The Conversion of nonlocal one-body operators into local ones:

The Slater potential revisited

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(Dated: January 27, 2022)

Abstract

One-particle Schrödinger equations are considered, e.g., the Hartree–Fock equations, that contain a nonlocal operator, e.g., the Hartree–Fock exchange operator, where this operator depends on the one-particle density-matrix of a determinantal state. One-body nonlocal operators of this type are converted into approximate local potentials that depend on the kernel of the nonlocal operator and, also, the one-particle density matrix that, as mentioned above, the nonlocal operator also depends on. When the non-local operator is the exchange operator, the method yields the Slater potential.

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I. INTRODUCTION

There is a considerable interest in the conversion of nonlocal, one-body operators into local, multiplicative operators, or potentials. For example, using a local, multiplicative operator to replace a nonlocal one can lead to significant computational savings when solving the Hartree–Fock equations, or other similar one-body, coupled equations. In addition, the Kohn-Sham approach of density functional theory (DFT) requires the noninteracting state to be obtained from a local potential, since this formalism invokes the Hohenberg-Kohn theorem, even though, according to the adiabatic connection, the exact exchange energy is the same one-particle density-matrix functional as the one from Hartree–Fock theory, except that the one-particle functions are Kohn–Sham orbitals.

Other possible applications of nonlocal to local conversions is for one-particle density-matrix approaches that employ a nonlocal operator. For example, in the reference-state one-particle density-matrix formalism, the conversion of the nonlocal exchange-correlation potential into a local operator leads naturally to a density functional theory, since the one-particle density matrix of the determinantal reference state obtained from a local potential is a unique functional of its electron density, according to the Hohenberg-Kohn theorem.

A classical example of the conversion of a nonlocal operators into a local one is Slater’s local exchange-operator, derived from a uniform electron gas. A very similar approximate functional has also been derived by Gasper, where this one only differs by a constant from the one derived by Slater. The $X\alpha$ approach includes a semiempirical parameter that yields Slater’s original prescription with $\alpha = 1$, and the one by Gasper for $\alpha = \frac{2}{3}$. Gasper’s exchange operator is also used within the local density approximation (LDA) of DFT. When the Gasper potential is combined with Becke’s exchange correction, derived in 1988, a very accurate approximation is obtained, and this two component exchange potential is used within the very successful DFT hybrid approach known as the B3LYP method.

The optimized potential method (OPM) is an approach to convert a nonlocal operator into a local potential. This method, unfortunately, leads to rather complicated functionals that depend on the individual orbitals. Below we introduce...
an approach that converts one-body nonlocal operators into approximate local potentials that depend on the kernel of the nonlocal operator and, also, the one-particle density matrix that the nonlocal operator also depends on. When the non-local operator is the exchange operator, the method yields the Slater potential \[22, 23, 36\], which also appears as the leading term from the Krieger–Li–Iafrate (KLI) approximation of the OPM \[29, 32, 36, 37\].

II. THE CLOSED-SHELL RESTRICTED SPIN-ORBITAL FORMALISM

Consider a set of spatially restricted spin-orbitals \[38\]:

\[
\psi_{i\sigma}(r, \omega) = \chi_i(r)\sigma(\omega), \; \sigma = \alpha, \beta, \tag{1}
\]

where the spin and spatial coordinates are given by \(r\) and \(\omega\), respectively. Consider also the following spinless, one-particle Schrödinger equation:

\[
\hat{F}_{\rho_1}\chi_i(r) = \epsilon_i\chi_i(r), \tag{2}
\]

where this Hermitian one-body operator is given by

\[
\hat{F}_{\rho_1} = -\frac{1}{2}\nabla^2 + v_{\rho_1} + \hat{w}_{\rho_1}, \tag{3}
\]

and \(v_{\rho_1}\) and \(\hat{w}_{\rho_1}\) are local and nonlocal operators, respectively; these operators depend on the spinless one-particle density matrix \(\rho_1\) of a closed shell single-determinantal state, say \(|\Phi\rangle\); that is, we have \[3, 21, 39\]

\[
\rho_1(r_1, r_2) = 2\sum_w \chi_w(r_1)\chi_w^*(r_2), \tag{4}
\]

where the same spatial-orbitals appearing in this summation are doubly occupied within \(|\Phi\rangle\); henceforth, \(w, x\) denote these occupied orbitals from \(|\Phi\rangle\); \(r, s\) denote the unoccupied orbitals.

