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Approximation of Meanfield Terms in MCTDHF Computations by H -Matrices

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APPROXIMATION OF MEANFIELD TERMS IN MCTDHF COMPUTATIONS BY \mathcal{H} -MATRICES

OTHMAR KOCH

ABSTRACT. We discuss the approximation of the meanfield terms appearing in computations of the time-dependent Hartree–Fock method for the solution of the time-dependent multi-particle (electronic) Schrödinger equation by hierarchical matrices. This report gives theoretical error bounds for the *cross approximation* defined by low rank approximations of admissible matrix sub-blocks.

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1. INTRODUCTION

In this paper we discuss numerical aspects of the multi-configuration time-dependent Hartree–Fock method (MCTDHF) for the approximate solution of the time-dependent Schrödinger equation

$$(1) \quad i \frac{\partial \psi}{\partial t} = H \psi,$$

where the complex-valued *wave function* $\psi = \psi(x^{(1)}, \dots, x^{(f)}, t)$ explicitly depends on time t and, in the case considered here, the positions $x^{(1)}, \dots, x^{(f)} \in \mathbb{R}^3$ of

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electrons in an atom or molecule. The Hamiltonian H is time-dependent and has the form

$$(2) \quad H(t) := \sum_{k=1}^f \left(\frac{1}{2} \left(-i\nabla^{(k)} - A(t) \right)^2 + U(x^{(k)}) + \sum_{l < k} V(x^{(k)}, x^{(l)}) \right) = T(t) + V,$$

where

$$(3) \quad U(x) := -\frac{Z}{|x|}, \quad Z \in \mathbb{N},$$

$$(4) \quad V(x, y) := \frac{1}{|x - y|},$$

$$(5) \quad A(t) := (a_1(t), a_2(t), a_3(t)).$$

$A(t)$ is a smooth (vector-valued) function of t modeling an ultrafast laser pulse, and $\nabla^{(k)}$ is the nabla operator w. r. t. $x^{(k)}$ only.

2. THE MCTDHF METHOD

In MCTDHF as put forward in [12, 30, 31], the multi-electron wave function ψ from (1) is approximated by a function satisfying the ansatz

$$(6) \quad u = \sum_{(j_1, \dots, j_f)} a_{j_1, \dots, j_f}(t) \phi_{j_1}(x^{(1)}, t) \cdots \phi_{j_f}(x^{(f)}, t) =: \sum_J a_J(t) \Phi_J(x, t).$$

Using (6) for the *electronic* Schrödinger equation, the Pauli principle implies that only solutions u are considered which are antisymmetric under exchange of any pair of arguments $x^{(j)}$, $x^{(k)}$. This assumption is particular to the MCTDHF approach, as compared to the multi-configuration time-dependent Hartree method (MCTDH) proposed in [6, 7, 27, 28] for quantum molecular dynamics. Antisymmetry reduces the number of equations considerably. Particularly, the assumption implies antisymmetry in the coefficients a_J . Formally, multi-indices $J = (j_1, \dots, j_f)$ vary for $j_k = 1, \dots, N$, $k = 1, \dots, f$. Due to the simplifications resulting from the antisymmetry assumption, only $\binom{N}{f}$ equations for a_J have to be solved in the actual computations, however.

The Dirac–Frenkel variational principle [13, 14] is used to derive differential equations for the coefficients a_J and the *single-particle functions* ϕ_j . This yields equations of motion for the coefficients and single-particle functions in (6), see [25]:

$$(7) \quad i \frac{da_J}{dt} = \sum_K \langle \Phi_J | V | \Phi_K \rangle a_K, \quad \forall J,$$

$$(8) \quad i \frac{\partial \phi_j}{\partial t} = T \phi_j + (I - P) \sum_{k=1}^N \sum_{l=1}^N \rho_{j,l}^{-1} \bar{V}_{l,k} \phi_k, \quad j = 1, \dots, N,$$

where

$$(9) \quad \psi_j := \langle \phi_j | u \rangle,$$

$$(10) \quad \rho_{j,l} := \langle \psi_j | \psi_l \rangle,$$

$$(11) \quad \bar{V}_{j,l} := \langle \psi_j | V | \psi_l \rangle,$$

and P is the orthogonal projector onto the space spanned by the functions ϕ_j .

