Computational materials design often profits from the fact that a part of the complicated interaction contributions is not calculated for the real material, but replaced by results of models such as the homogeneous electron gas. We turn this approximation into a very general and an in principle exact theory by introducing the concept of a connector, which is a prescription of how to use the results of a model system in order to simulate a real system. We set the conditions that must be fulfilled for the existence of an exact connector. We demonstrate that, and why, this approach is a very convenient starting point for approximations. We also show that the connector theory can be used to design new functional, for example for density functional theory. We illustrate our purposes with simple examples.

The following formal developments will be illustrated by the complexity of materials and by interaction effects. This hampers both calculations and understanding. The fundamental problem lies in the fact that the effects of the Coulomb interaction and of the specific material cannot be separated. Otherwise, one could calculate the interaction contributions once and forever, store them and add them every time a new material is calculated. This is an unreachable dream, but it still indicates an intriguing direction of thinking: in some model systems the effects of the Coulomb interaction can be treated exactly, or at least to a much better extent than in real systems, and attempts to use model results in order to simulate interaction effects in real materials are widespread. The most prominent example is the local density approximation (LDA) to density functional theory (DFT) [4], where the Kohn-Sham exchange-correlation potential at a point \( r \) is taken from a homogeneous electron gas (HEG) that is calculated at the density of the real system in the same point \( r \). In this way, DFT profits from the existence of tabulated and interpolated Quantum Monte Carlo (QMC) results [5]. Similarly, dynamical mean field theory (DMFT) in the single site approximation takes the effective local self-energy from the Anderson impurity model (AIM), and although in this case results have not been tabulated, the procedure has enabled a realistic description of correlated materials [6]. However, in spite of numerous studies and attempts [4, 7, 23] it is very difficult to go beyond these simple schemes.

The big obstacle on this route is the fact that using results of the HEG (for the case of DFT) or the single site AIM (for the case of DMFT) is considered from the very beginning as an approximation [45]. Breakthrough is instead often based on an exactification: a recent example is the exact factorization of the many-body wavefunction [46, 48] that includes the Born-Oppenheimer approximation as limiting case [49] and allows developments beyond it [50]. In a similar spirit, one may try to situate the LDA as an approximation of a much more general, in principle exact, approach. We keep this idea as broad as possible and therefore pose the following questions:

Can one exactify the idea of recycling results from one system, for example a model, to describe another system? If yes, under which conditions? And does this suggest strategies for systematic approximations? These are the questions at the heart of our work, and as we will show, there are positive answers. Our connector theory, which tells how one can in principle connect different systems, and how to find good approximations in practice, is very general. It is applicable to overcome numerous different complications (not only the problem of the Coulomb interaction). Besides the promise of an enormous speedup of calculations, as we will demonstrate it is also a powerful tool to design improved functionals, for example for DFT.

Formally, the kind of problems which this work is aimed at is the following: suppose one wishes to calculate a quantity \( Q(x) \) which is evaluated for a set of arguments \( x \) (such as points in space, frequency, temperature etc.). This quantity \( Q \) can be any observable or any other object, such as the Kohn-Sham potential. It can be difficult to calculate in a real system, but we suppose that it is accessible in the case of a model. In this model, it takes values given by \( Q(\tilde{x}) \): since the model is by definition simpler than the real system, \( \tilde{Q} \) will in general depend on a reduced set of arguments \( \tilde{x} \) that is often (but not necessarily) a subset of \( x \). Our aim is now to establish a connection between the model results and the values of \( Q \) in the real system.

The following formal developments will be illustrated in parallel with a simple example, where the real system consists of one electron in a one-dimensional (1D) potential of shape \( V(x) = \frac{1}{2} m \omega_0^2 (|x| - L)^2 \theta (|x| - L) \), with \( \omega_0 \) and \( L \) real positive parameters [51]. For \( L \to 0 \) this is the oscillator potential, while for \( \omega_0 \to \infty \) one recovers the infinite potential well \( V_\infty(x) = V_0 \theta (|x| - \frac{L}{2}) \),
with $V_0 \to \infty$. We are interested in the energy levels $E(\omega_0, L, n)$, where $n$ labels the levels. In this example, the energy $E$ plays the role of the quantity $Q$, and the set of arguments $(\omega_0, L, n)$ that fully describes the result stands for $x$. As model potential we choose the potential well $V(x) = V_\infty(x)$ with energy levels $E(L, \tilde{n})$, which represent $\tilde{Q}(\tilde{x})$. The parameter $L$ describes the model system, whereas $\tilde{n}$ labels a particular solution. One can then solve a series of model systems for different $L$, and create tables $E_\tilde{n}(L)$. Analogously, in the general case we divide $\tilde{x}$ into two sets of arguments $\tilde{x} = (\tilde{x}_1, \tilde{x}_2)$, where $\tilde{x}_1$ describes the model system, and $\tilde{x}_2$ characterizes the solution, as highlighted by the change in notation, $\tilde{Q}(\tilde{x}) \to \tilde{Q}_{\tilde{x}_2}(\tilde{x}_1)$.

