Quantum Embedding Theories to Simulate Condensed Systems on Quantum Computers

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Abstract

Quantum computers hold promise to improve the efficiency of quantum simulations of materials and to enable the investigation of systems and properties more complex than tractable at present on classical architectures. Here, we discuss computational frameworks to carry out electronic structure calculations of solids on noisy intermediate scale quantum computers using embedding theories, and we give examples for a specific class of materials, i.e., spin defects in solids. These are promising systems to build future quantum technologies, e.g., computers, sensors and devices for quantum communications. Although quantum simulations on quantum architectures are in their infancy, promising results for realistic systems appear to be within reach.

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I. INTRODUCTION

Quantum simulations of the physical properties of molecules and solids on classical computers are routinely used to tackle many problems in materials science and chemistry [1–6]. These simulations are aimed at understanding a variety of complex systems, in diverse fields such as catalysis [7, 8] and quantum information science [9–11], as well as at generating data for computations based on machine learning and artificial intelligence [12–14]. The use of quantum computers promises to improve the efficiency of quantum simulations and to enable the adoption of high level theories for systems more complex than tractable at present [15–19].

A fundamental step in the calculation of the electronic structure of molecules and solids at the quantum-mechanical level of theory is the solution of the time-independent Schrödinger equation describing interacting electrons in the field of the nuclei; such solution provides the basis for the evaluation of numerous properties, including total and excitation energies and optimized geometries. A common strategy adopted on the quantum hardware available at present, namely noisy intermediate scale quantum computers (NISQ), is that of writing the electronic structure problem in terms of second-quantized Hamiltonians, whose parameters are determined on a classical computer from quantum chemistry [20] or density functional theory (DFT) and many-body perturbation theory [21, 22] (MBPT) calculations. The Hamiltonian is then represented in terms of qubits and quantum gates, using, for instance, the Jordan-Wigner transform [23], the parity encoding [24, 25], the Verstraete-Cirac mapping [26] or the Bravyi-Kitaev transform [24]; these mappings are implemented in several open-source codes (e.g., Qiskit [27], OpenFermion [28]). Finally, the lowest eigenvalues of the Hamiltonian are computed with an algorithm compatible with the number of available qubits and circuit depths of the hardware. Topics of active research include the study of the scaling of the algorithms used in the diagonalization of the Hamiltonian, for example variational quantum eigensolver (VQE) [29, 30] and quantum phase estimation [31], with specific attention to the dimensionality of the problem and whether shallow or deep circuits are employed [32].

Progress has been reported in the past decade in solving the Schrödinger equation for molecular systems on quantum computers [29, 33–57] ranging from simple ions, including H_3^+ and HHe^+ to molecules such as water, alkali hydrides and hydrogen chains with up

to 12 atoms, for which Hartree-Fock solutions have been recently published [51]. An interesting summary of calculations of molecular systems on quantum computers is given in Ref. [6], which also discusses the algorithms used to solve the molecular Hamiltonian in second quantization.

Recently progress has also been reported in quantum computations of model Hamiltonians, such as the Hubbard [58–62] and Heisenberg Hamiltonians [35, 62, 63], infinite hydrogen chains [64, 65], and a two-dimensional electron gas in a strong magnetic field (Hamiltonian describing quantized Landau levels) [66, 67]. Most of these calculations have been carried out on a quantum simulator (i.e., the quantum computer is simulated on a classical one), with just few examples [59, 60, 62, 63] using quantum hardware. In addition, periodic Hubbard models have been solved on quantum simulators [68–75] either within dynamical mean field theory (DMFT)[76–80] or density matrix embedding theory (DMET) [81–86], with three recent examples of DMFT [87–89] and DMET [54, 90] calculations reported on quantum computers as well. DMFT and DMET are powerful approaches [76–80] to map the strongly-correlated states of a solid onto a self-consistent quantum impurity problem [71]. A review of algorithms used for DMFT and DMET calculations of strongly correlated systems is presented in Ref. [91]. In addition, quantum simulations have been applied to solve tight-binding Hamiltonians of weakly correlated solids [92–94] on quantum simulators and quantum computers.