3. EFFICIENT NUMERICAL EVALUATION

To make the numerical solution of the equations of motion (7), (8) computationally tractable, some care is required in the evaluation of the right-hand side of the differential equations. The computationally most demanding part is represented by the evaluation of the meanfield operators, see also [24, Fig. 2.3]. This becomes clear when we realize that the computations involve the evaluation of integrals of the form¹

$$(12) \quad \left\langle \phi_1(x) \left| \frac{1}{|x-y|} \right| \phi_2(x) \right\rangle_{L^2(x)} \phi_3(y),$$

$$(13) \quad \left\langle \phi_1(x) \tilde{\phi}_1(y) \left| \frac{1}{|x-y|} \right| \phi_2(x) \tilde{\phi}_2(y) \right\rangle_{L^2(x,y)},$$

where $\phi_i, \tilde{\phi}_i$ are any single-particle functions from (6). To reduce the computational effort necessary for the evaluation of these terms, a procedure based on discretization and low rank approximation is proposed in [12], which approximates the full integrals by operators of low rank. In [23], bounds for the error introduced by this approximation are given. In fact, the analysis deals with terms of the form

$$(14) \quad \langle \phi_1(x) | V(x, y) | \phi_2(y) \rangle_{L^2(x,y)} = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \overline{\phi_1(x)} V(x, y) \phi_2(y) dy dx,$$

which are however representative for the treatment of the actually appearing quantities, see also [12]. Thus, we are going to concentrate on the analysis of (14) first, and indicate the extensions to (12), (13) in Appendix B.

In the present paper, we are going to extend the analysis of [23] to the case where the meanfield operators are alternatively approximated by \mathcal{H} -matrices. These were first introduced in [19, 20], and compress the data represented by a matrix of a particular structure by using *cluster trees*. Storage requirements and complexity of arithmetic operations involving \mathcal{H} -matrices scale *almost linearly* with the dimension (that is, linearly with logarithmic terms) [16]. Appendix A gives a short description of the most important features of \mathcal{H} -matrices.

Following [12], we choose a discretization in terms of a set of basis functions $\mathcal{B} = \{|i\rangle = i(r) : i = 1, \dots, L\}$ and approximate V by

$$(15) \quad V \approx V_{\text{app}} = RVR,$$

where R is the orthogonal projection onto the subspace B spanned by \mathcal{B} . As basis functions we use real-valued functions with finite support defined on the spatial grid used to solve (7), (8). In general, it is natural to use polynomial finite elements on a suitable subdivision of the spatial domain. The details may vary from case to case. Here, we want to give error bounds under the assumption that the space partition is sensible and the choice of finite elements corresponds with the task at hand. The notions used in the subsequent presentation are explained for example in [11].

We consider for \mathcal{B} the *nodal basis* for globally continuous finite elements consisting of piecewise polynomials of degree $\leq m - 1$. The resulting finite elements are *conforming*, i. e., $B \subseteq H^1$ [10, Thm. II.5.2]. We will always assume that our spatial subdivision is *quasi-uniform* [11, Def. (4.4.13)], where the diameters of the elements are proportional to $h = 1/L$, also referred to as *mesh width*.

¹Subscripts of inner products $\langle \cdot | \cdot \rangle$ refer to the respective integration variables, and likewise for norms $\| \cdot \|$, see also Appendix C. We will drop the subscripts where the arguments are clear.

Now, the projection R used in (15) is characterized by

$$(16) \quad R = \sum_{i,j=1}^L |i\rangle [Q^{-1}]_{i,j} \langle j|,$$

with the *mass matrix* Q given as

$$(17) \quad Q_{i,j} = \langle i|j\rangle.$$

Obviously, Q is real, symmetric and nonsingular, and thus Q^{-1} is also symmetric. Moreover, we have $\|Q^{-1}\|_2 = O(1/h)$ from [2, Sec. 5.5] for the spectral norm $\|\cdot\|_2$ of the matrix Q^{-1} . It is easy to show that $R^2 = R$ and R is symmetric, $\langle \phi_1 | R \phi_2 \rangle = \langle R \phi_1 | \phi_2 \rangle$. Consequently, R is indeed the orthogonal projection onto B . Note also that, since R is bounded, R is self-adjoint.

