Reduced Density Matrix Functional Theory for Bosons

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Based on a generalization of Hohenberg-Kohn's theorem, we propose a ground state theory for bosonic quantum systems. Since it involves the one-particle reduced density matrix γ as a variable but still recovers quantum correlations in an exact way it is particularly well suited for the accurate description of Bose-Einstein condensates. As a proof of principle we study the building block of optical lattices. The solution of the underlying v-representability problem is found and its peculiar form identifies the constrained search formalism as the ideal starting point for constructing accurate functional approximations: The exact functionals $\mathcal{F}[\gamma]$ for this N-boson Hubbard dimer and general Bogoliubov-approximated systems are determined. For Bose-Einstein condensates with $N_{\mathrm{BEC}} \approx N$ condensed bosons, the respective gradient forces are found to diverge, $\nabla_\gamma \mathcal{F} \propto 1/\sqrt{1-N_{\mathrm{BEC}}/N}$, providing a comprehensive explanation for the absence of complete condensation in nature.

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Introduction.—One of the striking features of quantum many-body systems is that their elementary constituents interact only by two-body forces. As a consequence, the corresponding ground state problem can in principle be solved in terms of the two-particle reduced density matrix replacing the exponentially complex N-particle wave function [1–4]. Furthermore, in each scientific field all systems of interest are characterized by the same *fixed* interaction W between the particles (e.g., Coulomb interaction in quantum chemistry and contact interaction in the field of ultracold gases). The class of N-particle Hamiltonians is thus parametrized solely by the external potential v. Since the conjugate variable of v is the (particle or charge) density, this heuristic reasoning identifies density functional theory as the most economic approach in each scientific field for addressing the ground state problem. Indeed, density functional theory has become in the past few decades the method of choice for electronic structure calculations in physics, chemistry, and materials science [5]. It is, however, not suitable for describing in a direct way Bose-Einstein condensation (BEC), one of the most fascinating phenomena of quantum physics. This is due to the fact that the particle density does, in general, not provide sufficient insights into the presence or absence of BEC, quite in contrast to the one-particle reduced density matrix (1RDM)

$$\gamma \equiv N\mathrm{Tr}_{N-1}[\Gamma] \equiv \sum_\alpha n_\alpha |\alpha\rangle\langle\alpha|, \tag{1}$$

which is obtained from the N-boson density operator Γ by integrating out all except one boson: BEC is present whenever the largest eigenvalue $n_{\max} = \max_\varphi \langle\varphi|\gamma|\varphi\rangle$ of the 1RDM is proportional to N [6]. This criterion is more general than the one referring to off-diagonal long-range order of $\gamma(\vec{r},\vec{r}') = \langle\vec{r}|\gamma|\vec{r}'\rangle$ [7], since it also applies to nonhomogeneous systems.

Based on Bose's work [8], Einstein in 1925 predicted the existence of BEC [9]. Its experimental realization for cold atoms in 1995 [10–12] has led to a renewed interest. Since then, the respective field of ultracold atomic gases has even become one of the most active fields in quantum physics (see, e.g., Refs. [13–16]) with a broad range of applications in quantum technologies (see, e.g., Refs. [17–20]). It is also this development that urges us to propose and work out in the following a computationally feasible method that is capable of describing strongly interacting bosons in general and BEC in particular. This bosonic one-particle reduced density matrix functional theory (RDMFT) is based on a generalization of the famous Hohenberg-Kohn theorem [21]. It therefore recovers quantum correlations in an effective but exact manner and is not restricted to the low-density regime, quite in contrast to the Gross-Pitaevskii [22–24] or Bogoliubov theory [24,25]. The study of two concrete systems shall serve as a proof of principle: We succeed in determining their universal functionals. Moreover, we solve the underlying v- and N-representability problem which have partly hampered the development of RDMFT in fermionic quantum

systems [26,27]. A comprehensive explanation for the absence of complete BEC in nature follows, highlighting the potential of our novel method.

