Density-Wavefunction Mapping in Degenerate Current-Density-Functional Theory

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We show that the particle density, \(\rho(r)\), and the paramagnetic current density, \(\mathbf{j}^p(r)\), are not sufficient to determine the set of degenerate ground-state wave functions. This is a general feature of degenerate systems where the degenerate states have different angular momenta. We provide a general strategy for constructing Hamiltonians that share the same ground state density, yet differ in degree of degeneracy. We then provide a fully analytical example for a noninteracting system subject to electrostatic potentials and uniform magnetic fields. Moreover, we prove that when \((\rho, \mathbf{j}^p)\) is ensemble \((v, \mathbf{A})\)-representable by a mixed state formed from \(r\) degenerate ground states, then any Hamiltonian \(H(v', \mathbf{A}')\) that shares this ground state density pair must have at least \(r\) degenerate ground states in common with \(H(v, \mathbf{A})\). Thus, any set of Hamiltonians that shares a ground-state density pair \((\rho, \mathbf{j}^p)\) by necessity has at least have one joint ground state.

A cornerstone of modern density-functional theory (DFT) is the Hohenberg-Kohn theorem [1], which states that the ground-state particle density of a quantum-mechanical system determines up to an additive constant the one-body potential \(v\) of the same system. The original argument was limited to systems that have unique ground states. Although DFT can be formulated without recourse to the Hohenberg-Kohn theorem, using the constrained-search and Lieb’s convex analysis formalisms [2,3], the result strengthens and adds insight to the theory. Firstly, the alternative DFT formulations establish only that densities determine various contributions to the total energy; in particular, the exchange-correlation energy, and properties given as functional derivatives of the energy with respect to the scalar potential. The stronger statement that the wave function and Hamiltonian, and consequently all properties of a system, are determined still requires the Hohenberg-Kohn theorem. Secondly, whereas alternatives are known for ground-state DFT, the available formulation of time-dependent DFT is most closely related to the Hohenberg-Kohn formulation [4].

When the Hamiltonian contains a magnetic vector potential in addition to the scalar potential, the particle density alone is no longer sufficient for a rigorous formulation of DFT. The most well-established extension is current-density-functional theory (CDFT), where it has been proven that the particle density, \(\rho\), and the paramagnetic current density, \(\mathbf{j}^p\), determine the non-degenerate ground-state [5,6] (see Eqs. (1) and (3) for the definition of \(\rho\) and \(\mathbf{j}^p\), respectively). We use the term weak Hohenberg-Kohn theorem (cf. [7], Sec. III D) for this result and, following Dreizler and Gross [8], denote the invertible map from non-degenerate ground states to densities by \(\mathcal{D}\). The reason for the term weak is that such a result would be implied by the stronger but false statement that \((\rho, \mathbf{j}^p)\) determines \((v, \mathbf{A})\) [6,9,10]. Thus, the map, denoted \(\mathcal{C}\), from \((v, \mathbf{A})\) to non-degenerate ground states is not invertible. The situation can be summarized as

\[
(v, \mathbf{A}) \xrightarrow{\mathcal{C}} \psi \xrightarrow{\mathcal{D}} (\rho, \mathbf{j}^p). \tag{1}
\]

The fact that the map \(\mathcal{C}\) is not invertible does not preclude a density-functional formulation in terms of \(\rho\) and \(\mathbf{j}^p\). Indeed, the existence of the map \(\mathcal{D}^{-1}\) in non-degenerate paramagnetic CDFT is enough to define a corresponding Hohenberg-Kohn functional [5]. Furthermore, the Hohenberg-Kohn variational principle holds for the density pair \((\rho, \mathbf{j}^p)\) and a theory of density functionals can be based on these variables [5,6]. For further discussion on the choice of variables for current-density functionals we refer to [9,10], see also the mathematical analyses in [11,13] and the related [7]. For the status of the Hohenberg-Kohn theorem for physical current density instead of the paramagnetic current density, we refer to previous work showing that existing attempted proofs are flawed [9,10] and the recent progress towards a positive result using the total current density [14,15].