Now consider the possibility of replacing the nonlocal operator \(\hat{w}_{\rho_1}\) by a local one, say \(z_{\rho_1}\); so, we have

\[
z_{\rho_1}(r_1)\chi_x(r_1) = \int dr_2 \; w_{\rho_1}(r_1, r_2)\chi_x(r_2), \tag{5}
\]

where \(w_{\rho_1}(r_1, r_2)\) is the kernel of \(\hat{w}_{\rho_1}\).
Our interest here is in the one-particle density-matrix \( \rho_1 \) that arises from solving Eq. (2). Therefore, we only consider the operator \( \hat{W}_{\rho_1} \) acting upon an occupied orbital, \( \hat{W}_{\rho_1}\chi_x \) in the above equation. In other words, \( \rho_1 \) does not depend on \( \hat{W}_{\rho_1}\chi_r \), where \( \chi_r \) is an excited orbital. We do, however, require \( \hat{W}_{\rho_1} \) to be Hermitian.

Multiplying the previous equation by \( \chi_x^* (r_3) \) and summing over the orbital indices gives

\[
z_{\rho_1}(r_1)\rho_1(r_1, r_3) = \int dr_2 w_{\rho_1}(r_1, r_2)\rho_1(r_2, r_3). \tag{6}
\]

Setting \( r_3 = r_1 \) yields the desired result:

\[
z_{\rho_1}(r_1) \approx \rho^{-1}(r_1) \int dr_2 w_{\rho_1}(r_1, r_2)\rho_1(r_2, r_1), \tag{7}
\]

where \( \rho(r) \) is the electron density, \( \rho_1(r, r) \). For example, the exact exchange operator from Hartree–Fock theory yields the Slater potential \([22, 23, 36]\),

\[
v_{\rho_1}^x(r_1) \approx -\frac{1}{2}\rho^{-1}(r_1) \int dr_2 r_{12}^{-1} |\rho_1(r_1, r_2)|^2, \tag{8}
\]

where the kernel of the exchange operator is \(-\frac{1}{2}r_{12}^{-1} \rho_1(r_1, r_2)\).

In the two previous expressions above we have changed the equality to an approximation, since these are apparently not identities, where this conclusion arises, in part, since, in our derivation of Eq. (6) we have summed over all occupied orbitals. Now if Eq. (5) is valid, of course, Eqs. (6) and (7) must be satisfied, but, not vice versa. So if we define \( z_{\rho_1} \) by Eq. (7) we will probably not satisfy Eq. (5). For example, consider a simple case of only two occupied orbitals, say \( \chi_w \) and \( \chi_x \), where instead of Eq. (5) being satisfied, we have the following relations:

\[
\begin{align*}
z_{\rho_1}(r_1)\chi_x(r_1) &= \int dr_2 w_{\rho_1}(r_1, r_2)\chi_x(r_2) + \chi_y^*(r_1)\phi(r_1), \\
z_{\rho_1}(r_1)\chi_y(r_1) &= \int dr_2 w_{\rho_1}(r_1, r_2)\chi_y(r_2) - \chi_x^*(r_1)\phi(r_1),
\end{align*}
\tag{9a,b}
\]

where \( \phi(r_3) \) is an arbitrary function. Multiplying the first equation by \( \chi_x(r_3)^* \) and the second one by \( \chi_y(r_3)^* \) removes the last terms from both equations when the two equations are added, yielding Eq. (6).