Foundation of bosonic RDMFT.—Because of Gilbert [21], a generalization of the Kohn-Hohenberg theorem to Hamiltonians of the form

$$H(h) \equiv h + W \tag{2}$$

with a fixed interaction W proves the existence of a universal 1RDM-functional $\mathcal{F}[\gamma]$: The ground state energy and ground state 1RDM follow for any choice of the one-particle Hamiltonian h from the minimization of the total energy functional

$$\mathcal{E}_h[\gamma] = \mathrm{Tr}[h\gamma] + \mathcal{F}[\gamma]. \tag{3}$$

The functional $\mathcal{F}$ is universal in the sense that it does not depend on $h \equiv t + v$ but only on the fixed interaction W. This is due to the fact that the 1RDM γ allows one to determine not only the external potential energy $\mathrm{Tr}[v\gamma]$, but also the kinetic energy $\mathrm{Tr}[t\gamma]$. Because of the significance of bosonic quantum systems and the importance of γ as an indicator for BEC it is surprising that RDMFT has been developed only for *fermionic* systems (see, e.g., the reviews [28–31]). In this Letter we take the first steps towards realizing a bosonic RDMFT and in particular observe that some obstacles in the case of fermionic systems do not hamper its bosonic counterpart.

Let us first recall that the universal functional $\mathcal{F}$ is defined on the set $\mathcal{P}_v$ of 1RDMs which correspond to ground states of Hamiltonians $H(h)$. But for which γ does there exist a corresponding h? Unfortunately, no solution to this so-called v-representability problem is known, neither for fermions nor for bosons. To circumvent the v-representability problem, Levy suggested an extension of RDMFT to including nonphysical 1RDMs as well [26] (see also Ref. [32]). Expressing the ground state energy as $E(h) \equiv \min_\Gamma \mathrm{Tr}_N[H(h)\Gamma]$, and using the fact that the expectation value of h is determined by γ, allows one to replace $\mathcal{F}$ in Eq. (3) by [26,27,32,33]

$$\mathcal{F}^{(p/e)}[\gamma] = \min_{\Gamma \mapsto \gamma} \mathrm{Tr}_N[W\Gamma]. \tag{4}$$

The minimization in Eq. (4) may either be restricted to the *pure* (p) or all ensemble (e) N-boson states Γ mapping to the given 1RDM, $\gamma = N\mathrm{Tr}_{N-1}[\Gamma]$. Consequently, the functional $\mathcal{F}^{(p/e)}$ is defined on the domain $\mathcal{P}_{p/e}$ of pure or ensemble N-representable 1RDMs, where $\mathcal{P}_v \subseteq \mathcal{P}_p \subseteq \mathcal{P}_e$. A far-reaching observation is that for *every* 1RDM [recall Eq. (1)] there exists a corresponding bosonic pure state $\Gamma \equiv |\Phi\rangle\langle\Phi|$, e.g., $|\Phi\rangle = 1/\sqrt{N}\sum_\alpha \sqrt{n_\alpha}|\alpha, \ldots, \alpha\rangle$. Hence, in contrast to fermions [1,34–36], the one-body pure N-representability problem is trivial. Consequently, it will not hamper the development of bosonic functionals, and one has in particular $\mathcal{P}_p = \mathcal{P}_e$.

Hubbard dimer.—To illustrate the potential of bosonic RDMFT we discuss as a first example the Hubbard dimer for an arbitrary number N of spinless bosons. This building block of the Bose-Hubbard model is realized [37] and prominently used in the context of ultracold bosonic atoms, whose parameters can be tuned by laser light [14–16,38]. Similarly to the two-electron Hubbard dimer in the context of fermionic functional theories [39–44], its bosonic counterpart will serve as a theoretical laboratory system, eventually providing crucial insights into larger systems. Its Hamiltonian reads

$$H = -t(b_L^\dagger b_R + b_R^\dagger b_L) + \sum_{j=L/R} v_j \hat{n}_j + U \sum_{j=L/R} \hat{n}_j(\hat{n}_j - 1), \tag{5}$$

where the operators $b_j^\dagger$ and b_j create and annihilate a boson on site $j = L/R$, and $\hat{n}_j$ is the corresponding particle-number operator. The first term in Eq. (5) describes the hopping between both sites while the second one represents the external potential and the third one the on-site repulsion ($U > 0$).

