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The optimal size of the exchange hole and reduction to one-particle Hamiltonians

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Abstract. We use the concept of the exchange hole introduced by Slater to bound the energy of atoms, molecules, and other systems interacting by Coulomb forces from below by one-particle Hamiltonians with an effective screening potential and an exchange hole around each electron. Interestingly enough the optimal size of the exchange hole is smaller than Slater proposed: the best lower bound is obtained when the exchange hole carries charge $1/2$ instead of 1. To highlight the quality of our estimate we show that the Dirac exchange energy with a slightly different constant bounds the exchange–correlation energy from below, an estimate previously derived by Lieb and later improved by Lieb and Oxford.

Keywords: Exchange hole – correlation energy – exchange energy – Lieb-Oxford inequality – Coulomb systems

1 Introduction

Slater [1] simplified the Hartree–Fock equations by introducing a ball around each electron that carries a unit charge modeling the self-interaction and the exchange energy of a system of N electrons. This ball, called an "exchange hole" for brevity, replaces the exchange term in the Hartree–Fock equations and thus leads to a substantial simplification. Because of this importance it has attracted considerable interest since the pioneering work of Slater. We need to restrict ourselves for brevity but would like to mention the recent works of Buijse and Baerends [2], Springborg et al. [3], Becke and Roussel [4], and the references therein.

The novelty of our result is that it does not only give an expression for the exchange–correlation energy of atoms and molecules that becomes exact in the limit of large (neutral) atoms [5, 6, 7, 8]; it also yields a rigorous lower bound on the exact energy.

The observation relevant for us is due to Hughes [9, 10]. He noted that the classical Coulomb interaction of N point particles at positions $\mathbf{x}_1, \ldots, \mathbf{x}_N$ with unit charge can be estimated from below as follows

$$\sum_{1\leq n<m\leq N} \frac{1}{|\mathbf{x}_n-\mathbf{x}_m|} \geq \sum_{n=1}^{N} \int\limits_{|\mathbf{y}-\mathbf{x}_n|>R_1(\mathbf{x}_n)} \frac{\sigma(\mathbf{y})\mathrm{d}\mathbf{y}}{|\mathbf{y}-\mathbf{x}_n|} - D(\sigma,\sigma) + \sum_{n=1}^{N} \frac{1}{2R_1(\mathbf{x}_n)} \quad , \tag{1}$$

where we use the following notation: given any charge density, σ, in three-dimensional space, $\mathbb{R}^3$, we denote its electrostatic self-energy by $D(\sigma,\sigma)$, i.e.,

$$D(\sigma,\sigma) := \frac{1}{2}\int\limits_{\mathbb{R}^3} \mathrm{d}\mathbf{x} \int\limits_{\mathbb{R}^3} \mathrm{d}\mathbf{y} \frac{\sigma(\mathbf{x})\sigma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} \quad . \tag{2}$$

Here and in the following we assume that the integral exists (Eq. 2) even when σ is replaced by its absolute value $|\sigma|$. We also assume that $\int_{\mathbb{R}^3} \mathrm{d}\mathbf{y}|\sigma(\mathbf{y})|/|\mathbf{x}-\mathbf{y}|$ is finite for almost all $\mathbf{x}$.

Furthermore, we fix any nonnegative density and define $R_\xi(\mathbf{x})$ to be the radius of the smallest ball with center at $\mathbf{x}$ containing charge ξ, i.e., the smallest R fulfilling

$$\int\limits_{|\mathbf{y}-\mathbf{x}|\leq R} \sigma(\mathbf{y})\mathrm{d}\mathbf{y} = \xi \quad . \tag{3}$$

We assume, of course, $0 < \xi < \int \sigma$. For $R_{1/2}(\mathbf{x})$ we write simply $R(x)$.

Let us note the following:

1. The assumption that the exchange hole contains a unit charge was strongly influenced by Slater's heuristic arguments.
2. Although the inequality is true for any charge density σ, good results will be only obtained if it is picked to be a realistic density. In fact, using the Thomas–Fermi density allows us to obtain lower

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bounds that are correct up to second order in $Z^{-1/3}$ (Scott correction) [6, 7, 8, 9, 10]. It is also possible to determine σ self-consistently, i.e., setting $\sigma := |u_1(x)|^2 + \ldots + |u_N(x)|^2$, where the u_n are the solutions of the corresponding one-particle problem.
3. The inequality Eq. (1) implies strong simplifications for the treatment of interacting systems: it allows us to replace two-particle operators by one-particle operators, since their ground states are known to be Slater determinants. It is therefore of utmost importance to obtain a bound of this type that is as tight as possible.