As in any operator, our operators are completely defined by their matrix elements. If the
following identities are satisfied, then the local and nonlocal operators are equivalent:
\[
\int dr_1 \chi_y(r_1) z_{\rho_1}(r_1) \chi_x(r_1) = \int dr_1 \int dr_2 \chi_y(r_1) w_{\rho_1}(r_1, r_2) \chi_x(r_2), \quad (10a)
\]
\[
\int dr_1 \chi_x(r_1) z_{\rho_1}(r_1) \chi_x(r_1) = \int dr_1 \int dr_2 \chi_x(r_1) w_{\rho_1}(r_1, r_2) \chi_x(r_2), \quad (10b)
\]
\[
\int dr_1 \chi_x(r_1) z_{\rho_1}(r_1) \chi_s(r_1) = \int dr_1 \int dr_2 \chi_x(r_1) w_{\rho_1}(r_1, r_2) \chi_s(r_2), \quad (10c)
\]
and we can replace the one-body operator, given by Eq. (3), by the following:
\[
\hat{F}_{\rho_1} = -\frac{1}{2} \nabla^2 + v_{\rho_1} + z_{\rho_1}. \quad (11)
\]
However, for our purposes, we do not need all three relations given by Eqs. (10) to be satisfied. In particular, if Eq. (10c) is not satisfied, Eq. (2) is still satisfied for the same occupied orbitals and, as mentioned previously, the one-particle density-matrix $\rho_1$ is not changed. Furthermore, if Eq. (10a) is not satisfied, we will get different occupied orbitals but they will differ only by a unitary transformation as long as Eq. (10b) remains valid, and, again, the one-particle density-matrix $\rho_1$ is not changed. Hence, we only need Eq. (10b) to be a reasonable approximation.

### III. THE OPEN-SHELL UNRESTRICTED SPIN-ORBITAL FORMALISM

We now generalize the previous derivation to the case where the determinantal state is composed of orbitals that are spatially unrestricted; that is, we have
\[
\psi_{i\sigma}(x_1) = \chi_{i\sigma}(r_1)\sigma(\omega), \quad \sigma = \alpha, \beta, \quad (12)
\]
where the spatial $r_1$ and spin coordinates $\omega_1$ are denoted collectively by $x_1$; furthermore, we have a different one-body operator for each spin-function:
\[
\hat{F}_\sigma^\gamma \chi_{i\sigma}(r_1) = \epsilon_{i\sigma} \chi_{i\sigma}(r_1), \quad (13)
\]
where the Hermitian one-body operators are given by
\[
\hat{F}_\gamma^\sigma = -\frac{1}{2} \nabla^2 + v_\gamma^\sigma + \hat{w}_\gamma^\sigma, \quad (14)
\]
and $v_\gamma^\sigma$ and $\hat{w}_\gamma^\sigma$ are local and nonlocal operators, respectively; these operators depend on the one-particle density matrix $\gamma$ of the single-determinantal state $|\Phi\rangle$; that is, we have
\[
\gamma(x_1, x_2) = \gamma(r_1, \omega_1; x_2, \omega_2) \delta_{\omega_1 \omega_2}, \quad (15)
\]
where

\[
\gamma(r_1, \omega; x_2, \omega) = \sum_\sigma |\sigma(\omega)|^2 \rho_{1\sigma}(r_1, r_2),
\]

and for \(N_\sigma\) occupied \(\sigma\) orbital, the spin-components of \(\gamma\) are given by

\[
\rho_{1\sigma}(r_1, r_2) = \sum_{w} N_\sigma \chi_{w\sigma}(r_1) \chi_{w\sigma}^*(r_2).
\]

Our one-body operators \(\hat{F}_\gamma^\sigma\), and potential, \(v_\gamma^\sigma\) and \(\hat{w}_\gamma^\sigma\), depend upon \(\gamma\). However, \(\gamma\) is an explicit functional of its components, \(\rho_{1\alpha}\) and \(\rho_{1\beta}\); furthermore, we require \(\hat{F}_\gamma^\sigma\) not to depend on the spin variable \(\omega\), since this dependence is easily removed. So, we could, instead write, for example, \(\hat{F}_{\rho_{1\alpha} \rho_{1\beta}}\), however, for a less cluttered notation, we will continue to indicate a \(\gamma\) dependence. This is also not inaccurate, since if we know \(\gamma\), we also know \(\rho_{1\alpha}\) and \(\rho_{1\beta}\).