In [23], a bound

$$(18) \quad |\langle \phi_1(x) | V(x, y) - V_{\text{app}}(x, y) | \phi_2(y) \rangle_{L^2(x, y)}| = \begin{cases} O(h^m) & \text{for } V \text{ bounded,} \\ O(h^{m-1}) & \text{for } V \text{ Coulomb} \end{cases}$$

is shown for the discretization error if $\phi_1, \phi_2 \in H^m$.

Subsequently, the discrete operator V_{app} is approximated by a suitable operator whose application is computationally cheap. The global approximation put forward in [12] is analyzed in [23]. Here, we propose an approximation by a hierarchical matrix instead.

First, we rewrite (15) as

$$V_{\text{app}} = \sum_{i,j=1}^L \sum_{i',j'=1}^L |i\rangle [Q^{-1}]_{i,i'} \tilde{V}_{i',j'} [Q^{-1}]_{j',j} \langle j| = \sum_{i,j=1}^L |i\rangle [Q^{-1} \tilde{V} Q^{-1}]_{i,j} \langle j|$$

with

$$\tilde{V}_{i,j} = \int \int i(x) V(x, y) j(y) dx dy.$$

Obviously, the matrix \tilde{V} is symmetric. We now rewrite \tilde{V} as follows: define a matrix S by

$$S_{i,j} := \int i(x) g(x) j(x) dx$$

with a real function $g > 0$ which is large in regions which shall be emphasized, usually near the core. Obviously, S is symmetric, and it is easy to see that S is positive definite. Note that $\|\tilde{V}\|_2, \|S\|_2 = O(h)$, since $\|\tilde{V}\|_2 \leq \sqrt{\|\tilde{V}\|_1 \|\tilde{V}\|_\infty}$ ([15]) and the row sums and the column sums are $O(h)$, see also [2, Sec. 5.5].

In [12, 23], the Cholesky decomposition

$$S = (S^{1/2})^T S^{1/2},$$

is used to compute a low rank approximation of \tilde{V} , where the cut-off parameter can be chosen independently of the discretization parameter h , see [23]. This is realized by resorting to the transformed standard eigenvalue problem

$$(19) \quad (S^{-1/2})^T \tilde{V} S^{-1/2} \tilde{u} = \lambda \tilde{u},$$

with $\tilde{u} := S^{1/2} u$. Discarding eigenvalues smaller than a tolerance ε , finally leads to an approximation V_{low} satisfying an error bound

$$(20) \quad |\langle \phi_1(x) | V_{\text{app}}(x, y) - V_{\text{low}}(x, y) | \phi_2(y) \rangle_{L^2(x, y)}| = O(\varepsilon).$$

This corresponds to a low rank approximation of V_{app} . By computing this low rank approximation via (19), we obtained an approximation error which is independent of the mesh width.

In order to apply this concept also in the context of hierarchical matrices described in Appendix A, we adapt the idea of (19) for the approximation of the respective matrix blocks $\tilde{V}_{\mathcal{I} \times \mathcal{J}}$ (for the notation, see Appendix A) to obtain an \mathcal{H} -matrix approximation $\tilde{V}_{\mathcal{H}, \varepsilon}$. Thus, for an *admissible* block $\tilde{V}_{\mathcal{I} \times \mathcal{J}}$ with corresponding diagonal blocks $S_{\mathcal{I} \times \mathcal{I}}$ and $S_{\mathcal{J} \times \mathcal{J}}$ of S , we compute the singular value decomposition of

$$(S_{\mathcal{I} \times \mathcal{I}}^{-1/2})^T \tilde{V}_{\mathcal{I} \times \mathcal{J}} S_{\mathcal{J} \times \mathcal{J}}^{-1/2}.$$