The connector is defined as the prescription of how to choose the position $\tilde{x}^c_1$ in the table $\tilde{Q}$, such that one can replace $Q$ of the real system by $\tilde{Q}$ of the model system:

$$Q(x) = \tilde{Q}_{\tilde{x}_2}(\tilde{x}^c_1).$$

Formally,

$$\tilde{x}^c_1(x, \tilde{x}_2) = \tilde{Q}^{-1}_{\tilde{x}_2}(Q(x)), \quad (2)$$

where $\tilde{Q}^{-1}_{\tilde{x}_2}$ is the inverse function of $\tilde{Q}_{\tilde{x}_2}(\tilde{z})$, such that $\tilde{Q}^{-1}_{\tilde{x}_2}(\tilde{z}) = \tilde{q}$ when $\tilde{Q}_{\tilde{x}_2}(\tilde{q}) = \tilde{q}$. Now Eq. (1) reads

$$Q(x) = \tilde{Q}_{\tilde{x}_2}(\tilde{x}^c_1(x, \tilde{x}_2)). \quad (3)$$

using the table $\tilde{Q}$ via the connector is a way to reconstruct the full $x$-dependence of $Q(x)$. In our illustration, the connector $L^c$ is the width of the model square potential that guarantees $E(\omega_0, L, n) = E_n(L^c)$, i.e., one can replace a level $n$ of the real system by a level $\tilde{n}$ of the tabulated model system. The exact connector is $L^c(\omega_0, L, n, \tilde{n}) = E_n^{-1}(E(\omega_0, L, n))$.

The principle advantage of such an approach is clear: once the table $\tilde{Q}$ is stored and a connector function given, for any real system it is sufficient to use the table instead of calculating $Q$. This route is promising for three reasons: exact constraints can be defined straightforwardly, approximations are suggested by the structure of the equations, and the approach allows an interpretation of results in terms of physically meaningful building blocks.

Let us start with the first point: can the connector approach really be turned into an exact framework? This requires Eq. (1) to have a solution, which poses a condition:

- **[A]** On its domain of definition, the function $\tilde{Q}$ must yield all values that the function $Q$ can take on its domain of interest.

The domain of interest of $Q$ is set by the range of physical systems one wants to explore; this range does not necessarily include all possible physical systems. The domain of $\tilde{Q}$, on the other hand, defines the model system.

If for certain $x$ Eq. (1) cannot be fulfilled, we have to change model. In some cases, this can be achieved by extending the domain of $\tilde{Q}$. In the example of the 1D potential, one can limit the range of $L$ in order to describe the level $n = 1$ for some limited range of $L$ and $\omega_0$, but the range of $L$ has to be extended to $(0, +\infty)$ in order to describe all $n$ for all real and positive $L$ and $\omega_0$. In this way, the extension of domain would allow condition [A] to be fulfilled.

- **[B]** A unique inverse $\tilde{Q}^{-1}$ of $\tilde{Q}$ must exist over the domain spanned by all desired values of $Q$, or it must at least be possible to specify a unique choice within several possible functions $\tilde{Q}^{-1}$.

In our example we impose $\tilde{n} = n$, which is the simplest and most intuitive choice. Still, Eq. (1) is, for fixed $n$, a quadratic equation for $L$, but one of its two solutions is negative and therefore outside of the physical domain of the model.

Conditions [A] and [B] settle the framework, but nothing has been gained in practice: the unknown $Q$ still enters the calculation of the connector $\tilde{x}^c_1 = \tilde{Q}^{-1}(Q)$ in (2), and we have to proof that this is a clever starting point for approximations. The fundamental idea is to make an equivalent approximation to $Q$ and $\tilde{Q}$ which exploits the structure of (2):

$$\tilde{x}^{c, \text{approx}}_1(x, \tilde{x}_2) = (\tilde{Q}_{\tilde{x}_2}^{\text{approx}})^{-1}(Q^{\text{approx}}(x)).$$

Indeed, it is crucial to use in the calculation of the connector an approximation that is simple enough to be applied to both $Q$ and $\tilde{Q}$, although $Q$ is supposed to be well known: by imposing a similar approximation benefits from strong error canceling. The closer the model system resembles the real system, the closer are $Q$ and $\tilde{Q}$ and by consequence, the more we move towards perfect error canceling - even using a very poor approximation. How far the model system can be chosen from the real system depends on the quality of the approximation, and viceversa, how rough the approximation is that one can tolerate depends on the closeness of the model and the real system. This double dependence is a source of the power of the connector approach.