For most molecular and solid-state systems, the solution of the electronic structure problem using the full many-body Hamiltonian is still out of reach on both classical and near term quantum architectures, due to the large size of the Hilbert space. Interestingly, there are myriad of important problems in condensed matter physics, materials science and chemistry that can naturally be formulated in terms of active regions surrounded by a host medium, for example point defects in materials, active site of catalysts, molecular adsorbates on surfaces and nanostructures embedded in condensed systems, including matrices or solvents, to name a few. In addition strongly correlated states arising from d and f orbitals in oxides and other solids may be described by an active space embedded in a condensed medium. Hence, all of these problems may be addressed using embedding theories [79, 81–86, 95–112] which separate the electronic structure problem of an active region from that of the periodic, host environment. In particular, using embedding theories, one may define second-quantized Hamiltonians and formulate the electronic structure problem of active regions in solids in a

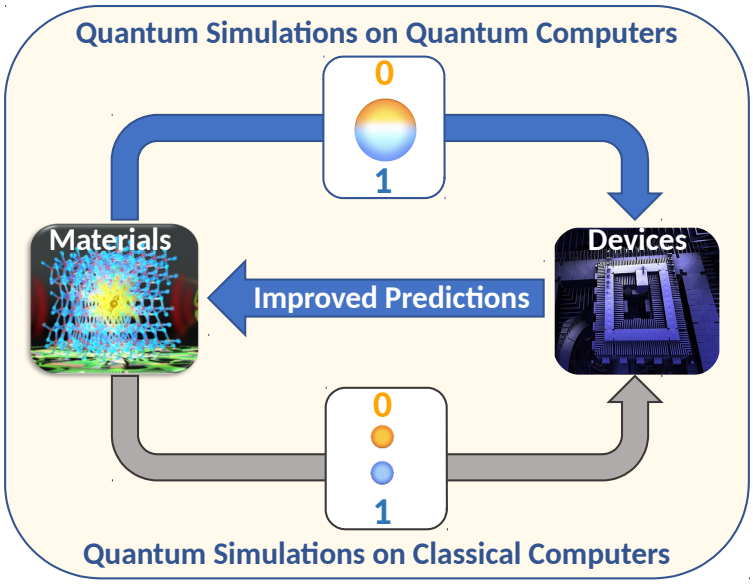

FIG. 1. From materials to devices and back again: the bottom and top arrows indicate quantum simulations of materials carried out on a classical or quantum computer, respectively, leading to the prediction and design of components for quantum architectures; the latter may then be used to perform quantum simulations (as indicated by the middle arrow) and in turn improve predictive capabilities for materials and devices.

fashion similar to that of molecular systems.

In this perspective we discuss frameworks to carry out quantum-mechanical calculations for solids on near-term quantum computers using embedding theories, with examples on a specific class of materials, i.e., spin-defects in solids (see Fig. 1), for which calculations of ground and excited state properties on a quantum computer have been recently reported. A spin-defect, i.e. a point defect with specific spin properties [9], is a promising system to realize a qubit and hence to build future quantum technologies, e.g., computers, sensors and novel devices for quantum communications [10, 11, 48, 113–116]. We discuss hybrid classical/quantum calculations of the electronic structure of spin defects and we envision a general feedback loop, where quantum simulations of materials properties on a quantum device may lead to the prediction of new materials and properties for the design of improved quantum devices, which will in turn lead to enhanced property predictions (see Fig. 1). We conclude with a discussion of current open challenges.