The aim of this work is to investigate a weak Hohenberg-Kohn result in CDFT without the assumption of a unique ground state. Given an N-electron wave function \(\psi\), define the particle density and the paramagnetic current density according to

\[
\rho_\psi(r_1) = N \int |\psi|^2 \, d\mathbf{r}_1, \tag{2}
\]

\[
\mathbf{j}_\psi^p(r_1) = N \text{Im} \int \overline{\psi} \nabla_1 \psi \, d\mathbf{r}_1, \tag{3}
\]

where \(\int d\mathbf{r}_1\) denotes integration over all space for all but one particle and \(\overline{\psi}\) denotes the complex conjugate of \(\psi\).

Furthermore, given a vector potential \(\mathbf{A}\) we may compute the total current density as the sum \(\mathbf{j} = \mathbf{j}^p + \rho \mathbf{A}\).

For vanishing \(\mathbf{A}\), the Hohenberg-Kohn theorem states that if \(\rho_1 = \rho_2\), then \(V_1 = V_2 + \text{constant}\), where \(V_k = \sum_j v_k(r_j)\) [1]. The proof of this result relies on the fact that if \(\psi\) is a ground state of both systems, then \((V_1 - V_2)\psi = \text{constant} \times \psi\). If \(\psi\) does not vanish on a
set of positive (Lebesgue) measure, we have $V_1 = V_2 + \text{constant}$ (almost everywhere). At any rate $V_1 = V_2$ up to a constant holds on the complement of $N_\psi = \{ \psi = 0 \}$. Assuming that the measure of $N_\psi$ is zero (i.e., assuming that the Schrödinger equation has the unique-continuation property from sets of positive measure), the proof can be completed by means of the variational principle as first suggested in [11]. A generalization of the original Hohenberg-Kohn theorem that includes degeneracy was given in [10]. (See also the work of Lammert [17] for further analysis of the set $N_\psi$ in connection with the Hohenberg-Kohn theorem in DFT.)

In the presence of a magnetic field, a ground state $\psi$ does not uniquely determine the Hamiltonian $H = H_0 + H_\omega$. This leads to complications in the following way: We demonstrate that a given pair $\rho$ and $j^p$ may arise from two different pairs of $v$ and $A$ that do not share the same set of ground states. This shows that the conclusion of Theorem 9 in [10] does not hold in general. Nonetheless, any set of ground-state density matrices that have the same density pair $(\rho, j^p)$ are ground states of the same set of Hamiltonians (see also [18] and the discussion that comes before Theorem 9 in [11]). We furthermore prove that $(\rho, j^p)$ at least determine one ground state, and under certain assumptions, the full set. This constitutes a weak ensemble Hohenberg-Kohn result in degenerate CDFT.

In what follows, our point of departure is a quantum mechanical system of $N$ (spinless) electrons subjected to both a magnetic field and a scalar potential. The Hamiltonian is

$$H(v, A) = H_0 + \sum_{j=1}^N \left( \frac{1}{2} \{-i\nabla_j, A(r_j)\} + v(r_j) + \frac{1}{2} A(r_j)^2 \right),$$

where $\{-\cdots\}$ denotes the anti commutator and $H_0$ is the universal part of $H$, independent of the external potentials $v$ and $A$. We let

$$H_0(\lambda) = \frac{1}{2} \sum_{j=1}^N \left( -\nabla_j^2 + \lambda \sum_{j\neq k} r_{jk}^{-1} \right), \quad 0 \leq \lambda \leq 1,$$

where $\lambda = 1$ corresponds to fully interacting electrons and $\lambda = 0$ the non-interacting case.

We start by demonstrating that $(\rho, j^p)$ does not determine the set of possibly degenerate ground states. The general idea is that for systems with cylindrical symmetry about the $z$-axis, degeneracy can either be introduced or lifted by the application of an external magnetic field. For example, consider a cylindrically symmetric Hamiltonian $H(v + A^2/2, 0)$ with a ground-state degeneracy, where the ground states are distinguished by different eigenvalues of $L_z$. The Hamiltonian $H(v, A)$ shares the same eigenstates, but the eigenvalue degeneracies are now lifted by the orbital Zeeman effect. At least for sufficiently weak magnetic fields along the $z$-axis, the state with minimal $L_z$ is then the unique ground state. The idea can also be applied in the other direction. That is, suppose a magnetic field has been tuned so that $H(v, A)$ has a ground state degeneracy, where the ground states are distinguished by different $L_z$ values. The degeneracy is then lifted in the spectrum of the Hamiltonian $H(v + A^2/2, 0)$.