The purpose of this paper is exactly this, i.e., to improve the above bound. We will no longer fix the amount of charge, ξ, in the exchange hole. Instead we will take it as a variational parameter. It will turn out that the bound on the interaction energy does not only simplify for $\xi = 1/2$; it will also improve and be tighter compared with all other values of ξ, including 1.

As an application we show in Sect. 3 that the resulting bound implies an inequality of Lieb [11] later improved by Lieb and Oxford [12].

2 An optimal lower bound on the Coulomb interaction via an exchange hole

Our main result is the following inequality:

Theorem 1.
Let σ be a charge density with $\int \sigma(\mathbf{y})\mathrm{d}\mathbf{y} \geq 1/2$. Then, for any given number N of points $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in space we have

$$\sum_{1\leq n<m\leq N} \frac{1}{|\mathbf{x}_n - \mathbf{x}_m|} \geq \sum_{n=1}^{N} \int_{|\mathbf{y}-\mathbf{x}_n|>R_\xi(\mathbf{x}_n)} \frac{\sigma(\mathbf{y})d\mathbf{y}}{|\mathbf{y}-\mathbf{x}_n|} - D(\sigma,\sigma) + \sum_{n=1}^{N} \frac{\xi - 1/2}{R_\xi(\mathbf{x}_n)} \quad . \tag{4}$$

2. *The right-hand side rhs of* Eq. (4) *has its maximum for* $\xi = 1/2$.

We would like to remark that we can replace $\sigma(\mathbf{x})\mathrm{d}\mathbf{x}$ by any signed measure $\mathrm{d}\mu(\mathbf{x})$ with the previously mentioned requirements on its interaction energy and its potential. Our main result would still be true. We leave this to the interested reader.

Our proof depends on a well-known formula that goes back to Newton [13]: for any spherically symmetric charge density, ρ, one has

$$\int_{\mathbb{R}^3} \frac{\rho(\mathbf{y})\mathrm{d}\mathbf{y}}{|\mathbf{x}-\mathbf{y}|} = \int_0^\infty \frac{4\pi r^2 \rho(r)\mathrm{d}r}{\max\{r, |\mathbf{x}|\}} \quad , \tag{5}$$

which is easily verified by integration in spherical coordinates.

Proof 1. It is convenient to introduce a charge density of total charge one which is smeared out uniformly on a sphere of radius R centered at $\mathbf{y} \in \mathbb{R}^3$:

$$\mathrm{d}\mu_{R,\mathbf{y}}(\mathbf{x}) := \frac{\delta(|\mathbf{x}-\mathbf{y}| - R)\mathrm{d}\mathbf{x}}{4\pi R^2} \quad . \tag{6}$$

We begin with the crucial observation that the Coulomb kernel is positive as an operator, i.e.,

$$D(\mu,\mu) \geq 0 \quad , \tag{7}$$

for any complex measure, μ, on the three-dimensional space provided the corresponding integral is absolutely convergent, i.e., $\int_{\mathbb{R}^3} \mathrm{d}|\mu|(\mathbf{x}) \int_{\mathbb{R}^3} \mathrm{d}|\mu|(y)|\mathbf{x}-\mathbf{y}|^{-1}$ is finite. Now, we choose

$$\mathrm{d}\mu(x) := \sigma - \mathrm{d}\mu_{R_\xi(\mathbf{x}_1),\mathbf{x}_1} - \ldots - \mathrm{d}\mu_{R_\xi(\mathbf{x}_N),\mathbf{x}_N} \quad .$$