In the following, we represent γ with respect to the lattice site states $|L\rangle, |R\rangle$ and assume real-valued matrix elements. We choose $\gamma_{LL} = 1 - \gamma_{RR}$ and $\gamma_{LR} = \gamma_{RL}$ as the two independent variables. Here, we normalize the 1RDM to unity since then the sets $\mathcal{P}_p = \mathcal{P}_e$ become independent of N (which allows the comparison of functionals for different values of N). As already stressed, the only constraint on those sets is that γ's eigenvalues are nonnegative, leading to

$$\gamma_{LR}^2 + \left(\gamma_{LL} - \frac{1}{2}\right)^2 \leq \frac{1}{4}. \tag{6}$$

Because of the circular symmetry of this disc it will prove convenient below to also introduce spherical coordinates: $\gamma_{LL} = \frac{1}{2}[1 + (1 - 2D)\cos\varphi]$ and $\gamma_{LR} = \frac{1}{2}(1 - 2D)\sin\varphi$. Hence, as illustrated in Fig. 1, D is γ's distance to the boundary $\partial\mathcal{P}_p$ and Eq. (6) reduces to $0 \leq D \leq 1/2$. The corresponding spectral decomposition of γ becomes

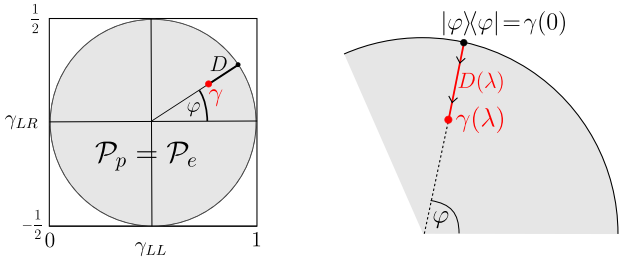

FIG. 1. Left: Illustration of the spherical representation (7) of the 1RDM γ. Right: Straight line $\gamma(\lambda)$ as constructed within the approach (10) at an angle φ.

$$\gamma(D,\varphi) = (1-D)|\varphi\rangle\langle\varphi| + D|\varphi^{\perp}\rangle\langle\varphi^{\perp}|, \tag{7}$$

with the natural orbitals $|\varphi\rangle = \cos(\varphi/2)|L\rangle + \sin(\varphi/2)|R\rangle$ and $|\varphi^{\perp}\rangle = \sin(\varphi/2)|L\rangle - \cos(\varphi/2)|R\rangle$.

To discuss and compare the three universal functionals $\mathcal{F}$, $\mathcal{F}^{(p)}$, and $\mathcal{F}^{(e)}$, respectively, we first need to address the underlying v-representability problem. Given its fundamental significance in functional theories, it is remarkable that no solution is known so far beyond the two-electron Hubbard dimer [45]. To solve here that problem for arbitrary particle numbers N, we first observe that the ground states for the hopping rate $t = 0$ are given by configuration states with n_L bosons on the left and $n_R = N - n_L$ on the right site. By varying the asymmetry $v_L - v_R$ of the external potential we can reach all values $n_L = 0, 1, \ldots, N$ and therefore each $\gamma = (n_L/N)|L\rangle\langle L| + (1 - n_L/N)|R\rangle\langle R|$ is v representable. Moreover, $v_L - v_R$ can be chosen such that the two configurations n_L and $n_L + 1$ are degenerate. By considering infinitesimal deformations of the respective Hamiltonian, one can thus reach any possible superposition $x|n_L, n_R\rangle \pm \sqrt{1-x^2}|n_L + 1, n_R - 1\rangle$. This leads to ellipses of v-representable 1RDMs. As is shown in the supporting information [46], the degeneracy of those specific ground states implies that all 1RDMs surrounded by such an ellipse (black solid ellipses in Fig. 2) are not v representable. Moreover, by anticipating the results on the presence of a diverging gradient, none of the 1RDMs on the boundary $\partial\mathcal{P}_p$ is v representable (except $\gamma = |L\rangle\langle L|, |R\rangle\langle R|$) but all points in its vicinity ($0 < D \ll 1$) can be obtained as ground state 1RDMs. Last but not least, each 1RDM between the boundaries of the black solid ellipses and $\partial\mathcal{P}_p$ can be reached. This can be confirmed by numerical investigations or mathematically by constructing corresponding connecting paths of ground state 1RDMs.