Its success is illustrated in Fig. 1 using the energy levels of the 1D potential. Our approximation is a first order perturbation expansion around a box $V_\infty$ of width $L$. The expansion parameter in the real system is $1/(L^2 \omega_0)$. Ordinary perturbation theory would directly yield energy levels $E_n^{\text{approx}}$. Fig. 1 shows that they are close to the exact $E_n$ for small $1/(L^2 \omega_0)$, but
for larger values the $E_{n}^{\text{approx}}$ strongly deviate. Below a critical value for $L^{2}\omega_{0}$, the $E_{n}^{\text{approx}}$ are even negative, which is unphysical. In the connector approach, instead, also the energy levels of the model box of width $\tilde{L}$ are expanded around those of the box of width $L$, yielding the approximate model levels $E_{n}^{\text{approx}}(\tilde{L})$. The connector $E_{n}^{\text{c,approx}}(n) = (E_{n}^{\text{approx}})^{-1}(E_{n}^{\text{approx}})$ from Eq. (4), and $E_{n}^{\text{c}} = E_{n}(E_{n}^{\text{c,approx}})$ from Eq. (3). Note that at this stage the exact tabulated model results are used for $E_{n}$. Results are shown in Fig. 1. Contrary to $E_{n}^{\text{approx}}$ obtained by direct first order perturbation theory, the connector results $E_{n}^{\text{c}}$ remain physical over the whole parameter range, and they are in much better agreement with the exact results everywhere. It must be stressed that the computational cost of the direct and the connector approximation is almost the same, especially when exact and approximate model results are tabulated. Finally, there is a physical interpretation: for a given energy level, the complicated potential acts like a simpler potential with a width that is a weighted average, given by the connector. Fig. 2 illustrates the connector strategy referring to this example.

This idea opens a huge range of computational possibilities. However, let us consider here another powerful aspect of the connector theory, which is the design of functionals. For the formal extension, it is sufficient to add to the vector $x$ a function $F$, which means that $Q$ is now also functional of $F$: $Q(x, [F])$. All previous equations remain valid, if $x$ is replaced by $x, [F]$. With this, Eq. (2) and (3) show that the connector and the target quantity $Q$, respectively, are expressed as functionals of $F$. An approximation for this functional $Q(x, [F])$ is finally obtained using (4) in (3). All steps and points of the previous discussion remain valid; therefore also this novel construction of functionals strongly benefits from error canceling.

To see what this means, let us suppose that we want to simplify the calculation of the Hartree potential $v^{H}(r, [n])$ of finite systems. As model system we choose a sphere of radius $R$ with homogeneous density $n_{h}$. The connector approach suggests to calculate and store the Hartree potential for a series of homogeneous spheres of different densities $n_{h}$, and to use this table in order to simulate the result of a real finite system. In this example, Eq. (1) reads

$$v^{H}(r, [n]) = \int dr' \frac{n(r')}{|r - r'|} = n_{h}^{\text{c}} \int_{R} dr' \frac{1}{|r - r'|}. \quad (5)$$

This yields the equivalent of (2),

$$n_{h}^{\text{c}}(r, [n], R) = \int dr' \frac{n(r')}{|r - r'|} / \int_{R} dr' \frac{1}{|r - r'|}. \quad (6)$$

which is always positive and real. It is a functional of the density that, using (3), would yield the exact results for all systems, but would still require calculation of their full Hartree potential. In the connector strategy, one instead makes the same approximation on the left and right hand sides of Eq. (5), in the spirit of (4). A rough illustration is to set $1 / |r - r'|$ to a constant $\beta$. In that case $v^{H,\text{approx}}(r) = \beta N$, where $N$ is the number of electrons. The connector result, instead, is

$$n_{h}^{\text{c,approx}}(r, [n], R) = \bar{n} \quad \text{and} \quad v^{H,\text{c}}(r) = \bar{n} \int_{R} dr' \frac{1}{|r - r'|}. \quad (7)$$

from (3), where $\bar{n}$ is the average density in the sphere. The comparison illustrates two points: first, the connector results are independent of $\beta$, i.e., they are more stable with respect to details of the approximation. Second, whereas the direct approximation screws up the result completely, the connector result still recovers the correct long range limit far from the system.