Rearranging the terms in Eq. (7) gives

$$2\sum_{1\leq n<m\leq N} D\left[\mu_{R_\xi(\mathbf{x}_n),\mathbf{x}_n}, \mu_{R_\xi(\mathbf{x}_m),\mathbf{x}_m}\right] \geq -D(\sigma,\sigma) - \sum_{n=1}^{N} D\left[\mu_{R_\xi(\mathbf{x}_n),\mathbf{x}_n}, \mu_{R_\xi(\mathbf{x}_n),\mathbf{x}_n}\right] + 2\sum_{n=1}^{N} D\left[\sigma, \mu_{R_\xi(\mathbf{x}_n),\mathbf{x}_n}\right]. \tag{8}$$

We evaluate and estimate the occurring expressions. By explicit computation using Newton's formula Eq. (5) we find

$$2D\left[\mu_{R_\xi(\mathbf{x}_n),\mathbf{x}_n}, \mu_{R_\xi(\mathbf{x}_m),\mathbf{x}_m}\right] \leq |\mathbf{x}_n - \mathbf{x}_m|^{-1} \quad , \tag{9}$$

which is also obvious from the physical point of view: it costs energy to contract the smeared-out unit charge to a point. This means, that we can estimate the left–hand side of Eq. (8) from above by $\sum_{1\leq n<m\leq N} |\mathbf{x}_n - \mathbf{x}_m|^{-1}$. Computing, the self-interaction of a unit charge smeared out on a sphere of radius R yields

$$D(\mu_{R,\mathbf{x}}, \mu_{R,\mathbf{x}}) = \frac{1}{2R} \quad . \tag{10}$$

Finally, the summands of the last term of the right side of Eq. (8) are again computed explicitly:

$$D(\sigma, \mu_{R_\xi(\mathbf{x}),\mathbf{x}}) = \frac{1}{2} \int_{|\mathbf{y}-\mathbf{x}|>R_\xi(\mathbf{x})} \frac{\sigma(\mathbf{y})}{|\mathbf{y}-\mathbf{x}|}\mathrm{d}\mathbf{y} + \frac{\xi}{2R_\xi(\mathbf{x})} \quad . \tag{11}$$

Inserting the estimates gives the desired first inequality

$$\sum_{1\leq n<m\leq N} \frac{1}{|\mathbf{x}_n - \mathbf{x}_m|} \geq \sum_{n=1}^{N} \int_{|\mathbf{y}-\mathbf{x}_n|>R_\xi(\mathbf{x}_n)} \frac{\sigma(\mathbf{y})}{|\mathbf{y}-\mathbf{x}_n|}\mathrm{d}\mathbf{y} - D(\sigma,\sigma) + \sum_{n=1}^{N} \frac{\xi - 1/2}{R_\xi(\mathbf{x}_n)} \quad . \tag{12}$$

Proof 2. To prove the second part of the theorem we compare the rhs of Eq. (4) at $\xi = 1/2$ with all other values of $\xi = 1/2 + \epsilon$: we have – assuming $\epsilon > 0$ –

$$\mathrm{rhs}(1/2+\epsilon) - \mathrm{rhs}(1/2) = \sum_{n=1}^{N} \int_{|\mathbf{y}-\mathbf{x}_n|>R_{1/2+\epsilon}(\mathbf{x}_n)} \frac{\sigma(\mathbf{y})}{|\mathbf{y}-\mathbf{x}_n|}\mathrm{d}\mathbf{y}$$

$$
\begin{aligned}
&-D(\sigma,\sigma)+\sum_{n=1}^{N}\frac{\epsilon}{R_{1/2+\epsilon}(\mathbf{x}_n)}\\
&-\sum_{n=1}^{N}\int\limits_{|\mathbf{y}-\mathbf{x}_n|>R_{1/2}(\mathbf{x}_n)}\frac{\sigma(\mathbf{y})}{|\mathbf{y}-\mathbf{x}_n|}\mathrm{d}\mathbf{y}+D(\sigma,\sigma)\\
&=-\sum_{n=1}^{N}\int\limits_{R_{1/2}(\mathbf{x}_n)<|\mathbf{y}-\mathbf{x}_n|<R_{1/2+\epsilon}(\mathbf{x}_n)}\frac{\sigma(\mathbf{y})}{|\mathbf{y}-\mathbf{x}_n|}\mathrm{d}\mathbf{y}\\
&+\sum_{n=1}^{N}\frac{\epsilon}{R_{1/2+\epsilon}(\mathbf{x}_n)}\\
&\le-\sum_{n=1}^{N}\int\limits_{R_{1/2}(\mathbf{x}_n)<|\mathbf{y}-\mathbf{x}_n|<R_{1/2+\epsilon}(\mathbf{x}_n)}\frac{\sigma(\mathbf{y})}{R_{1/2+\epsilon}(\mathbf{x}_n)}\mathrm{d}\mathbf{y}\\
&+\sum_{n=1}^{N}\frac{\epsilon}{R_{1/2+\epsilon}(\mathbf{x}_n)}\\
&=0\ , \qquad (13)
\end{aligned}
$$

since the annulus of integration contains exactly charge ϵ by definition of $R_\xi(x)$.