The solution of the v-representability problem provides additional crucial insights. In particular, the probability $p_N = 1 - \mathrm{Vol}(\mathcal{P}_v)/\mathrm{Vol}(\mathcal{P}_p)$ for finding non-v-representable 1RDMs does not vanish for large particle numbers N, $p_N \to \pi/8 \simeq 0.39$. Moreover, the domain $\mathcal{P}_v$ (orange) of the Gilbert functional $\mathcal{F}$ is getting arbitrarily complicated for larger N, as sketched in Fig. 2. This identifies Levy's constrained search (4) as the more suitable starting point for developing an RDMFT. The corresponding functional $\mathcal{F}_N^{(p)}$ can be determined analytically for $N = 2$ bosons,

$$\mathcal{F}_2^{(p)}[D,\varphi] = U[2 - (1 + 2\sqrt{D(1-D)})\sin^2(\varphi)], \tag{8}$$

and in the limit of large N (see the Supplemental Material [46]). For finite $N > 2$, one can easily determine the functional by an exact numerical calculation based on the minimization in Eq. (4). The ensemble functionals follow directly as the lower convex envelops, $\mathcal{F}_N^{(e)} = \mathrm{Conv}(\mathcal{F}_N^{(p)})$ [36].

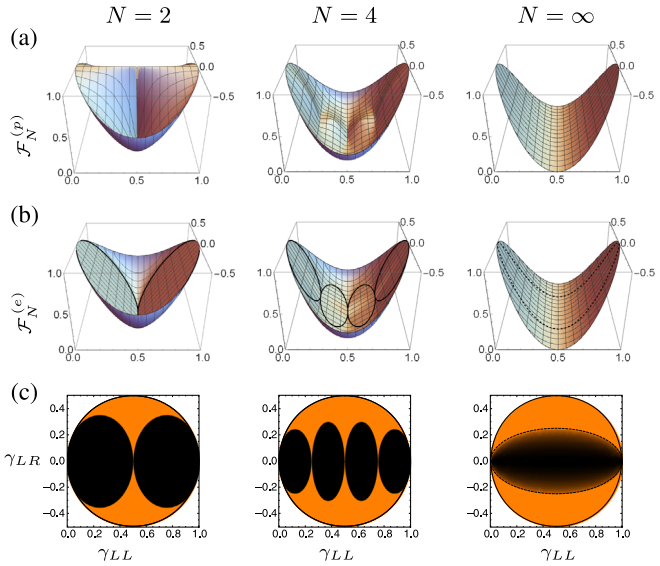

FIG. 2. For the Bose-Hubbard dimer we plot (a) the pure functional $\mathcal{F}_N^{(p)}$ and (b) the ensemble functional $\mathcal{F}_N^{(e)}$ (both renormalized to [0, 1]) as functions of the diagonal γ_{LL} and the off-diagonal entry γ_{LR} of the 1RDM for the particle numbers $N = 2, 4, \infty$. In (c) the v-representable 1RDMs are shown in orange and the nonphysical ones in black (see text for more details).