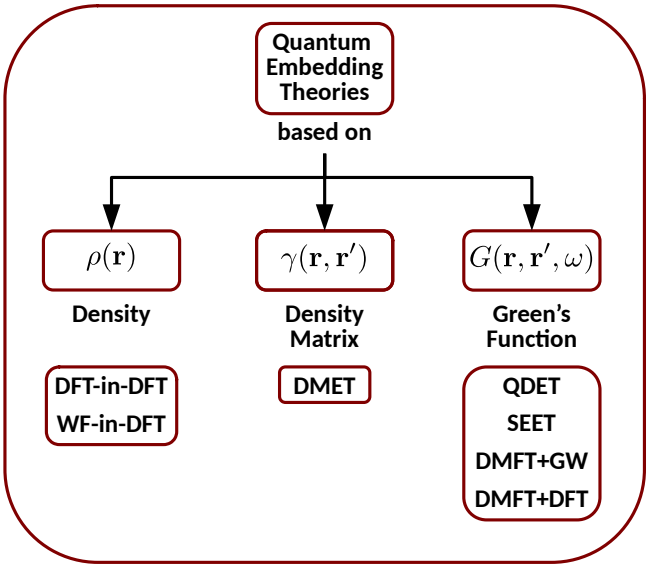

FIG. 2. A summary of quantum embedding theories used in condensed-matter physics and quantum chemistry. Density-based theories encompass density-functional-theory-in-density-functional-theory (DFT-in-DFT) and wavefunction-in-DFT (WF-in-DFT) embedding [95–97] schemes. Density-matrix embedding theory (DMET) [81–86] employs the density matrix (γ) to define an embedding protocol. Green's (G) function-based methods include quantum defect embedding theory (QDET) [98–100], self-energy embedding theory (SEET) [101–103], dynamical mean-field theory (DMFT)+GW [104–109], and DMFT+DFT [79, 110] embedding.

II. QUANTUM EMBEDDING THEORIES

As mentioned in the introduction, quantum embedding theories are frameworks to solve the time-independent Schrödinger equation for a system of electrons by separating the problem into the calculation of the energy levels or density of a so-called *active space* (or "fragment", "impurity") and those of the remaining *environment*. Each part of the system is described at the quantum-mechanical level [117, 118], with the active space being treated with a more accurate and computationally more expensive theoretical method than the environment [117]. In contrast, quantum embedding *models* describe only the active space with quantum-mechanical methods, while employing a classical description for the environment [118–121].

The three key ingredients of a quantum embedding theory are the strategy used to partition the full system into active space and environment, the computational method adopted

to describe the two portions, and the approximation for the interaction between active space and environment [122]. As illustrated in Fig. 2, we can classify embedding theories by identifying the key quantity used to realize the embedding [117, 118]. In density functional embedding theory (DFET), the active space is defined by a region in real space and the density of the system is partitioned into that of the active region and of the environment. DFT calculations for the environment yield an exchange-correlation embedding potential [95–97, 123] which then enters the Schrödinger equation for the active space; such equation is solved with a high-level quantum-chemical method. In density matrix embedding theories [81–86, 124–126], the active space is again defined by selecting a specific region of real space. However, the electronic structure of the active space is determined by solving a Schrödinger equation at a high level of theory with additional bath orbitals which account for the interaction with the environment. This framework is commonly known as the quantum impurity problem due to its similarity with the Anderson impurity problem [127]. The bath orbitals are obtained from a low-level calculation of the full system with an additional one-particle operator; the latter is constructed to satisfy the condition that the density matrix at the low- and high-level of theory be identical.

In Green's function embedding theories, such as dynamical mean-field theory embedding (DMFT+DFT [79, 110] and DMFT+GW [104–109]) or self-energy embedding theory (SEET) [101–103], the dynamical and non-local self-energy of the active space is expressed as a sum of terms evaluated at a high and low level of theory, with an additional double counting term. DMFT based methods and SEET approaches differ by the choice of high- and low-level methods and by the technique used to separate the terms of the total self-energy of the system.

Recently, we proposed a Green's function based quantum embedding theory for the calculation of defect properties in solids [98–100], which we call quantum defect embedding theory (QDET). Note that the term *defect* here is not restricted to defects in solids and simply denotes a *small guest* region embedded in a *large host* condensed system. Similar to all Green's function based methods, in QDET the active space is defined by a set of single particle electronic states. The set includes the states localized in proximity of the defect or impurity and, in some cases, contains additional single particle orbitals belonging to the host material. Within QDET, one constructs an effective Hamiltonian in second quantization which operates on the active space, using a potential which includes the ef-

fect of the environment through an effective many-body screening term. The Hamiltonian is solved using a full configuration interaction (FCI) approach, thus including correlation effects between the electronic states of the active space.

The vast majority of calculations for model solids or materials carried out on quantum simulators or quantum computers, have adopted Green's function embedding theories. Few exceptions include tight-binding Hamiltonians [92, 93] and the infinitely coordinated Bethe lattice Hubbard model treated within DMET [90]. Therefore it is instructive to compare in detail Green's function based quantum embedding theories before describing quantum computations, and such comparison is presented in the next section.