Now, as in Eq. (5), consider the possibility of replacing the nonlocal operator \(\hat{w}_\gamma^\sigma\) by a local one, say \(z_\gamma^\sigma\):

\[
z_\gamma^\sigma(r_1) = \int dr_2 w_\gamma^\sigma(r_1, r_2) \chi_{x\sigma}(r_2),
\]

where \(w_\gamma^\sigma(r_1, r_2)\) is the kernel of \(\hat{w}_\gamma^\sigma\). Multiplying this equation by \(\chi_{x\sigma}^*(r_3)\) and summing over the orbital indices gives

\[
z_\gamma^\sigma(r_1) \rho_{1\sigma}(r_1, r_3) = \int dr_2 w_\gamma^\sigma(r_1, r_2) \rho_{1\sigma}(r_2, r_3).
\]

Setting \(r_3 = r_1\) yields the desired result:

\[
z_\gamma^\sigma(r_1) \approx \rho_{\sigma}^{-1}(r_1) \int dr_2 w_\gamma^\sigma(r_1, r_2) \rho_{1\sigma}(r_2, r_1),
\]

where \(\rho_{\sigma}(r)\) is the \(\sigma\)-component of the electron density, given by \(\rho_{1\sigma}(r, r)\). For example, the exact exchange operator from Hartree–Fock theory yields the Slater potential \[22, 23, 36\],

\[
v_{\rho_{1\sigma}}^x(r_1) \approx -\rho_{\sigma}^{-1}(r_1) \int dr_2 r_{12}^{-1} |\rho_{1\sigma}(r_1, r_2)|^2,
\]

where the kernel of the exchange operator is \(-r_{12}^{-1} \rho_{1\sigma}(r_1, r_2)\).

**APPENDIX A: THE SLATER POTENTIAL**

The Slater potential is a local approximation of the exchange potential that was suggested by Slater and used to obtain the \(X\alpha\) approach with \((\alpha = 1)\). While it is well known in the
literature that Eq. (21) is the Slater potential, we are not familiar with a derivation demonstrating that is the case. Therefore, we have decided to present one here. In appendix B we present a derivation of the Xα exchange potential.

Using the notation by Slater 22, but in atomic units, Slater’s potential has the following form:

\[ v_s(x_1) = -\frac{\sum_j N^N \sum_{k} \int u_s^*(x_1) u_k^*(x_2) u_k(x_1) u_j(x_2) r_{12}^{-1} \, dx_2}{\sum_j u_j^*(x_1) u_j(x_1)}, \quad (A1) \]

where the sums are over the \( N \) occupied spin orbitals, given by Eq. (12), we have potential, form:

\[ \text{proving that is the case. Therefore, we have decided to present one here. In appendix B we present a derivation of the Xα exchange potential.} \]

Using the notation by Slater 22, but in atomic units, Slater’s potential has the following form:

\[ v_s(x_1) = -\frac{\sum_{\sigma} \sum_{i} \sum_{j} \int \psi_{i\sigma}^*(x_1) \psi_{j\sigma}^*(x_2) \psi_{j\sigma}(x_2) \psi_{i\sigma}(x_1) r_{12}^{-1} \, dx_2}{\sum_{\sigma} \sum_{i} \psi_{i\sigma}(x_1) \psi_{i\sigma}(x_1)}, \quad (A2) \]

where the sums are over the \( N_\alpha \) and \( N_\beta \) occupied spin orbitals, and from Eq. (12), we have

\[ v_s(x_1) = -\frac{\sum_{\sigma} \sum_{i} \sum_{j} \int \chi_{i\sigma}(r_1) \chi_{j\sigma}(r_2) \chi_{j\sigma}(r_1) \chi_{i\sigma}(r_1) r_{12}^{-1} \, dr_2}{\sum_{\sigma} \sum_{i} \chi_{i\sigma}(r_1) \chi_{i\sigma}(r_1) |\sigma(\omega_1)|^2}, \quad (A3) \]