In order to avoid relying on numerical results, we shall focus on a two-dimensional non-interacting system of $N$ electrons subject to a magnetic field. Define $r_j = (x_j, y_j)$, $v(r) = \frac{1}{2} \omega r^2$ and $A = (B/2)(-y, x, 0)$, where $B \geq 0$ is the strength of a uniform magnetic field perpendicular to the plane, i.e., $B = Bz$. Since $\{-i\nabla_j, A(r_j)\} = BL_{zj}$, the system’s Hamiltonian is given by

$$H = H_0(\lambda) + \sum_{j=1}^N \left( \frac{B}{2} L_{zj} + \left[ \frac{B^2}{8} + \omega^2 \right] r_j^2 \right).$$

Let $\lambda = 0$ such that $H_0 = \sum_{j=1}^N (-\nabla_j^2/2)$. We write $H = \sum_{j=1}^N h_j$, where (dropping the index $j$) the one-electron operator $h$ is given by

$$h = -\frac{1}{2} \nabla^2 + \frac{B}{2} L_z + \left[ \frac{B^2}{8} + \omega^2 \right] r^2.$$

Let $\omega = \sqrt{(B/2)^2 + \omega^2}$. The eigenfunctions of $h$ in polar coordinates fulfill (see for instance [19])

$$\phi_{n,m}(r, \varphi) = C_{n|m|} e^{i m \varphi} L_n^{|m|}(\omega r^2) e^{-\omega r^2/2},$$

where $L_n^{|m|}$ are the associated Laguerre polynomials, $n = 0, 1, \ldots$ and $m = 0, \pm 1, \ldots$ The corresponding eigenvalues, or orbital energies, are given by

$$\varepsilon_{n,m} = (2n + 1 + |m|) \omega + \frac{mB}{2}.$$

The first few $\varepsilon_{n,m}$ are plotted in Fig. 1 for a fixed $\omega = \omega_0$.

To prove our claim, Fig. 1 shows that it is enough to study a system with $N = 3$ electrons (other particle numbers are also possible). Let $|n, m\rangle$ be the abstract state vector corresponding to the single-particle wave function $\phi_{n,m}$. Set $\omega = \omega_0$, $B = B_0 = \omega_0/\sqrt{8}$, $\varepsilon_0 = 15\omega_0/\sqrt{8}$ and

$$\psi_0 = |0, 0 \rangle \otimes |0, -1 \rangle \otimes |0, 1 \rangle,$$

$$\psi_1 = |0, 0 \rangle \otimes |0, -1 \rangle \otimes |0, -2 \rangle,$$

where $\otimes$ denotes antisymmetrized tensor product. Then by direct computation, using $B_0 = \omega_0/\sqrt{2}$,

$$H_0 \psi_0 = (\varepsilon_{0,0} + \varepsilon_{0,-1} + \varepsilon_{0,1}) \psi_0 = \varepsilon_0 \psi_0,$$

$$H_0 \psi_1 = (\varepsilon_{0,0} + \varepsilon_{0,-1} + \varepsilon_{0,-2}) \psi_0 = \varepsilon_0 \psi_0,$$

and $\psi_1$ and $\psi_0$ are both degenerate ground states of $H$, with energy $\varepsilon_0$. See also Fig. 1 where $\varepsilon_{0,1} = \varepsilon_{0,-2}$ at the point $(B_0, 7B_0/2) \approx (0.57, 1.98)$ for $\omega_0 = 0.8$. Furthermore, $L_z \psi_0 = 0$ whereas $L_z \psi_1 \neq 0$.

Next, let $H'$ be a Hamiltonian of the form (4) for a different system of the same number of electrons, but with
existence of level-crossings does not depend on the presence or absence of the spin-Zeeman term. In particular, the lithium atom in a homogeneous magnetic field exhibits such a level crossing: In [22] that includes the spin-Zeeman term (see Sec. IV A and Fig. 1, Table II and Table III), the ground-state has \( L_z = 0 \) for field strengths up to a certain value after which a level crossing occurs and there are ground states with both \( L_z = 0 \) and \( L_z \neq 0 \). Arguing as above, we can find a system without a magnetic field that shares the ground-state with \( L_z = 0 \) and furthermore, for this system, the ground state is unique.