A. Comparison between Green's function based quantum embedding theories

As discussed below, although in principle QDET, DMFT+GW and SEET are related methods, these three frameworks target vastly different properties and hence applications, and can handle systems of different sizes.

Dynamical Mean Field Theory was originally proposed to solve interacting lattice models, such as the Hubbard and the periodic Anderson model [77, 128]. Building on the original formulation, the framework commonly known as DMFT+GW aims at describing correlated bands in periodic solids, e.g., transition-metal compounds with correlated $3d$- and lanthanides with correlated $4f$-bands [80, 129], for example $SrVO_3$ [106, 130–132], La_2CuO_4, and NiO [107]. The approach is designed to yield thermodynamical properties and charged excitations, which can be obtained from the one-body Green's function. Current DMFT+GW calculations on classical computers can tackle cells of the order of 5-20 atoms and dense grids of k-points.

Within this approach, the states of a chosen active space (e.g., the $3d$ bands in transition metal compounds [80, 129]) are mapped onto an effective impurity problem, which by construction reproduces the Green's function of the active space. The impurity and the states of the full solid are connected through a so called hybridization self-energy Δ, which is determined self-consistently by requiring the impurity Green's function be identical to the local Green's function of the active space. The influence of the environment on the active space is described within MBPT, using a diagrammatic expansion of the self-energy (Σ) in terms of the screened Coulomb potential W. Vertex corrections are usually neglected and

hence $\Sigma = \mathrm{i}GW$ [133–137], where G is the Green's function [107, 108, 131, 132, 138, 139]. Within DMFT+GW, the self-energy of the active space is given by the sum of the DMFT and GW self-energies plus a double counting term. The latter is necessary to remove the contribution of diagrams that are contained in both the GW and DMFT self-energies. Additionally, the interaction within the active space is screened by the polarizability of the environment, and evaluated, e.g., by using the constrained random-phase approximation (cRPA) method [140–142].

Various schemes have been proposed in the literature to evaluate the dynamical screening, as well as the charge self-consistency [143, 144], and double counting terms [108, 139, 145]. While early implementations assumed the local interactions to be static within DMFT, dynamical interactions are now included in DMFT+GW [105] calculations. These interactions may be computed using quantum Monte Carlo (QMC) solvers [128, 146–148] or exact diagonalization (ED) [149] methods; however, the implementation of QMC and ED solvers has been only reported for approximate dynamically screened interactions [105, 132, 150]. An approximation to DMFT+GW was introduced more than twenty years ago [79, 110], where the environment is described by DFT instead of many body perturbation theory; the approach is now known as DMFT+DFT. The combination of DMFT for a correlated subspace of orbitals and DFT for the remaining non-correlated states in the solid has become a widespread technique to study strongly correlated systems [80, 151]. An exact double counting scheme has been derived [152] for DMFT+DFT, although approximate double counting schemes are most often employed in the literature [79, 153–155].

While DMFT+GW targets the properties of solids, SEET was originally introduced to describe correlated states in molecular systems. However, an extension to periodic systems has recently been proposed [103, 156, 157], and applied to hydrogen chains, and to unit cells of oxides with 2 to 5 atoms, including $SrVO_3$, $SrMO_3$, MnO and NiO. SEET yields ground state properties at zero temperature, for example total energies. In (SEET) [101, 102, 158, 159] an active space is defined by a subspace of the full electronic Hilbert space, and is used to separate the independent-particle Green's function G^0 into that of the active space and its environment. Using the Dyson equation $G = G^0 + G^0\Sigma G$, where G is the full Green's function, one then defines an impurity problem for the active space, with an explicit hybridization term (Δ) with the environment. The interaction within the active space is given by the bare Coulomb potential. The self-energy of the active space is obtained as

the sum of the impurity self-energy, the self-energy computed at a low-level of theory (e.g., GW [133–136]) and a double counting term. The quantum impurity problem is solved by FCI [102, 158, 160].