The results for $\mathcal{F}_N^{(p)}$ and $\mathcal{F}_N^{(e)}$ together with the solution of the v-representability problem are presented in Fig. 2. Panel (b) confirms that $\mathcal{F}_N^{(e)}$ is indeed given as the largest convex function fulfilling $\mathcal{F}_N^{(e)} \leq \mathcal{F}_N^{(p)}$ on the entire domain $\mathcal{P}_p$. While for v-representable 1RDMs, $\gamma \in \mathcal{P}_v$, both functionals $\mathcal{F}_N^{(p)}, \mathcal{F}_N^{(e)}$ necessarily coincide [36,45,47,48] (they are equal to $\mathcal{F}$), this is remarkably also the case in the limit of large N for non-v-representable 1RDMs. The most surprising insight, however, is that the gradients of the functionals seem to diverge repulsively on the boundary $\partial\mathcal{P}_p$, which prevents the system from ever reaching *complete* condensation in any state $|\varphi\rangle = b_\varphi^\dagger|0\rangle$ (as corresponding to $D = 0$). For instance, for $N = 2$ [recall Eq. (8)] one finds $\partial\mathcal{F}_2^{(p)}/\partial D \simeq -U\sin^2(\varphi)/\sqrt{D}$. Does this result generalize to larger systems and in that sense provide a comprehensive explanation for the absence of *complete* BEC in nature (quantum depletion)?

In the following we confirm the existence of this "Bose-Einstein condensation-force" also for $N > 2$. For this, we propose and work out an approach which allows one to determine exact functionals in the vicinity of the boundary $\partial\mathcal{P}_p$ which corresponds to N-boson states close to complete BEC. We first observe that the value $\mathcal{F}^{(p)}[\gamma_h]$ of the functional at a v-representable "point" γ_h [with corresponding Hamiltonian $H(h)$ and ground state energy $E(h)$] follows directly from the energy relation

$$E(h) = \mathcal{F}^{(p)}[\gamma_h] + \mathrm{Tr}[h\gamma_h]. \tag{9}$$

The second crucial ingredient is that each $\gamma = |\varphi\rangle\langle\varphi| \in \partial\mathcal{P}_p$ has a unique corresponding N-boson state which is given by $1/\sqrt{N!}(b_\varphi^\dagger)^N|0\rangle$. We could identify those states as the unique ground states of the one-particle Hamiltonians $h^{(0)} \equiv -b_\varphi^\dagger b_\varphi$. As illustrated in Fig. 1, the idea is then to construct for fixed φ a curve $H(\lambda,\varphi)$ of auxiliary Hamiltonians,

$$H(\lambda,\varphi) \mapsto |\Phi(\lambda,\varphi)\rangle \mapsto \gamma(\lambda,\varphi), \tag{10}$$

whose ground state 1RDMs $\gamma(\lambda,\varphi) \equiv \mathrm{Tr}_{N-1}[|\Phi(\lambda,\varphi)\rangle\times\langle\Phi(\lambda,\varphi)|]$ describe a straight line at an angle φ starting at $|\varphi\rangle\langle\varphi| = \gamma(\lambda=0,\varphi)$. To calculate the functional $\mathcal{F}^{(p)}[\gamma(D,\varphi)]$ for $D \ll 1$ according to Eq. (9) we expand the Hamiltonian, $H(\lambda,\varphi) \equiv h(\lambda,\varphi) + \lambda W = h^{(0)} + \lambda(h^{(1)} + W) + \mathcal{O}(\lambda^2)$. The purpose of the higher orders of the one-particle Hamiltonian $h(\lambda,\varphi)$ is to ensure that $\gamma(\lambda,\varphi)$ remains diagonal in the basis $|\varphi\rangle, |\varphi^\perp\rangle$, at least up to second order in λ. As it is shown in the supporting information [46], the eigenvalue problem $H(\lambda,\varphi)|\Phi(\lambda,\varphi)\rangle = E(\lambda,\varphi)|\Phi(\lambda,\varphi)\rangle$ can systematically be solved in several orders of λ, while the enforced diagonality of γ determines the required higher order terms of $h(\lambda,\varphi)$. Comparison of the 1RDM of the ground state $|\Phi(\lambda,\varphi)\rangle$ with Eq. (7) fixes $\lambda \equiv \lambda(D,N,\varphi)$. Plugging all results from the perturbation theoretical calculation into Eq. (9) yields (for $D \ll 1$):

$$\mathcal{F}_N^{(p)}[\gamma(D,\varphi))] \simeq E_N^{(0)}(\varphi) + E_N^{(1)}(\varphi)D - U\sin^2(\varphi)N\sqrt{N-1}\sqrt{D}, \tag{11}$$