It is interesting to note that the above situation cannot arise for the hydrogen atom in a uniform magnetic field. Let \( H = \frac{1}{2}(-i\nabla + A)^2 - |r|^{-1} \), be the Hamiltonian that models a hydrogen atom in a uniform magnetic field generated by the vector potential \( A \equiv \frac{2}{r}r_\perp, B > 0 \) and \( r_\perp = (-y, x, 0) \). We denote the ground-state energy \( e_0 \) and let \( \lambda_m = \inf_{L_z = m} \langle \psi, H \psi \rangle \), \( \lambda_0 < \lambda_{-1} < ... \), since \( \lim_{r_\perp \to \infty} v = 0 \). Thus, no level crossing occurs in this system.

Now we turn to a positive result. To obtain a weak ensemble Hohenberg-Kohn result, denote \( \Omega_H \) the set of ground states belonging to \( H \) and let \( \{ \psi_k \}_{k=1}^m \) be an orthonormal basis of \( \Omega_H \). We here assume that \( m < +\infty \), i.e., the multiplicity of the ground-state energy \( e_0 \) is finite. For a basis \( \{ \psi_k \}_{k=1}^m \), \( 0 \leq \lambda_k \leq 1 \) and \( \sum_{k=1}^m \lambda_k = 1 \), let \( \Gamma_H(\lambda_1, \ldots, \lambda_m) = \sum_{k=1}^m \lambda_k \langle \psi_k, \rho \psi_k \rangle \) be a density matrix of \( H \). A ground-state particle density \( \rho \) and paramagnetic current density \( j^p \) of \( H \) are then given by \( \rho = \text{Tr} \Gamma_H \hat{\rho} = \sum_{k=1}^m \lambda_k \rho \psi_k \psi_k^* \) and \( j^p = \text{Tr} \Gamma_H \hat{j}\rho = \sum_{k=1}^m \lambda_k j^p \psi_k \). Conversely, given a particle density \( \rho \) and paramagnetic current density \( j^p \) we say that they are \((\rho, j^p)\)-ensemble-representable if there exists \( H \) with a \( \Gamma_H \) such that \( \Gamma_H \mapsto (\rho, j^p) \). We use the standard shorthand \( \Gamma_H \mapsto (\rho, j^p) \) to denote \( \rho = \sum_{k=1}^m \lambda_k \rho \psi_k \psi_k^* \) and \( j^p = \sum_{k=1}^m \lambda_k j^p \psi_k \). Here, of course, \( \{ \psi_k \}_{k=1}^m \) is a basis for \( \Omega_H \).

We have: Suppose that \( \Gamma_k \) is a ground-state density matrix of \( H_k \) and moreover that \( \Gamma_k \mapsto (\rho, j^p) \) for \( k = 1, 2 \). Then \( \Gamma_1 \) is a ground-state density matrix for \( H_2 \) and vice versa.

We can prove this claim as follows. Writing \( H_l = H_k + (H_l - H_k) \), we have for \( l \neq k \)

\[
\text{Tr} \Gamma_k H_l = e_k + \int j^p \cdot (A_l - A_k) dr + \int (\rho(\nu_l - \nu_k + (A_l^2 - A_k^2)/2)) dr.
\]

Consequently \( \text{Tr} \Gamma_1 H_2 + \text{Tr} \Gamma_2 H_1 = e_1 + e_2 \). Moreover, since \( e_l \leq \text{Tr} \Gamma_l H_l \) it follows \( e_l = \text{Tr} \Gamma_k H_l \) and \( \Gamma_k \) is also a ground-state density matrix of \( H_l \). The result is illustrated in Fig. 2.

There are some immediate consequences of the above
That Ω₁ is a ground-state density matrix of H₁. Assume further that they map to the same density, Γ₁ → (ρ, j₁) and Γ₁ → (ρ, j₂). Then it follows that Γ₁ is also a ground state of H(v₂, A₂) and that Γ₂ is also a ground state of H(v₁, A₁). Thus, both Γ₁ and Γ₂ are located in the intersection of the two ellipses.

Fact. In particular, we stress that a Hohenberg-Kohn functional can still be constructed in the degenerate case, since \( F_{HK}(\rho, j) = \text{Tr} \Gamma H \) has a unique value independent of which ground state \( \Gamma \mapsto (\rho, j) \) that is used. Furthermore, if the ground states of \( H₁ \) and \( H₂ \) are non-degenerate, then \( \rho₁ = ρ₂ \) and \( j₁ = j₂ \) implies \( \Omega₁ = \Omega₂ \). This is the result of Vignale and Rasolt [5].