Finally, QDET is designed to determine correlated electronic states of active regions in periodic solids, e.g., those of point defects embedded in a periodic crystal, and to obtain neutral excitations within the active space, for example the excited states of a spin defect with localized single particle states within a host crystal. The approach has recently been applied to defects in diamond and silicon carbide [98–100], as well as hexagonal BN [161], with periodic cells containing between 215 atoms and 511 atoms. The specific steps of a QDET calculation are summarized in Fig. 3). After performing a (hybrid) DFT calculation for the full solid using a plane-wave basis set, an active space is defined by selecting a number of Kohn-Sham states (e.g., by choosing four localized orbitals in the proximity of the negatively-charged nitrogen vacancy center (NV^-) in diamond as in Ref. [98]). The reduced polarizability χ^R and screening W^R are calculated without explicit summations over empty states (for example using the WEST code [162–165]). This is an important feature which makes QDET scalable to large supercells. Using the reduced screening as well as a double counting correction, an effective potential and an effective Hamiltonian H^{eff} are derived, describing the states belonging to the active space in the field of the environment (the rest of the crystal). For a given active space, H^{eff} is unique. Note that screening effects may be evaluated either within the RPA or explicitly taking into account the derivative of the exchange-correlation potential (f^{xc}) [98]. We also note that an exact double counting correction within the G_0W_0 approximation, which is fully consistent with those employed in DMFT+GW, has been rigorously derived, implemented and tested for QDET [166].

In the following, we clarify the connection between DMFT+GW, SEET, and QDET with an instructive example, and we discuss how correlation effects are treated by the different methods. We consider a set of localized electronic states of a defect in an insulator or semiconductor in the dilute limit (i.e. in the limit where there is a single defect within the crystal and hence no interaction between defects is present). This specific case is known as the quantum impurity problem in the atomic limit [105, 167, 168]. Ground and excited states of some of these defects are of interest for the realization of qubits, that are building blocks of quantum technologies, including quantum sensing, computing, and communication [10, 11, 48, 113–116]. While defect states in semiconductors do not form correlated bands and

hence are not commonly studied using DMFT-based frameworks, they represent a useful example to illustrate similarities and differences between methods.

Consider a supercell of a periodic solid in real space and assume the reciprocal space is sampled using only the Γ=(0,0,0) point. The mapping of the active space (localized electronic states of the mean-field Hamiltonian) to the impurity problem is exact and the hybridization vanishes, i.e., $\Delta = 0$. As such, a single, non-self-consistent solution of the impurity problem yields the electronic states of the active space. Assuming the interactions to be instantaneous, the solution of the impurity problem can be obtained by exact diagonalization, which is equivalent to full configuration interaction (FCI). Under these specific conditions, the DMFT+*GW* and QDET frameworks are identical. However, the properties that can be computed using these two frameworks and their respective regimes of validity do differ, due to the different approximations adopted in practice when carrying out calculations. Most notably, the two methods differ in their treatment of the impurity Hamiltonian: DMFT+*GW* targets correlated bands in crystalline solids, where the onsite repulsion U is the dominant term; hence the effective impurity Hamiltonian is commonly approximated by the Anderson impurity model [127] which only includes density-density repulsion terms. Some multi-orbital implementations of DMFT have been proposed in the literature, however they are rather challenging, from a computational standpoint [169, 170]. QDET, on the other hand, is specifically designed to compute neutral excitations of localized correlated states, where the treatment of exchange interactions is crucial (for example in multiplet excitations), and therefore no approximations to the effective Hamiltonian are applied.

For a defect in a periodic supercell, both QDET and SEET obtain the self-energy as the sum of a quantum impurity self-energy, the *GW* self-energy, and a double counting term. If the active space is chosen to be a subset of the quasi-particle states obtained from the *GW* calculation of the full system, then the hybridization term vanishes; in this case the SEET+*GW* framework reduces to the atomic impurity problem for the active space and becomes similar to QDET. The main difference resides in the screening of the interaction in the active space which is the bare Coulomb potential in SEET+*GW*; it is instead the screened Coulomb interaction within QDET. This difference also leads to different expressions for the double counting correction to the active-space self-energy [102].