The case of negative ϵ is analogous.

To emphasize the charge-optimized bound we state it explicitly:

$$
\boxed{\sum_{1\le n<m\le N}\frac{1}{|\mathbf{x}_n-\mathbf{x}_m|}\ge\sum_{n=1}^{N}\int\limits_{|\mathbf{y}-\mathbf{x}_n|>R(\mathbf{x}_n)}\frac{\sigma(\mathbf{y})\mathrm{d}\mathbf{y}}{|\mathbf{y}-\mathbf{x}_n|}-D(\sigma,\sigma)\ ,} \qquad (14)
$$

which holds for arbitrary charge density σ fulfilling merely the general requirements of the Introduction.

3. The correlation bound of Lieb and Oxford

We would like to show that the inequality (Eq. 14) implies an exchange–correlation bound in terms of the Dirac exchange term that goes back to Lieb [11] and Lieb and Oxford [12].

The main technical tool will be the Hardy–Littlewood maximal function $(Mf)(\mathbf{x})$ of a function f. It is defined to be the biggest spherical average of f over balls of radius R, i.e.,

$$
(Mf)(\mathbf{x}):=\sup_{R>0}\frac{\int_{|\mathbf{x}-\mathbf{y}|<R}|f(\mathbf{y})|\mathrm{d}\mathbf{y}}{\frac{4\pi}{3}R^3}\ . \qquad (15)
$$

It is a classical fact that the L^p norm of the maximal function can be estimated in terms of the L^p norm of the function itself ([14]) . We will need this fact in the case where $p=4/3$. This estimate reads

$$
\int\limits_{\mathbb{R}^3}(Mf)(\mathbf{x})^{4/3}\mathrm{d}\mathbf{x}\le A_{4/3}^{4/3}\int\limits_{\mathbb{R}^3}|f(\mathbf{x})|^{4/3}\mathrm{d}\mathbf{x}\ . \qquad (16)
$$

Note that the best constant $A_{4/3}$ in this inequality does not exceed 17.57 (Stein and Strömberg [15]). We also need an inequality that appears in the spherical symmetric case in Lieb [11]:

Lemma 1. If f is an integrable function, then

$$
\int\limits_{\mathbb{R}^3}|f(\mathbf{x})|/|\mathbf{x}|\mathrm{d}\mathbf{x}\le\left(\frac{9}{2}\pi(Mf)(\mathbf{0})\right)^{1/3}\left(\int\limits_{\mathbb{R}^3}|f(\mathbf{x})|\mathrm{d}\mathbf{x}\right)^{2/3}\ . \qquad (17)
$$

Proof. Obviously, it is enough to prove the result for nonnegative spherically symmetric functions. Integrating by parts we get

$$
\begin{aligned}
\int\limits_{\mathbb{R}^3}f(\mathbf{x})/|\mathbf{x}|\mathrm{d}\mathbf{x}&=\frac{1}{4\pi}\int\limits_{\mathbb{R}^3}\mathrm{d}\mathbf{x}|\mathbf{x}|^{-4}\int\limits_{|\mathbf{y}|<|\mathbf{x}|}\mathrm{d}\mathbf{y}f(\mathbf{y})\\
&=\frac{1}{3}\int\limits_{|\mathbf{x}|<R}\mathrm{d}\mathbf{x}|\mathbf{x}|^{-1}\int\limits_{|\mathbf{y}|<|\mathbf{x}|}\mathrm{d}\mathbf{y}f(\mathbf{y})\frac{4\pi}{3}|\mathbf{x}|^3\\
&+\frac{1}{4\pi}\int\limits_{|\mathbf{x}|>R}\mathrm{d}\mathbf{x}|\mathbf{x}|^{-4}\int\limits_{|\mathbf{y}|<|\mathbf{x}|}\mathrm{d}\mathbf{y}f(\mathbf{y})\\
&\le\frac{2\pi}{3}R^2(Mf)(\mathbf{0})+\int\limits_{\mathbb{R}^3}\mathrm{d}\mathbf{y}f(\mathbf{y})/R\ . \qquad (18)
\end{aligned}
$$