Returning to the degenerate case, as demonstrated in the first part of this work \( Ω₁ = \Omega₂ \) is not true in general even though \( Γ_k \mapsto (\rho, j) \). We next introduce a definition. Given a \( (v, A) \)-ensemble-representable density pair \( (\rho, j) \), there exists an \( H \) with ground state \( Γ_H \) such that \( ρ = \text{Tr} Γ_H \hat{ρ} \) and \( j = \text{Tr} Γ_H \hat{j} \). Let \( r(Γ_H) \) denote the rank of \( Γ_H \), i.e., the number of nonzero eigenvalues \( λ_k \) of \( Γ_H \). We have the following weak ensemble Hohenberg-Kohn result:

Assume that \( H₁ \) and \( H₂ \) have the sets of ground-state densities \( Ω₁ \) with (orthonormal) basis \( ψ₁, ψ₂, ..., ψ_m \) and \( Ω₂ \) with (orthonormal) basis \( φ₁, φ₂, ..., φ_n \). Assume \( Γ₁ \mapsto (ρ₁, j₁) \) and \( Γ₂ \mapsto (ρ₂, j₂) \), where \( Γ_k \) is a ground-state density matrix of \( H_k \). If \( ρ₁ = ρ₂ \) and \( j₁ = j₂ \), it follows that \( Ω₁ \cap Ω₂ \neq \emptyset \). Moreover, with the notation \( r_k = r(Γ_k) \) then there are at least \( \max(r₁, r₂) \) linearly independent common ground states of the two systems and

\[
\dim Ω₁ \cap Ω₂ \geq \max(r₁, r₂).
\]

If in addition \( r₁ = \dim Ω₁ \) and \( r₂ = \dim Ω₂ \), then \( Ω₁ = Ω₂ \).

To prove the above, assume that \( ρ₁ = ρ₂ = ρ \) and \( j₁ = j₂ = j \). For the first part, suppose \( Ω₁ \cap Ω₂ = \emptyset \) and let \( \{λ_k\}_k \) satisfy \( 0 ≤ λ_k ≤ 1 \) and \( \sum_k λ_k = 1 \) such that \( ρ = \sum_k λ_k ψ_k \) and \( j = \sum_k λ_k j ψ_k \). We then have strict inequality

\[
e₁ < \sum_{k=1}^m λ_k (ψ_k, H₂ψ_k) = e₁ - \int j \cdot (A₂ - A₁) \, dr + \int ρ (v₂ - v₁ + (A₂^2 - A₁^2) / 2) \, dr.
\]

On the other hand, let \( \{μ_i\}_i \) satisfy \( 0 ≤ μ_i ≤ 1 \) and \( \sum_i μ_i = 1 \) and \( j' = \sum_i μ_i j \). Again using \( Ω₁ \cap Ω₂ = \emptyset \), it holds

\[
e₁ < \sum_{i=1}^n μ_i (φ_i, H₁φ_i) = e₁ - \int j' \cdot (A₁ - A₂) \, dr + \int ρ (v₂ - v₁ + (A₂^2 - A₁^2) / 2) \, dr.
\]

Adding (6) and (7) gives \( e₁ + e₂ < e₁ + e₂ \), which is a contradiction and \( Ω₁ \cap Ω₂ \neq \emptyset \).

For the second part, we use that \( Γ_k \mapsto (ρ, j) \) implies that \( Γ_k \) is a ground-state density matrix of \( H₂ \) (and vice versa). To obtain a contradiction, assume \( \dim Ω₁ \cap Ω₂ < r₁ \). Without loss of generality, let \( ψ₁, ψ₂, ..., ψ_m ∈ Ω₁ \) and \( ψ_{m+1}, ψ_{m+2}, ..., ψ_m \not∈ Ω₂ \), where \( m' < r₁ ≤ m \). This implies

\[
\text{Tr} Γ₁H₂ = \left( \sum_{k=1}^{m'} + \sum_{k=m'+1}^m \right) λ_k (ψ_k, H₂ψ_k) > e₂
\]

and \( Γ₁ \) is not a ground-state density matrix of \( H₂ \). By above, this is a contradiction. Hence, there are at least \( r₁ \) ground states \( ψ_k ∈ Ω₂ \).

The proof that there are at least \( r₂ \) ground states \( φ_k ∈ Ω₁ \) is completely analogous, and we can conclude that there are at least \( \max(r₁, r₂) \) common ground states of two systems and \( \dim Ω₁ \cap Ω₂ ≥ \max(r₁, r₂) \).