In summary in the atomic limit, that is in the case of a single defect embedded in a

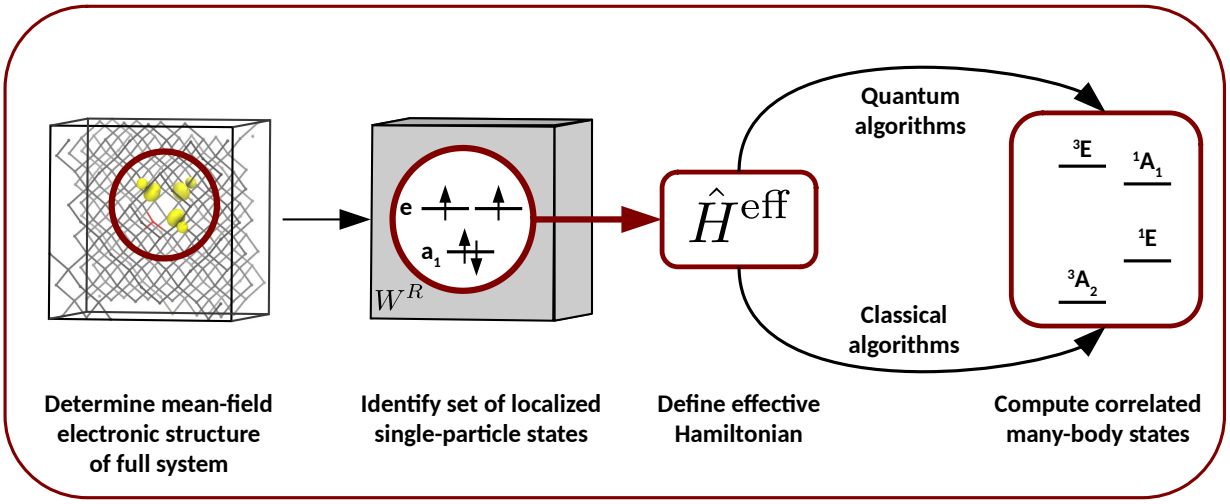

FIG. 3. Layout of materials simulations using the quantum defect embedding theory (QDET) of Ref. [98–100] on a classical and quantum computer. In the second and fourth panel from the left, representative single particle and many body states are shown, respectively. The term W^{E} (see text) denotes the screening that the environment exerts on the active space. The effective Hamiltonian H^{eff} describes the active space (see text).

surrounding host with which it does *not* hybridize, the DMFT+GW and QDET methods coincide. SEET and QDET also turn out to be similar frameworks in the case of zero hybridization, however they differ by the type of interactions (bare or screened) entering the total potential acting on the active space.

III. QUANTUM EMBEDDING ELECTRONIC STRUCTURE CALCULATIONS ON A QUANTUM COMPUTER

By reducing the complexity of electronic structure calculations of solids, quantum embedding theories lend themselves to possible implementations on quantum computers, which hold promises to reduce the exponential scaling of FCI or ED calculations. Although quantum advantage for useful chemistry and physics problems has not yet been demonstrated, the use of quantum hardware is expected to eventually pave the way to implement algorithms with a polynomial instead of exponential scaling as a function of the system size for