Let us finally examine how this will help the design of functionals in areas of intense research, for example of the Kohn-Sham exchange-correlation (xc) potential $v_{xc}(r, [n])$. For illustration we suppose to use the HEG as model system, so (1) is $v_{xc}(r) = v_{xc}(n^{c}(r))$. The LDA
approximates \( n_{h}^{\text{app}}(\mathbf{r}) = n(\mathbf{r}) \). Starting from the exact expression allows us to go beyond the LDA in a systematic way. One possibility to obtain a highly nonlocal density functional is to expand the real and model potentials around a given homogeneous density \( \bar{n} \) \[11–14\]. By definition, the variation in the HEG is limited to homogenetic way. One possibility to obtain a highly nonlocal

approximate density functional by extrapolating from the homogeneous electron gas, we propose an in principle exact and very general approach. Its aim is to calculate every target quantity, and must be approximated. How-

ever, we show that, and why, a given approximation is much more powerful when used within the connector theory than when directly applied to the quantity of interest. The approach is not merely a very efficient computational trick, but it can also be used to design functionals. We have illustrated this point using as example density functionals derived from the homogeneous electron gas, but we stress that the connector theory is not limited to density functional theory, nor to the choice of the homogeneous electron gas as model system. It may be used, for example, to approximate observables as functionals of the external potential, or one might decide to choose silicon as model system for a wide range of semiconductors in the perspective of high-throughput calculations. The present work sets the framework, elucidates the fundamentals and suggests directions for practical application, with a potentially huge impact on computational mate-

\[
E_{xc}^{\text{WDA}}[\bar{n}] = \int d\mathbf{r} d\mathbf{r}' \frac{n(\mathbf{r}) n(\mathbf{r}')}{2|\mathbf{r}' - \mathbf{r}|} C(\bar{n}(\mathbf{r}, \mathbf{r}')) \left( 1 - e^{-\frac{\lambda(\bar{n}(\mathbf{r}, \mathbf{r}'))}{|\mathbf{r}' - \mathbf{r}|}} \right),
\]

(10)

where \( C \) and \( \lambda \), that depend on \( \bar{n} \), make \( E_{xc} \) exact in the HEG and guarantee the validity of the sum rule \( \int d\mathbf{r} n_{xc}(\mathbf{r}, \mathbf{r}' - \mathbf{r}) = -1 \). Note that what matters here is not the quality of this approximated xc functional, but only how well and how efficiently we will be able to describe it through the connector. To check the performance of our approach, we consider an inhomogeneous “real system” with periodic density \( n(\mathbf{r}) = A \cos(\mathbf{a} \cdot \mathbf{r}) + B \), that depends on the parameters \( A \) and \( B \), and the reciprocal lattice vector \( \mathbf{a} \). In this system, the xc potential \( v_{xc}^{\text{WDA}} \) derived from (10) is very different from the LDA, as shown in Fig. 3 where \( \mathbf{a} \) and the maximum density correspond to the case of solid argon. We now expand \( v_{xc}^{\text{WDA}}(\mathbf{r}) \) at each point \( \mathbf{r} \) linearly in the density variation with respect to a homogeneous density that equals \( \bar{n} = n(\mathbf{r}) \), i.e. around the LDA, using \( f_{xc} \) derived from (10). Fig. 3 shows that the WDA potential is well described by the linear approximation in regions of high density (large \( |v_{xc}| \)), but not where the density is low. Instead, using the very same linear expansion in the connector through (3) and (4) takes into account a significant amount of non-locality and gives by far the best results (Results for another set of parameters are given in [54]).

In conclusion, inspired by a historically used strategy to approximate density functionals by extrapolating from the homogeneous electron gas, we propose an in principle exact and very general approach. Its aim is to calculate once and forever a given quantity in a model system with high precision. The results are tabulated and can be used to determine the same quantity in real systems, via a procedure termed connector. The connector is different for every target quantity, and must be approximated. However, we show that, and why, a given approximation is much more powerful when used within the connector theory than when directly applied to the quantity of interest. The approach is not merely a very efficient computational trick, but it can also be used to design functionals. We have illustrated this point using as example density functionals derived from the homogeneous electron gas, but we stress that the connector theory is not limited to density functional theory, nor to the choice of the homogeneous electron gas as model system. It may be used, for example, to approximate observables as functionals of the external potential, or one might decide to choose silicon as model system for a wide range of semiconductors in the perspective of high-throughput calculations. The present work sets the framework, elucidates the fundamentals and suggests directions for practical application, with a potentially huge impact on computational mate-
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* Present address: Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

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