Lastly, with \( r₁ = m \) and \( r₂ = n \), we obtain from the previous step

\[
\min(m, n) ≥ \dim Ω₁ \cap Ω₂ ≥ \max(m, n).
\]

This can only hold when \( m = n \), and consequently \( Ω₁ = Ω₂ \). This completes the proof.

To summarize, we have proved that a density pair \( (ρ, j) \) in general does not determine the full set of ground states. The counterexample we have provided demonstrates that a given \( (ρ, j) \) may correspond to either a system with a unique ground state, or a system with degenerate ground states. All that is known is that any system that has \( (ρ, j) \) as a ground-state density pair must at least share one ground state. While a fully analytical proof is tractable in special cases, such as noninteracting systems, the counterexample only requires that a level-crossing can be tuned by a magnetic field. Hence, this situation is common and can be established numerically in many systems, such as the lithium atom. Moreover, we have proved a positive result. When \( (ρ, j) \) is ensemble \( (v, A) \)-representable by a mixed state formed
from $r$ degenerate ground states, then any Hamiltonian $H(v', A')$ that shares this ground state density pair must have at least $r$ degenerate ground states in common with $H(v, A)$. Finally, we emphasize that the complications in CDFT due to degeneracy does not effect the generalized Hohenberg-Kohn functional since any ground-state $\Gamma \mapsto (\rho, j^\rho)$ has the same expectation value $\text{Tr} \Gamma H_0$.

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[1] P. Hohenberg and W. Kohn, Phys. Rev. B 1964, 136, 864.
[2] M. Levy, Proc. Natl. Acad. Sci. U.S.A. 1979, 76, 6062.
[3] E. H. Lieb, Int. J. Quant. Chem. 1983, 24, 243.
[4] E. Runge and E. K. U. Gross, Phys. Rev. Lett. 1984, 52, 997.
[5] G. Vignale and M. Rasolt, Phys. Rev. Lett. 1987, 59, 2360.
[6] K. Capelle and G. Vignale, Phys. Rev. B 2002, 65, 113106.
[7] E. I. Tellgren, A. Laestadius, T. Helgaker, S. Kvaal and A. M. Teale, J. Chem. Phys. 2018, 148, 024101.
[8] R. M. Dreizler and E. K. U. Gross, Density Functional Theory: An Approach to the Quantum Many-Body Problem (Springer-Verlag 1990)
[9] E.I. Tellgren, S. Kvaal, E. Sagvolden, U. Ekström, A. M. Teale and T. Helgaker, Phys. Rev. A 2012, 86, 062506.
[10] A. Laestadius and M. Benedicks, Int. J. Quant. Chem. 2014, 114, 782.
[11] A. Laestadius, Int. J. Quant. Chem. 2014, 114, 1445.
[12] A. Laestadius, J. Math. Chem. 2014, 52, 2581.
[13] S. Kvaal and T. Helgaker, J. Chem. Phys. 2015, 143, 184106.
[14] E. I. Tellgren, Phys. Rev. A 2018, 97, 012504.
[15] M. Ruggenthaler, Ground-State Quantum-Electro-dynamical Density-Functional Theory, 2017 arXiv:1509.01417
[16] H. Englisch and R. Englisch, Physica A 1983, 121, 253.
[17] P.E. Lammert, A Gamut of Hohenberg-Kohn properties 2016, preprint arXiv:1412.3876
[18] K. Capelle, C. A. Ulrich and G. Vignale, Phys. Rev. A 2007, 76, 012508.
[19] M. Taut, J. Phys. A: Math. Gen. 1994, 27, 1045.
[20] M. Taut, P. Machon and H. Eschrig, Phys. Rev. A 2009, 80, 022517.
[21] S. Viefers, P. Koskinen, P. Singha Deo and M. Manninen, Physica E 2004, 21, 1.
[22] O.-A. Al-Hujaj and P. Schmelcher, Phys. Rev. A 2004, 70, 033411.
[23] S. Stopkowicz, J. Gauss, K. K. Lange, E. I. Tellgren and T. Helgaker, J. Chem. Phys. 2015, 143, 074110.
[24] K. K. Lange, E. I. Tellgren, M. R. Hoffmann and T. Helgaker 2012, 337 327.
[25] J. E. Avron, I. W. Herbst and B. Simon, Commun. Math. Phys. 1981, 79, 529.