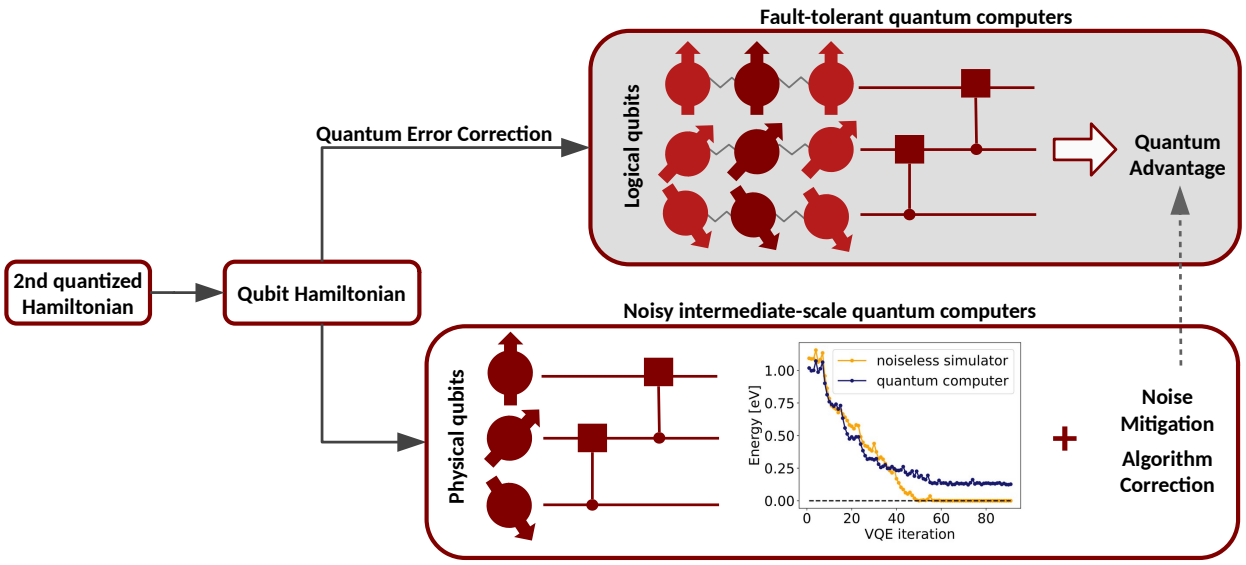

FIG. 4. Schematic representation of a quantum simulation: A second-quantized Hamiltonian is mapped to a spin Hamiltonian with a qubit representation. In the current NISQ era, the calculation with physical qubits requires noise mitigation and algorithm corrections (see text). In the future, quantum error correction is expected to lead to a logical qubit representation, and in turn to quantum advantage.

the solution of the time independent Schröedinger equation. Indeed, in a classical computer N classical bits can represent one N-bit number, but N quantum bits (qubits) can represent 2^N bit numbers on a quantum computer, providing a powerful memory scaling. Hence, it is interesting to explore how to obtain ground and excited states of second-quantized Hamiltonians and how to evaluate spectral functions on a quantum computer (see Fig. 4).

The computational complexity of quantum-embedding calculations based on Green's functions is determined by the size of the active space. In DMFT for example, the large Hilbert space of correlated $4f$ or $5f$ orbitals (14 partially occupied states) makes the study of lanthanide and actinide compounds numerically challenging. Similar challenges arise when the correlated orbitals of several atomic sites are included in the active space in cellular DMFT [171, 172] (CDMFT). In CDMFT calculations reported so far on classical hardware, typically one uses supercells or clusters with up to 100 sites [173, 174], and the maximum number of sites strongly depends on the temperature of the system. In QDET and SEET, large Hilbert spaces may arise from systems with a large number of localized defect states

or from active regions containing, for example, multiple defects.

At present, SEET, DMFT+*GW* or DMFT+DFT calculations of solids have not yet been implemented on quantum computers. Recently, first-principles DMFT calculations for La_2CuO_4 have carried out on a quantum emulator [175]. However, model Hamiltonians derived within DMFT have been diagonalized both on quantum simulators [68, 69, 71, 72] and quantum hardware [87–89]. Note that the Hubbard and Heisenberg model Hamiltonians considered so far for quantum computations are finite-site models with typically 2 sites or orbitals, which can be directly encoded on quantum hardware; instead, the infinite Hubbard lattice cannot be directly encoded and DMFT has been used to map the infinite lattice to a finite-size problem. DMFT calculations on quantum computers have so far been performed only for the single-band Hubbard model on the Bethe lattice [87–89]. These calculations, using either the variational quantum eigensolver (VQE) [87, 89] or explicit time evolution techniques [88] to obtain the impurity Green's function, have shown that quantum computing can yield results in good agreement with known analytical limits. However, the quantum noise of NISQ-era hardware leads to erroneous contributions to the self-energy Σ, which may prevent the DMFT calculation from converging [87, 88]. Thus, regularization by applying sum rules [87] or by approximations to $\Sigma(\omega)$ [88] are currently required. The noise can introduce unphysical poles in the spectral function, which in turn prevents DMFT calculations from reaching self-consistency. [68, 70, 72, 73, 87–89, 176].