Using a cutoff parameter ε to define the low rank approximation of each block, it is found that the overall error committed in the approximation of \tilde{V} results in

$$\|\tilde{V} - \tilde{V}_{\mathcal{H}, \varepsilon}\|_2 = |\ln(h)|O(\varepsilon),$$

see Theorem A.1 which is proven in [17]. Consequently, it is possible to write²

$$\tilde{V} - \tilde{V}_{\mathcal{H}, \varepsilon} = \hat{U} \Lambda \hat{U}^T,$$

with a unitary matrix \hat{U} and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_L)$ with $\lambda_j = |\ln(h)|O(\varepsilon h)$. Thus, the error analysis proceeds analogously to [23],

$$\begin{aligned} & |\langle \phi_1(x) | V_{\text{app}}(x, y) - V_{\mathcal{H}, \varepsilon}(x, y) | \phi_2(y) \rangle_{L^2(x, y)}| = \\ & \left| \sum_{i, j=1}^L \langle \phi_1 | i \rangle \langle j | \phi_2 \rangle \sum_{\mu=1}^L [Q^{-1} \hat{U}]_{i, \mu} \lambda_{\mu} [\hat{U}^T Q^{-1}]_{\mu, j} \right| \\ & \leq \|\phi_1\| \|\phi_2\| \sum_{i, j=1}^L \|i\| \|j\| \left| \sum_{\mu=1}^L [Q^{-1} \hat{U}]_{i, \mu} \lambda_{\mu} [\hat{U}^T Q^{-1}]_{\mu, j} \right| \\ & \leq \text{const. } \varepsilon |\ln(h)| h^3 \sum_{i, j=1}^L \sum_{\mu=1}^L |[Q^{-1} \hat{U}]_{i, \mu}| |[\hat{U}^T Q^{-1}]_{\mu, j}| \\ & \leq \text{const. } \varepsilon |\ln(h)| h^3 \sum_{i, j=1}^L [|Q^{-1} \hat{U}| |\hat{U}^T Q^{-1}|]_{i, j} \\ & \leq \text{const. } \varepsilon |\ln(h)| h^3 L \|Q^{-1} \hat{U}\|_2^2 \leq \text{const. } \varepsilon |\ln(h)| h^3 L \|Q^{-1}\|_2^2 \|\hat{U}\|_2^2 \\ & \leq \text{const. } \varepsilon |\ln(h)|, \end{aligned}$$

where the absolute value of a matrix, $|A|$, is meant entry-wise. For this estimate, we have used a simple property proven in [23, Lemma 2.1]:

Let $X \in \mathbb{R}^{L \times L}$ be a nonsingular matrix. Then,

$$\sum_{i, j=1}^L [|X^T| |X|]_{i, j} \leq L \|X\|_2^2.$$

Thus, the error of our low rank approximation is bounded in terms of the error margin ε , (almost) uniformly in the diameters of the spatial partition. We formulate this fact in the following theorem:

²Note that by construction, $\tilde{V}_{\mathcal{H}, \varepsilon}$ is symmetric, and consequently, $\tilde{V} - \tilde{V}_{\mathcal{H}, \varepsilon}$ has a symmetric singular value decomposition.

Theorem 3.1. For $\phi_1, \phi_2 \in L^2$, and an underlying spatial partition which is quasi-uniform, the error introduced by the approximation by \mathcal{H} -matrices satisfies

$$|\langle \phi_1(x) | V_{\text{app}}(x, y) - V_{\mathcal{H}, \varepsilon}(x, y) | \phi_2(y) \rangle_{L^2(x, y)}| = O(\varepsilon \ln(N)),$$

where ε is an error margin which can be freely chosen.

Remark: The logarithmic growth of this error bound can be avoided if additionally the assumptions of Corollary A.1 can be verified.

APPENDIX A. HIERARCHICAL MATRICES

Let $\mathcal{S} = \{1, \dots, n\}$ be an index set. The elements of \mathcal{S} are called *degrees of freedom*. Associate with each index i a point $x_i \in \mathbb{R}^n$. Non-empty subsets $\sigma \subseteq \mathcal{S}$ are referred to as *clusters* and associated with a bounded domain $\cup \sigma$. The latter is assumed to be contained in an axis oriented *bounding box* B_σ of minimal size.