where $E_N^{(0)}(\varphi) \equiv UN(N-1)[1-\frac{1}{2}\sin^2(\varphi)]$, $E_N^{(1)}(\varphi) \equiv UN(N-2)[3\sin^2(\varphi)-2]$ depend on φ and N only. The key result (11) confirms the existence of a "BEC-force" on the boundary of the domain $\mathcal{P}_p$. Indeed, we find that

$$\frac{\partial\mathcal{F}_N^{(p)}}{\partial D} = -\frac{U}{2}N\sqrt{N-1}\sin^2(\varphi)D^{-1/2} + \mathcal{O}(D^0) \tag{12}$$

diverges repulsively for $D \to 0$, for all N and φ (except $\varphi = 0,\pi$).

To fully appreciate the scope of the surprising finding (12), let us recall that the functional $\mathcal{F}_N^{(p)}$ is universal. Its form and features therefore provide insights into the ground states of *all* Hamiltonians $H(h)$ (2) *simultaneously*. To illustrate this in the Hubbard dimer, we choose an arbitrary h [i.e., t and $\Delta v \equiv (v_L - v_R)/2t$]. The energy functional follows as $N\mathrm{Tr}[h\gamma] + \mathcal{F}_N^{(p)}[\gamma]$. Its minimization yields the corresponding ground state energy and the ground state 1RDM (described by φ_0 and $D_0 \equiv 1 - N_{\mathrm{BEC}}/N$), as a function of $\Delta v, u = U/t$ and N. For the number N_{BEC} of bosons condensed in the one-particle state $|\varphi_0\rangle$ we obtain

$$N_{\mathrm{BEC}} \simeq N\left[1 - \frac{(N-1)\sin^4(\varphi_0)}{16[\sin(\varphi_0) - \Delta v\cos(\varphi_0)]^2}u^2\right]. \tag{13}$$

The required condition of BEC, $D_0 = 1 - N_{\mathrm{BEC}}/N \ll 1$ implies $u \ll 1/\sqrt{N-1}$. The corresponding natural orbital $|\varphi_0\rangle$ typically deviates from the lowest eigenstate of h, but its concrete form is here not relevant.

Bogoliubov-approximated systems.—As a second example, we discuss homogeneous dilute Bose gases with an arbitrary pair interaction $W(|\vec{r}_i - \vec{r}_j|)$ in a cubic box of length L. We exploit the commonly used s-wave scattering approximation and recall that the pair interaction simplifies in the dilute regime to $(W_0/2L^3)\hat{n}_0(\hat{n}_0-1) + (W_0/2L^3)\sum_{\boldsymbol{p}\neq 0}(2\hat{n}_0\hat{n}_{\boldsymbol{p}} + b_{\boldsymbol{p}}^\dagger b_{-\boldsymbol{p}}^\dagger b_0 b_0 + \mathrm{H.c.})$, where W_0 denotes the zeroth Fourier coefficient of $W(\cdot)$ [24]. As a consequence, the functional $\mathcal{F}[\{n_{\boldsymbol{p}}\}_{\boldsymbol{p}\neq 0}]$ separates, $\mathcal{F}[\{n_{\boldsymbol{p}}\}] = \sum_{\boldsymbol{p}\neq 0}\mathcal{F}_{\boldsymbol{p}}[n_{\boldsymbol{p}}]$. Moreover, the contribution $E_{\epsilon_{\boldsymbol{p}}}$ of each pair mode $(\boldsymbol{p},-\boldsymbol{p})$ to the ground state energy is known for any choice of the kinetic energy $\sum_{\boldsymbol{p}}\epsilon_{\boldsymbol{p}}\hat{n}_{\boldsymbol{p}}$, $E_{\epsilon_{\boldsymbol{p}}} = \frac{1}{2}[\sqrt{\epsilon_{\boldsymbol{p}}^2 + 2nW_0\epsilon_{\boldsymbol{p}}} - (\epsilon_{\boldsymbol{p}} + nW_0)]$, where $n \equiv N/L^3$ denotes the particle density. This allows us to determine $\mathcal{F}_{\boldsymbol{p}}[n_{\boldsymbol{p}}]$ more directly as the Legendre-Fenchel transform of $E_{\epsilon_{\boldsymbol{p}}}$ [cf. Eq. (3) and Refs. [32,36]], leading to $\mathcal{F}_{\boldsymbol{p}}[n_{\boldsymbol{p}}] = E_{\epsilon_{\boldsymbol{p}}(n_{\boldsymbol{p}})} - \epsilon_{\boldsymbol{p}}(n_{\boldsymbol{p}})n_{\boldsymbol{p}}$. $\epsilon_{\boldsymbol{p}}(n_{\boldsymbol{p}}) = (nW_0/2)[(2n_{\boldsymbol{p}}+1)/\sqrt{n_{\boldsymbol{p}}(n_{\boldsymbol{p}}+1)} - 2]$ follows from the inversion of the known relation $n_{\boldsymbol{p}} \equiv n_{\boldsymbol{p}}(\epsilon_{\boldsymbol{p}})$ [24]. Eventually, this yields

