The many-body theory, computed at the level of $M = 2$ orbitals in the expansion (4), improves as one would expect the accuracy of excitations unveiled by Bogoliubov–de Gennes theory. More important, it unravels additional excitations. We see the capability of the LR-MCTDHB theory to describe numerically-exactly the center-of-mass and relative coordinates' excitations. The physical distinction here for the excitations missing in the Bogoliubov–de Gennes theory is that all consist of one quantum of center-of-mass excitation plus at least one additional quantum of excitation. The latter can be either another center-of-mass or a relative coordinates' excitation, see the rightmost column of Table 1. We stress again that the computation is done in the

	M=1	M=2	Exact analytical	n_{CM}, n_{rel}
E_{GS}	<u>447.26949371</u>	<u>447.26638194</u>	447.26638190	0, 0
ω_1	1.00000000	1.00000000	1.00000000	1, 0
ω_2	<u>1.78907797</u>	<u>1.78885443</u>	1.78885438	0, 2
ω_3	n/a	<u>2.00004476</u>	2.00000000	2, 0
ω_4	<u>2.68361696</u>	<u>2.68328168</u>	2.68328157	0, 3
ω_5	n/a	<u>2.78888891</u>	2.78885438	1, 2
ω_6	n/a	<u>3.00007751</u>	3.00000000	3, 0
ω_7	<u>3.57815595</u>	<u>3.57771028</u>	3.57770876	0, 4
ω_8	n/a	<u>3.68397387</u>	3.68328157	1, 3

Table 1. Spectrum of the one-dimensional harmonic-interaction model with $N = 1000$ bosons and repulsion $K = -0.0001$. Comparisons of LR-MCTDHB and the exact results for the ground, E_{GS} , and excited states, $\omega_k = E_k - E_{GS}$. The last column assigns the excitations in terms of center-of-mass and relative coordinates' quantum numbers. Some excitations are first uncovered at the $M = 2$ level of theory, i.e., they are not available (n/a) within Bogoliubov–de Gennes theory ($M = 1$). Convergence with the number of orbitals M to the exact results is clearly seen. Underlined digits indicate the difference to the exact result. All quantities are dimensionless.

	M=1	M=2	Exact analytical	n_{CM}, n_{rel}
E_{GS}	<u>547.67691206</u>	<u>547.67483497</u>	547.67483495	0, 0
ω_1	1.00000000	1.00000000	1.00000000	1, 0
ω_2	n/a	<u>2.00003648</u>	2.00000000	2, 0
ω_3	<u>2.19070765</u>	2.19089026	2.19089023	0, 2
ω_4	n/a	<u>3.00006435</u>	3.00000000	3, 0
ω_5	n/a	<u>3.19091687</u>	3.19089023	1, 2
ω_6	<u>3.28606147</u>	<u>3.28633542</u>	3.28633535	0, 3
ω_7	n/a	<u>4.00129579</u>	4.00000000	4, 0
ω_8	n/a	<u>4.28580642</u>	4.28633535	1, 3

Table 2. Same as Table 1 but for $N = 1000$ bosons with attraction $K = +0.0001$. Some excitations are first uncovered at the $M = 2$ level of theory, i.e., they are not available (n/a) within Bogoliubov–de Gennes theory ($M = 1$). Convergence with M to the exact results is clearly seen. Note the interchange of order of some center-of-mass and relative coordinates' excitations in comparison with the repulsive system. All quantities are dimensionless.

laboratory frame, where all bosons are equivalent, i.e., the separability to center-of-mass and relative coordinates, which is special for harmonic traps, is not exploited.

We now move to attractive interaction and compute the excitation spectrum of $N = 1000$ bosons with $K = +0.0001$. The results are collected in Table 2 and show, as above, the capability of LR-MCTDHB to uncover the missing excitations and to numerically-exactly converge to the analytical results. The physical distinction of the missing excitations having one quantum of center-of-mass excitation plus at least one additional quantum of excitation is readily seen in Table 2. When comparing the repulsive and attractive systems, please note the interchange of order of some center-of-mass and relative coordinates' excitations.

4. Concluding remarks

The linear-response theory of the multiconfigurational time-dependent Hartree for bosons method for computing many-body excitations of trapped Bose-Einstein condensates has been implemented for systems with general interparticle interaction. This allows us to investigate the excitation spectrum of interacting bosons with, for instance, long-range interaction. As illustrative examples we considered, separately, repulsive and attractive bosons within the one-dimensional harmonic-interaction model. The many-body theory improves the accuracy of excitations unveiled within Bogoliubov–de Gennes theory. Chiefly, the many-body linear-response theory is capable of identifying all excitations, including the excitations which are not unraveled within Bogoliubov–de Gennes equations, and to numerically converge to their exact values. The results of the present work serve to benchmark the LR-MCTDHB method.