Definition A.1. \mathcal{T} is a cluster tree for the index set \mathcal{S} , if for a parameter C there holds

- (1) \mathcal{S} is the root of \mathcal{T} .
- (2) Each node $\sigma \in \mathcal{T}$ is a subset of \mathcal{S} .
- (3) If $\sigma \in \mathcal{T}$ is a leaf, then $|\sigma| \leq C$.
- (4) If $\sigma \in \mathcal{T}$ is not a leaf, then there are two unique non-empty clusters σ', σ'' satisfying $\sigma' \cap \sigma'' = \emptyset$, $\sigma' \cup \sigma'' = \sigma$, called sons.

A cluster tree can be constructed from purely geometrical information as follows: Starting with the index set \mathcal{S} , in each step the index set is recursively split in two by halving the associated bounding box along the longest edge and partitioning the index set according to the resulting new bounding boxes. This is repeated until the size of the remaining index sets is smaller than the constant C .

Remark: It is also possible to construct the cluster tree based on the cardinality of the associated index set instead of geometric information, see [17, (5.4.11)]. This ensures that the cluster tree is *balanced*, i. e. has minimal depth. Thus, the constant C reliably controls the minimal block size, which may be desirable from the viewpoint of optimal allocation of computer memory.

For the elements of a cluster tree, we define the *level* recursively by associating with the index set \mathcal{S} the level 0 and defining the level of σ' as the level of σ plus one, if σ' is a son of σ . The *depth* of a cluster tree is the maximal level of its members. Note that, excluding pathological cases when the geometrical construction is chosen, the depth of \mathcal{T} is proportional to $\log(n)$. This property always holds when the construction is based on cardinality.

As a next step, a hierarchical partition of $\mathcal{S} \times \mathcal{S}$ is derived. If σ, τ are clusters with respective bounding boxes B_σ, B_τ , then the *block* (σ, τ) is *admissible* as long as

$$(21) \quad \max(\text{diam}(B_\sigma), \text{diam}(B_\tau)) < \eta \text{dist}(B_\sigma, B_\tau),$$

where diam denotes the diameter of a box (in Euclidean distance) and dist is the distance between the boxes. Otherwise, the block is *inadmissible*.

Remark: More general admissibility conditions are also conceivable, see [17, (5.2.9)]. When dealing with a singular potential (4), the geometric criterion (21) seems to give a good indication of the possibility to approximate the block $\tilde{V}_{\mathcal{I} \times \mathcal{J}}$ of low rank.

It should be stressed that the choice of the admissibility condition is independent of whether a geometric or cardinality based construction of the cluster tree is adopted.

The algebraic structure just derived is now applied for the approximation of a matrix $A \in \mathbb{R}^{n \times n}$, where each block in the sense of the definition given above corresponds with a submatrix $A_{\mathcal{I} \times \mathcal{J}}$ of A , where \mathcal{I} , \mathcal{J} denote subsets of the index set \mathcal{S} . In the method of *cross approximation*, a low rank approximation of each admissible block is computed by some suitable method. Instead of interpolation [8, 9], truncated Taylor expansion [19, 20] or *adaptive cross approximation* [3, 5], in our case we can simply use a truncated singular value decomposition, as the computational cost of setting up the \mathcal{H} -matrix approximation is negligible as compared to the application of this matrix in the course of the time integration of the MCTDHF equations.

In our analysis in §3, we make use of the following error bound resulting from cross approximation. A proof of this result and the subsequent corollary is given in [17], see also [4].

Theorem A.1. *Let a matrix $A \in \mathbb{R}^{n \times n}$ be approximated by a hierarchical matrix $A_{\mathcal{H}}$, where on each admissible block $A_{\mathcal{I} \times \mathcal{J}}$,*

$$\|A_{\mathcal{I} \times \mathcal{J}} - A_{\mathcal{H}, \mathcal{I} \times \mathcal{J}}\|_2 \leq \varepsilon$$

holds with an error margin ε which can be freely chosen. Then,

$$\|A - A_{\mathcal{H}}\|_2 \leq \text{const.} \ln(n)\varepsilon.$$

The assertion of the last theorem can be improved, if additionally the error in each block decays exponentially with its corresponding level in the cluster tree:

Corollary A.1. *Under the assumptions of Theorem A.1 with the additional requirement that*

$$\|A_{\mathcal{I} \times \mathcal{J}} - A_{\mathcal{H}, \mathcal{I} \times \mathcal{J}}\|_2 \leq \text{const.} q^{\ell-1} \varepsilon, \quad q < 1,$$

if $A_{\mathcal{H}, \mathcal{I} \times \mathcal{J}}$ is a block of level ℓ , we have the improved bound

$$\|A - A_{\mathcal{H}}\|_2 \leq \text{const.} \varepsilon.$$

APPENDIX B. FURTHER ESTIMATES

It is easy to extend the analysis given in this report for terms of the form (14) to the terms (12) and (13) which actually appear in the MCTDHF equations. For estimates of (13) it is sufficient to replace norms of ϕ -s by norms of products of ϕ 's, for both the discretization error and the low rank approximation. By inequalities given in Corollary C.1 in Appendix C (see also [1, 21, 26]), we find that the constant in the estimate (18) now depends on $\|\phi\|_{H^2} := \max\{\|\phi_1\|_{H^2}, \|\tilde{\phi}_1\|_{H^2}, \|\phi_2\|_{H^2}, \|\tilde{\phi}_2\|_{H^2}\}$, and the constant in Theorem 3.1 on $\|\phi\|_{H^1}$. Due to the analysis given in [26], it is clear that the latter is bounded.

For estimates of (12), we proceed as follows: Clearly, for the discretization of $V = V(x, y)$ as $V_{\text{app}} = RV R$, we find

$$\begin{aligned}
& \left\| \langle \phi_1(x) | (V - V_{\text{app}})(x, y) | \phi_2(x) \rangle_{L^2(x)} \phi_3(y) \right\|_{L^2(y)} \\
& \leq \left\| \langle \phi_1(x) | (V - V_{\text{app}})(x, y) | \phi_2(x) \rangle_{L^2(x)} \right\|_{L^\infty(y)} \|\phi_3(y)\|_{L^2(y)} \\
& \leq \left(\left\| \langle \phi_1 | V | \phi_2 - R\phi_2 \rangle_{L^2(x)} \right\|_{L^\infty(y)} + \left\| \langle \phi_1 - R\phi_1 | V | R\phi_2 \rangle_{L^2(x)} \right\|_{L^\infty(y)} \right) \|\phi_3\|_{L^2} \\
& \leq \text{const.} (\|\phi_1\|_{H^1} \|\phi_2 - R\phi_2\|_{L^2} + \|\phi_1 - R\phi_1\|_{L^2} \|R\phi_2\|_{H^1}) \|\phi_3\|_{L^2} \\
& = O(h^{m-1}),
\end{aligned}$$

analogously to (18), and the constant depends on $\|\phi\|_{H^m}$, see [11, (4.4.24)].

For the effect of the \mathcal{H} -matrix approximation, we compute

$$\begin{aligned}
(22) \quad & \left\| \langle \phi_1(x) | (V_{\text{app}} - V_{\mathcal{H},\varepsilon})(x, y) | \phi_2(x) \rangle_{L^2(x)} \phi_3(y) \right\|_{L^2(y)} \\
& \leq \left\| \langle \phi_1(x) | (V_{\text{app}} - V_{\mathcal{H},\varepsilon})(x, y) | \phi_2(x) \rangle_{L^2(x)} \right\|_{L^2(y)} \|\phi_3\|_{L^\infty} \\
& \leq \text{const.} \left\| \langle \text{Id} | (V_{\text{app}} - V_{\mathcal{H},\varepsilon})(x, y) | \overline{\phi_1}(x) \phi_2(x) \rangle_{L^2(x)} \right\|_{L^2(y)} \|\phi_3\|_{H^2} \\
& \leq \|\overline{\phi_1}\phi_2\|_{L^2} \|\phi_3\|_{H^2} \sum_{i,j=1}^L \|i\| \|j\| \left| \sum_{\mu=1}^L [Q^{-1}\hat{U}]_{i,\mu} \lambda_\mu [\hat{U}^T Q^{-1}]_{\mu,j} \right| \\
& \leq \text{const.} \|\phi_1\|_{H^1} \|\phi_2\|_{H^1} \|\phi_3\|_{H^2} \varepsilon \ln(h) h^3 \sum_{i,j=1}^L \sum_{\mu=1}^L |[Q^{-1}\hat{U}]_{i,\mu}| |[\hat{U}^T Q^{-1}]_{\mu,j}| \\
& \leq \text{const.} \varepsilon |\ln(h)| h^3 \sum_{i,j=1}^L |[Q^{-1}\hat{U}][\hat{U}^T Q^{-1}]_{i,j}| \\
& \leq \text{const.} \varepsilon |\ln(h)| h^3 L \|Q^{-1}\hat{U}\|_2^2 \leq \text{const.} \varepsilon |\ln(h)| h^3 L \|Q^{-1}\|_2^2 \|\hat{U}\|_2^2 \\
& \leq \text{const.} \varepsilon |\ln(h)|,
\end{aligned}$$