Picking $R=\sqrt{3\int_{\mathbb{R}^3}\mathrm{d}\mathbf{y}f(\mathbf{y})/[4\pi(Mf)(\mathbf{0})]}$ yields the desired inequality.

Lemma 2. Let σ be as required in the Introduction. Then

$$
\int\limits_{|\mathbf{x}-\mathbf{y}|\le R(\mathbf{x})}\mathrm{d}\mathbf{y}\frac{\sigma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\le\frac{(9\pi)^{1/3}}{2}(M\sigma)(\mathbf{x})^{1/3}\ . \qquad (19)
$$

Proof. We set $\sigma_{\mathbf{x}}(\mathbf{y}):=\sigma(\mathbf{x}+\mathbf{y})\chi_{R(\mathbf{x})}(\mathbf{y})$, where $\chi_{R(\mathbf{x})}(\mathbf{y})$ is 1, if $|\mathbf{y}|<R(\mathbf{x})$ and vanishes otherwise. We apply lemma 1 with $f=\sigma_x$ and get

$$
\begin{aligned}
\int\limits_{|\mathbf{y}-\mathbf{x}|<R(\mathbf{x})}\mathrm{d}\mathbf{y}\frac{\sigma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}&=\int\limits_{\mathbb{R}^3}\mathrm{d}\mathbf{y}\frac{\sigma_{\mathbf{x}}(\mathbf{y})}{|\mathbf{y}|}\\
&\le\left(\frac{9}{2}\pi(M\sigma_{\mathbf{x}})(\mathbf{0})\right)^{1/3}\left(\int\limits_{\mathbb{R}^3}|\sigma_{\mathbf{x}}(\mathbf{y})|\mathrm{d}\mathbf{y}\right)^{2/3}\\
&=\left(\frac{9}{2}\pi(M\sigma)(\mathbf{x})\right)^{1/3}\left(\frac{1}{2}\right)^{2/3}\ , \qquad (20)
\end{aligned}
$$

where the last inequality holds because of the definition of $R(\mathbf{x})$. The last term of the chain of inequalities is easily seen to give the claim.

Assume ψ to be a normalized wave function of N particles with spin q each, i.e., ψ depends on the variables $\vec{x} := (x_1, , ..., x_N)$, where each $x_n = (\mathbf{x}_n, \tau_n)$ is a space–spin variable, i.e.,

$$\int |\psi(\vec{x})|^2 d\vec{x} := \int_{\mathbb{R}^3} d\mathbf{x}_1 \sum_{\tau_1=1}^{q} \ldots \int_{\mathbb{R}^3} d\mathbf{x}_N \sum_{\tau_N=1}^{q} |\psi(\vec{x})|^2 = 1 \ .$$

We do not assume that ψ fulfills any symmetry requirements but we do assume that

$$I_\psi := \sum_{1 \le n < m \le N} \int d\vec{x} \frac{|\psi(\vec{x})|^2}{|\mathbf{x}_n - \mathbf{x}_m|} < \infty$$

and that the one-particle density, ρ_ψ, of the state ψ is integrable when raised to the power 4/3, i.e., $\int \rho_\psi^{4/3} < \infty$. Note that all these requirements are naturally fulfilled for quantum states with finite kinetic energy. Then

$$I_\psi \ge 2D(\rho_\psi, \sigma) - D(\sigma, \sigma) - L \left(\int_{\mathbb{R}^3} \rho_\psi(\mathbf{x})^{4/3} d\mathbf{x} \right)^{3/4} \left(\int_{\mathbb{R}^3} \sigma(\mathbf{x})^{4/3} d\mathbf{x} \right)^{1/4} , \quad (21)$$

with $L = (9\pi)^{1/3} A_{4/3}^{4/9}/2$. (Using the upper bound of Stein and Strömberg on $A_{4/3}$ shows that $L \le 3.96$.) Picking $\sigma = \rho_\psi$ yields the inequality of Lieb [11] and Lieb and Oxford [12]

$$I_\psi \ge D(\rho_\psi, \rho_\psi) - L \int_{\mathbb{R}^3} \rho_\psi(\mathbf{x})^{4/3} d\mathbf{x} \ . \quad (22)$$