Using the following identity:

\[ \sigma^*(\omega_1) \sigma'(\omega_1) = \delta_{\sigma\sigma'} |\sigma(\omega_1)|^2, \quad (A4) \]

gives

\[ v_s(x_1) = -\frac{\sum_{\sigma} \sum_{i} \sum_{j} \int \chi_{i\sigma}(r_1) \chi_{j\sigma}(r_2) \chi_{j\sigma}(r_1) \chi_{i\sigma}(r_1) r_{12}^{-1} \, dr_2}{\sum_{\sigma} \sum_{i} \chi_{i\sigma}(r_1) \chi_{i\sigma}(r_1) |\sigma(\omega_1)|^2}, \quad (A5) \]

which can be rearranged,

\[ v_s(x_1) = -\frac{\sum_{\sigma} \sum_{i} \sum_{j} \int \chi_{i\sigma}(r_1) \chi_{j\sigma}(r_2) \chi_{j\sigma}(r_1) \chi_{i\sigma}(r_1) r_{12}^{-1} \, dr_2}{\sum_{\sigma} \sum_{i} \chi_{i\sigma}(r_1) \chi_{i\sigma}(r_1) |\sigma(\omega_1)|^2}, \quad (A6) \]

and by using Eq. (17), we have

\[ v_s(x_1) = -\frac{\sum_{\sigma} \sum_{i} \sum_{j} \int \chi_{i\sigma}(r_1) \chi_{j\sigma}(r_1) r_{12}^{-1} \, dr_2}{\sum_{\sigma} \sum_{i} \chi_{i\sigma}(r_1) \chi_{i\sigma}(r_1) |\sigma(\omega_1)|^2}, \quad (A7) \]

Furthermore, the following identity is readily verified:

\[ v_s(r_1, \omega_1) \chi_{i\sigma}(r_1) \sigma(\omega_1) = v_{\rho_{1\sigma}}^X(r_1) \chi_{i\sigma}(r_1) \sigma(\omega_1) \quad (A8) \]

indicating that the Slater potential \( v_s \), given by Eq. (A1) or (A2), is equivalent to our potential, \( v_{\rho_{1\sigma}} \), given by Eq. (21).
APPENDIX B: THE Xα EXCHANGE POTENTIAL

It is well known that the spinless, one-particle density matrix \( \rho_1(\mathbf{r}_1, \mathbf{r}_2) \) of a closed-shell unified electron-gas depends on its density \( \rho \), a constant. A generalized expression for \( \rho_1 \) is obtained by replacing the constant density with a non-constant one, say \( \rho(\mathbf{r}) \) [3]:

\[
\rho_1(\mathbf{r}_1, \mathbf{r}_2) = \rho_1(\mathbf{r}, s) = 3\rho(\mathbf{r}) \left( \frac{\sin [k_f(\mathbf{r}) s] - k_f(\mathbf{r}) s \cos [k_f(\mathbf{r}) s]}{[k_f(\mathbf{r}) s]^3} \right), \tag{B1}
\]

where

\[
k_f(\mathbf{r}) = \sqrt{3\pi^2 \rho(\mathbf{r})}, \tag{B2}
\]

and a change of coordinates is employed:

\[
\mathbf{r} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \tag{B3}
\]

\[
\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2, \tag{B4}
\]

\[
s = |\mathbf{s}| = r_{12} = [(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2]^{1/2}. \tag{B5}
\]

Using this expression for \( \rho_1 \), the exchange-energy functional for a closed shell system, given by

\[
E_x[\rho_1] = -\frac{1}{4} \int \int d\mathbf{r}_1 d\mathbf{r}_2 \ r_{12}^{-1} |\rho_1(\mathbf{r}_1, \mathbf{r}_2)|^2, \tag{B6}
\]

leads to the well known Dirac exchange-energy density-functional

\[
E_x[\rho] \approx -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} \int \rho^{4/3}(\mathbf{r}) d\mathbf{r}, \tag{B7}
\]

where in the derivation by Parr and Yang [3], the integration is expressed using the \( \mathbf{r} \) and \( \mathbf{s} \) coordinates and the integration is carried out over \( \mathbf{s} \). Analogous expressions for unrestricted orbitals and open shell systems are also readily derived [3, 6].