As a complementary result, we compactly represent the theory in a block-diagonal form. This is made possible by identifying a complex transformation, applicable also for complex wavefunctions and complex hermitian Hamiltonians. This will open up an avenue for treating larger systems. We expect the LR-MCTDHB theory and its implementation for general interparticle interaction to provide an important and proved probe into the many-body excitations involved in the out-of-equilibrium dynamics of trapped BECs.

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Appendix A. Block diagonalization by a complex transformation

Consider the eigenvalue system

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \omega \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \quad (\text{A.1})$$

where \mathbf{A}, \mathbf{B} and \mathbf{u}, \mathbf{v} are the blocks of a square matrix and its eigenvector, respectively. The eigenvalue ω is assumed to be real.

Let us examine the transformation matrix $\mathbf{Q} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & \mathbf{1}\theta \\ \mathbf{1} & -\mathbf{1}\theta \end{pmatrix}$, Eq. (7) of the main text. Interestingly, the transformation matrix \mathbf{Q} is neither a unitary nor an anti-unitary operator. Its inverse exists and reads

$$\mathbf{Q}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ \mathbf{1}\theta & -\mathbf{1}\theta \end{pmatrix}, \quad \mathbf{Q}\mathbf{Q}^{-1} = \mathbf{Q}^{-1}\mathbf{Q} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}. \quad (\text{A.2})$$

Multiplying with \mathbf{Q} from the left on both sides of Eq. (A.1) we find

$$\left\{ \mathbf{Q} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix} \mathbf{Q}^{-1} \right\} \left\{ \mathbf{Q} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \right\} = \begin{pmatrix} \mathbf{0} & \mathbf{A} - \mathbf{B}\theta \\ \mathbf{A} + \mathbf{B}\theta & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} = \omega \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}, \quad (\text{A.3})$$

where $\begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(\mathbf{u} + \mathbf{v}^*) \\ \frac{1}{\sqrt{2}}(\mathbf{u} - \mathbf{v}^*) \end{pmatrix}$. Multiplying now Eq. (A.3) from the left with the transformed matrix we obtain the desired result in a block-diagonal form

$$\begin{pmatrix} (\mathbf{A} - \mathbf{B}\theta)(\mathbf{A} + \mathbf{B}\theta) & \mathbf{0} \\ \mathbf{0} & (\mathbf{A} + \mathbf{B}\theta)(\mathbf{A} - \mathbf{B}\theta) \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} = \omega^2 \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}. \quad (\text{A.4})$$

This concludes our derivation.

Using the operation of complex conjugation θ above becomes redundant if \mathbf{A} and \mathbf{B} are real quantities. In this specific case, which is the only one considered within Bogoliubov–de Gennes equations in the literature, see, e.g., [31–33], \mathbf{Q} becomes a unitary and real transformation.

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- [30] The blocks of the linear-response matrix (6) are given by

$$\mathcal{L}^u = \begin{pmatrix} \mathbf{P}\rho^{+\frac{1}{2}}\mathcal{L}_{oo}^u\rho^{+\frac{1}{2}}\mathbf{P} & \mathbf{P}\rho^{+\frac{1}{2}}\mathcal{L}_{oc}^u\mathbf{P}_C \\ \mathbf{P}_C(\mathcal{L}_{oc}^u)^\dagger\rho^{+\frac{1}{2}}\mathbf{P} & \mathbf{P}_C(\cdot)^{\hat{H}-\varepsilon}\mathbf{P}_C \end{pmatrix}, \quad \mathcal{L}^v = \begin{pmatrix} \mathbf{P}\rho^{+\frac{1}{2}}\mathcal{L}_{oo}^v(\rho^*)^{+\frac{1}{2}}\mathbf{P}^* & \mathbf{P}\rho^{+\frac{1}{2}}\mathcal{L}_{oc}^v\mathbf{P}_C^* \\ \mathbf{P}_C(\mathcal{L}_{oc}^v)^\dagger(\rho^*)^{+\frac{1}{2}}\mathbf{P}^* & \mathbf{0} \end{pmatrix}.$$

The meaning of the ingredients is as follows: \mathbf{P} is a projector matrix on the subspace of one-particle functions orthogonal to the ground-state modes ϕ_j ; \mathbf{P}_C is a projector matrix on the subspace of permanents' coefficients orthogonal to the ground-state coefficients $C_{\vec{n}}$; ρ is the reduced one-particle density matrix [38] of the ground state; and $(\cdot)^{\hat{H}-\varepsilon}$ marks the operation of the Hamiltonian in Fock space utilizing mapping of permanents [39] and ε is the ground-state energy. Finally, the sub-blocks \mathcal{L}_{oo}^u , \mathcal{L}_{oc}^v and \mathcal{L}_{oc}^u , \mathcal{L}_{oc}^v collect, respectively, the couplings between the modes and the couplings between the modes and coefficients. Together with further details, they are given in [11, 14].

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