where the constant depends on $\|\phi\|_{H^2}$.

Remark: Note that the relation (see [11, (4.5.11)])

$$\|i\|_{H^m} \leq \text{const.} h^{1-m}$$

implies that estimates of (22) in Sobolev- H^m norms grow with negative powers of h . Consequently, estimates of observables depending on these norms are not bounded uniformly in h and are therefore not useful in practice.

APPENDIX C. TECHNICAL PREREQUISITES

Here, we repeat some elementary notions from functional analysis, see for example [11, 18, 22, 29].

The underlying space we consider is L^2 equipped with the inner product $\langle \cdot | \cdot \rangle$ and norm $\|\cdot\|$.

Definition C.1. $u \in L^2$ has a weak derivative $\partial u \in L^2$ if

$$\langle w | \partial u \rangle = -\langle \partial w | u \rangle$$

for all test functions w .

Definition C.2. *The set of all functions in L^2 having weak derivatives up to order $\leq k$ is denoted as the Sobolev space H^k . It is equipped with the norm*

$$\|u\|_{H^k} := \left(\sum \|\partial^\alpha u\|^2 \right)^{1/2},$$

where the sum is over all derivatives up to order k .

Furthermore, we will denote by $\|\cdot\|_{L^\infty}$ the supremum norm on the space of functions bounded almost everywhere.

If functions of several variables are considered, we will sometimes make clear what variables and spaces the inner products and norms refer to by writing

$$\langle \cdot | \cdot \rangle_{L^2(x)}, \quad \|\cdot\|_{H^k(x)}, \quad \dots$$

In our analysis we will make use of the following results, see for instance [11]. Our formulations are specific to \mathbb{R}^3 :

Theorem C.1. *Let $k, m \in \mathbb{N}$ such that $k - m > 3/2$. Then for $u \in H^k$ there is a C^m function in the L^2 equivalence class of u and*

$$\|u\|_{C^m} := \sum \|\partial^\alpha u\|_{L^\infty} \leq \text{const.} \|u\|_{H^k},$$

where the sum is over all derivatives of order up to m .

This implies the following inequalities [1], [11], [21], and [29], see also [26]:

Corollary C.1. *For functions u, v, w , the following inequalities hold:*

- (23) $|\langle u|v \rangle_{L^2}| \leq \|u\|_{L^2} \|v\|_{L^2}, \quad u, v \in L^2,$
- (24) $\|uv\|_{L^2} \leq \|u\|_{L^2} \|v\|_{L^\infty} \leq \text{const.} \|u\|_{L^2} \|v\|_{H^2}, \quad u \in L^2, v \in H^2,$
- (25) $\|uv\|_{L^2} \leq \text{const.} \|u\|_{L^4} \|v\|_{L^4} \leq \text{const.} \|u\|_{H^1} \|v\|_{H^1}, \quad u, v \in H^1.$
- (26) $\|uv\|_{H^1} \leq \text{const.} (\|u\|_{H^1} \|v\|_{H^2} + \|u\|_{H^2} \|v\|_{H^1}), \quad u, v \in H^2,$

Moreover, we will use *Hardy's inequality* [22]

$$(27) \quad \int_{\mathbb{R}^3} \frac{|u(y)|^2}{|x-y|^2} dy \leq 4 \int_{\mathbb{R}^3} |\nabla u(y)|^2 dy, \quad x \in \mathbb{R}^3.$$

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