Note that Lieb [11] estimated L as 8.52 using also the maximal inequality and Lieb and Oxford [12] estimated L as 1.68 using a somewhat more involved but elementary technique. That our result implies this inequality with a relatively good constant highlights the quality of our exchange–correlation estimate using the idea of the exchange hole.

We start the proof of the inequality in Eq. (21) by multiplying both sides of the inequality in Eq. (14) by $|\psi(\vec{x})|^2$ and integrate and sum over all space-spin variables:

$$\begin{aligned} I_\psi &\ge 2D(\rho_\psi, \sigma) - \int_{\mathbb{R}^3} d\mathbf{x} \rho_\psi(\mathbf{x}) \int_{|\mathbf{x}-\mathbf{y}|<R(\mathbf{x})} \frac{\sigma(\mathbf{y}) d\mathbf{y}}{|\mathbf{x} - \mathbf{y}|} - D(\sigma, \sigma) \\ &\ge 2D(\rho_\psi, \sigma) - D(\sigma, \sigma) \\ &\quad - \frac{(9\pi)^{1/3}}{2} \int_{\mathbb{R}^3} \rho_\psi(\mathbf{x}) (M\sigma)(\mathbf{x})^{1/3} d\mathbf{x} \ , \end{aligned} \quad (23)$$

where we have used Eq. (19) of lemma 2. Applying the Hölder inequality followed by the maximal inequality Eq. (16) gives

$$\begin{aligned} I_\psi &\ge 2D(\rho_\psi, \sigma) - D(\sigma, \sigma) \\ &\quad - \frac{(9\pi)^{1/3}}{2} \left(\int_{\mathbb{R}^3} \rho_\psi^{4/3} \right)^{3/4} \left(\int_{\mathbb{R}^3} (M\sigma)^{4/3} \right)^{1/4} \\ &\ge 2D(\rho_\psi, \sigma) - D(\sigma, \sigma) \\ &\quad - \frac{(9\pi)^{1/3}}{2} A_{4/3}^{4/9} \left(\int_{\mathbb{R}^3} \rho_\psi^{4/3} \right)^{3/4} \left(\int_{\mathbb{R}^3} \sigma^{4/3} \right)^{1/4} , \end{aligned} \quad (24)$$

which proves the inequality Eq. (21).

Approximate density functional

The inequality in Eq. (14) reduces the interacting N-particle problem to an approximate noninteracting one whose energy is a strict lower bound on the exact energy. Picking, in addition the occuring arbitrary density σ appropriately, allows us to construct a Kohn-Sham type density functional for the ground, state energy which is not only an approximation but gives a rigorous lower bound: we denote the Kohn-Sham orbitals of the N electrons by $\phi_1, ..., \phi_N$. Next we pick

$$\sigma(\mathbf{x}) := \rho(\mathbf{x}) := |\phi_1(\mathbf{x})|^2 + \cdots + |\phi_N(\mathbf{x})|^2 \ .$$

The approximate Kohn-Sham functional becomes in this case

$$\mathscr{E}_{KS}[\phi_1, \ldots, \phi_N] := \sum_{\nu=1}^{N} \int |\nabla \phi_\nu|^2 + D(\rho, \rho) - \int d\mathbf{x} \int d\mathbf{y}_{|\mathbf{y}-\mathbf{x}|<R(\mathbf{x})} \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} + \int V(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} \ ,$$

where V is the external electric potential. The corresponding Kohn–Sham equations are

$$-\Delta \phi_\nu + \left(V(\mathbf{x}) + \int_{|\mathbf{x}-\mathbf{y}|>R(\mathbf{x})} \frac{\rho(\mathbf{y}) d\mathbf{y}}{|\mathbf{x} - \mathbf{y}|} \right) \phi_\nu = \epsilon_\nu \phi_\nu \ .$$

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