$$\mathcal{F}_N^{(p)}[\{n_{\boldsymbol{p}}\}] \simeq -nW_0\sum_{\boldsymbol{p}\neq 0}\left[\sqrt{n_{\boldsymbol{p}}(n_{\boldsymbol{p}}+1)} - n_{\boldsymbol{p}}\right]. \tag{14}$$

In analogy to the dimer's result (11), any homogeneous dilute Bose gas exhibits a BEC-force which diverges repulsively on the boundary of $\mathcal{P}_p$. To illustrate this, we consider a straight path to the boundary $\partial\mathcal{P}_p$. Taking the derivative of the functional (14) along that path with respect to the distance $D \equiv 1 - N_{\mathrm{BEC}}/N$ close to complete BEC yields $\mathrm{d}\mathcal{F}_N^{(p)}/\mathrm{d}D \propto -1/\sqrt{1 - N_{\mathrm{BEC}}/N}$. Hence, the diverging BEC-force prevents the system from reaching complete BEC.

Conclusion.—Bose-Einstein condensation (BEC) is often described through the Gross-Pitaevskii mean-field theory [22–24]. We have proposed a reduced density matrix functional theory (RDMFT) which no longer discards the quantum correlations but recovers them in an exact way. In contrast to its fermionic counterpart [36], the underlying one-body N-representability problem is trivial and cannot hamper the development of bosonic RDMFT. By solving the v-representability problem for the building block of optical lattices (N-boson Hubbard dimer) we identified Levy's constrained search as the ideal starting point for constructing accurate functional approximations. This allowed us to determine for two classes of systems the

exact functionals $\mathcal{F}[\gamma]$. Remarkably, their gradients were found to diverge in the regime of Bose-Einstein condensation, $\nabla_\gamma \mathcal{F} \propto 1/\sqrt{1 - N_{\mathrm{BEC}}/N}$, providing a comprehensive explanation for the absence of *complete* BEC in nature. For its proof, we developed a general approach that facilitates the calculation of functionals close to the boundary of their domains. This key finding of a universal BEC-force can be seen as the bosonic analog of the recently discovered fermionic exchange force [49].

We also would like to reiterate that $\mathcal{F}[\gamma]$ is universal. It depends only on the interparticle interaction W while the one-particle terms h are covered by the linear functional $\mathrm{Tr}[h\gamma]$. Hence, determining or approximating $\mathcal{F}[\gamma]$ would represent the simultaneous (partial) solution of the ground state problem for *all* Hamiltonians of the form $H(h) = h + W$. This offers a range of new possibilities. For instance, any trap potential could be considered and linear response coefficients become accessible. Furthermore, in analogy to many-body localization for electrons (see, e.g., Ref. [50] and references therein), the influence of disorder and interparticle interactions on BEC and their competition [51,52] can be studied in a more direct manner. All those applications highlight the promising potential of bosonic RDMFT.

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