In the Kohn-Sham LDA [1, 3, 6], the functional derivative of the above exchange functional gives the following local exchange potential:

\[
v_x^\rho(\mathbf{r}) = -\left( \frac{3}{\pi} \rho(\mathbf{r}) \right)^{1/3}, \tag{B8}
\]

in agreement with Gasper’s potential [24]. However, it well known that this functional differs from the one obtained by Slater [22] by a factor of \( \frac{2}{3} \), where \( v_x^\rho(\mathbf{r}) \) is obtained directly from
the Hartree-Fock, nonlocal, exchange-operator and, in addition, Slater’s approach uses a sort of averaging over the occupied orbital states.

We now demonstrate that the $X_\alpha$ exchange potential, with original prescription of $\alpha = 1$, arises in our approach when considering a uniform electron gas, where we only consider the closed-shell spin restricted formalism, and the derivation in analogous to the one by Parr and Yang mentioned above. In our derivation, we also use Eq. \((B1)\) except that, at least for the moment, we leave the density as a constant:

$$\rho_1(r_1, r_2) = 3\rho \frac{1}{k_f s^3} (\sin(k_f s) - k_f s \cos(k_f s)).$$ \hfill (B9)

Substituting this expression into Eq. \((B8)\) and using Cartesian coordinates gives

$$v_{\rho_1}^x(r_1) = -\frac{9}{2} \rho \int \int \int dx_2 dy_2 dz_2 \frac{1}{s^3 k_f^5} (\sin(k_f s) - k_f s \cos(k_f s))^2. \hfill (B10)$$

Now as far as the integral is concerned, $x_1, y_1, z_1$ are constants. Therefore, by making the following substitution:

$$s_x = (x_2 - x_1) \hfill (B11)$$

as well as analogous ones for $s_y$ and $s_z$, where, for example $(ds_x = dx_2)$, we get

$$v_{\rho_1}^x(r_1) = -\frac{9}{2} \rho \int \int \int ds_x ds_y ds_z \frac{1}{s^3 k_f^5} (\sin(k_f s) - k_f s \cos(k_f s))^2, \hfill (B12)$$

which in spherical coordinates, can be written as

$$v_{\rho_1}^x(r_1) = -18\pi \rho \frac{1}{k_f^2} \int ds \frac{1}{s^5 k_f^5} (\sin(k_f s) - k_f s \cos(k_f s))^2. \hfill (B13)$$

Making the following substituting $t = k_f s$, where $ds = dt/k_f$, we have

$$v_{\rho_1}^x(r_1) = -18\pi \frac{\rho}{k_f^2} \int_0^\infty dt \frac{1}{t^5} (\sin t - t \cos t)^2. \hfill (B14)$$

and since the integral is $\frac{1}{4}$, we get

$$v_{\rho_1}^x(r_1) = v_\rho^x = -\frac{9}{2} \pi \frac{\rho}{k_f^2}, \hfill (B15)$$

where we have introduced a different notation for the exchange potential, since it is simply a constant that depends on $\rho$. Using Eq. \((B2)\), we obtain the following expression after some algebra and by replacing $\rho$ by a non-constant density, $\rho(r)$:

$$v_\rho^x(r) = -\frac{3}{2} \left( \frac{3}{\pi} \rho(r) \right)^{1/3}. \hfill (B16)$$
This expression is in agreement with Slater’s original prescription of $\alpha = 1$.

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