Seminal applications of quantum embedding theories to realistic materials on a quantum computer have been carried out using QDET. Ma et al. [99] reported calculations of the strongly correlated states of the NV^- in diamond on a NISQ computer using a minimum model, and they obtained results consistent with those of quantum emulators, the latter coinciding with the results of classical calculations. However, the energies obtained on a quantum computer turned out to be slightly higher than those computed with a quantum emulator, due to hardware noise.

Recently, Huang *et al.* calculated the excitations of the NV^- defect in diamond and the neutral divacancy (VV^0) in 4H-SiC [177] on a quantum computer within QDET using a combination of variational quantum eigensolver (VQE) [29] and quantum subspace expansion (QSE) [178] algorithms. They found that hardware noise leads to poor conservation of the number of electrons, thus violating the variational principle. A post-selection of results enforcing particle conservation was shown to significantly improve the accuracy of the cal-

culations. An additional error reduction was obtained through a zero noise extrapolation scheme (ZNE) [42, 179], an error mitigation scheme that doesn't require additional qubits.

Calculations on quantum computers using quantum embedding methods have been performed on a variety of quantum hardware, including IBM superconducting qubits [87, 88, 98, 177], ion trap quantum qubits at the University of Maryland [87], and the quantum cloud service by Rigetti [89]. Generally, the calculations are performed using 4 qubits [87, 88, 98, 177], with the exception of Ref. [89] which employed 2 qubits.

In spite of encouraging results on quantum computers, establishing which algorithms are better suited to obtain many-body energies of electronic states of solids on NISQ hardware remains an open problem [177, 180]. For example, recent papers have proposed alternative methods to find the eigenstates of a Fermionic Hamiltonian that are not based on the variational principle and therefore do not involve an optimization procedure [62]. In particular, Ref. [181] proposed an algorithm to prepare approximate ground states with shallow circuit and, interestingly, just one parameter to define trial wave-functions.

IV. OUTLOOK

In conclusion, we have discussed several quantum embedding theories[79, 81–86, 95–110] which are promising frameworks for quantum simulations of heterogeneous solids on near term quantum computers. Although limited to few systems (spin defects in semiconductors), the results obtained so far on quantum hardware indicate that quantum simulations of strongly-correlated sites in periodic systems are within reach for NISQ quantum computers. Spin qubits [9] represent just one of the possible applications of quantum embedding theories, which may in principle be applied to a variety of localized highly-correlated states, including those found in solvated ions and nanostructures, adsorbates on surfaces and catalytic sites at surfaces and interfaces.

The verdict is not yet out, on whether quantum computers will substantially improve the scaling of algorithms in use in classical computers to diagonalize the Hamiltonian of active sites or to compute spectral functions of realistic materials beyond model Hamiltonians. Several estimates [6, 29, 33, 70, 87, 182] point at a few hundreds *logical* qubits as the requirement to reach quantum advantage in terms of algorithmic scaling. Although the relatively small number of logical qubits is encouraging, all algorithms in use today require

large gate counts of at least millions of error-corrected gates [72, 182], going beyond the capability of current NISQ hardware [183] for the implementation of hundred logical qubits. Further development of improved quantum algorithms and error-mitigation will therefore be crucial to demonstrate improved scaling on NISQ machines.

In addition, since the lowest achievable scaling of quantum computational algorithms has not yet been fully determined, the size of the active space for which quantum simulations become advantageous over classical ones is still unknown. Fault-tolerant error correction schemes[184, and references therein], necessary to apply quantum simulations to realistic materials and to obtain full quantum advantage, are an active and yet relatively new field of research and questions regarding which kind of schemes might be needed to achieve chemical accuracy are still open questions. Furthermore, for all hybrid simulations where data are moved from classical to quantum computers, communication schemes need to be carefully engineered in order to avoid transfer bottlenecks.

Finally, we note that here we just briefly addressed the problem of solving the time-independent Schrödinger equation for electrons in solids, namely a basic electronic structure problem at fixed ionic coordinates. The calculations of additional properties of materials, including structural stability [185], electron-phonon interaction [186] and finite-temperature properties [187, 188] remain, as of yet, largely unexplored on quantum computers.

AUTHOR CONTRIBUTIONS

G.G. conceived this perspective and formulated the final content with all authors. All authors contributed to the writing of the manuscript.

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