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LETTER TO THE EDITOR

Exact relation between relativistic and non-relativistic Green functions for independent particles in a given external potential

R Baltin† and N H March‡

† Theoretical Chemistry Department, University of Ulm, Oberer Eselsberg, 7900 Ulm, Federal Republic of Germany

‡ Theoretical Chemistry Department, University of Oxford, 1 South Parks Road, Oxford OX1 3TG, UK

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Abstract. Well established integral equations already exist for both relativistic ($G^{(r)}$) and non-relativistic ($G^{(nr)}$) Green functions for independent particles moving in a given external potential V. In this paper, an exact integral equation giving $G^{(r)}$ in terms solely of $G^{(nr)}$ and known operators is derived, by eliminating V. The connection with relativistic density functional theory is emphasised.

In recent work, we have been concerned with relativistic density functional theory in the framework of (a) a square barrier model of an inhomogeneous electron gas [1] and (b) a linear response theory of perturbations in an initially uniform electron gas [2]. This latter work has been utilised more recently [3, 4] to exhibit a formal relation between relativistic and non-relativistic electron densities for independent particles moving in a given weak external potential.

The purpose of the present letter is to derive an exact relation between relativistic $G^{(r)}$ and non-relativistic $G^{(nr)}$ Green functions.

The starting point of the present work can be usefully taken as the defining equation for the components $G^{(r)}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s)$ of the relativistic Green's function. This can be written as (cf equation (2.9a) of [2])

$$\sum_{\gamma=1}^{4} (H^{(0)}_{\alpha\gamma} - s\delta_{\alpha\gamma}) G^{(r)}_{\gamma\beta}(\boldsymbol{x}, \boldsymbol{x}', s) + V(\boldsymbol{x}) G^{(r)}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s) = \delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{1}$$

where $H^{(0)}_{\alpha\gamma}$ are the components of the free-electron Hamilton operator

$$\mathsf{H}^{(0)} \equiv \begin{pmatrix} mc^2 & 0 & cp_z & cp_- \\ 0 & mc^2 & cp_+ & -cp_z \\ cp_z & cp_- & -mc^2 & 0 \\ cp_z & -cp_z & 0 & -mc^2 \end{pmatrix} \tag{2}$$

and

$$p_\pm \equiv p_x \pm \mathrm{i} p_y \tag{3}$$

with momentum operators $p_\alpha = -\mathrm{i}\hbar\partial/\partial x_\alpha$, $\alpha = x, y, z$. The procedure employed is to eliminate the external potential $V(\boldsymbol{x})$ from (1) by using the non-relativistic scalar Green function

$$G^{(nr)}(\boldsymbol{x}, \boldsymbol{x}', s) \equiv \sum_j \frac{\phi_j(\boldsymbol{x})\phi_j^*(\boldsymbol{x}')}{E_j - s} \tag{4}$$

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where $\phi_j(\boldsymbol{x})$ and E_j are eigenfunctions and eigenvalues of the Schrödinger equation for the given external potential energy $V(\boldsymbol{x})$.

As is readily seen, $G^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}', s)$ not only satisfies

$$[T(\boldsymbol{x})+V(\boldsymbol{x})-s]G^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}', s)=\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{5a}$$

but also

$$[T(\boldsymbol{x}')+V(\boldsymbol{x}')-s]G^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}', s)=\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{5b}$$

where

$$T(\boldsymbol{x})\equiv-\frac{\hbar^2}{2m}\nabla_x^2. \tag{6}$$

By relabelling the variables in (5b) by $\boldsymbol{x}''$ instead of $\boldsymbol{x}$ and $\boldsymbol{x}$ instead of $\boldsymbol{x}'$, this equation can be written as

$$G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)\,V(\boldsymbol{x})=\delta(\boldsymbol{x}''-\boldsymbol{x})-(T(\boldsymbol{x})-s)G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s). \tag{7}$$

The next step is to multiply (1) by $G^{(\mathrm{nr})}$ $(\boldsymbol{x}'', \boldsymbol{x}, s)$ and then to integrate over $\boldsymbol{x}\in\Omega$, where $\Omega\subseteq\mathbb{R}^3$ is the spatial domain accessible to the particle. The resulting equation is

$$\begin{aligned}\sum_{\gamma=1}^{4}\int_\Omega &\mathrm{d}^3x\,G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)[H^{(0)}_{\alpha\gamma}(\boldsymbol{x})-s\delta_{\alpha\gamma}]G^{(\mathrm{r})}_{\gamma\beta}(\boldsymbol{x}, \boldsymbol{x}', s)\\ &+\int_\Omega \mathrm{d}^3x[\delta(\boldsymbol{x}''-\boldsymbol{x})-(T(\boldsymbol{x})-s)G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)]G^{(\mathrm{r})}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s)\\ &=\delta_{\alpha\beta}G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}', s).\end{aligned} \tag{8}$$

In writing (8), the term

$$\int_\Omega \mathrm{d}^3x\,G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)\,V(\boldsymbol{x})G^{(\mathrm{r})}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s)$$

was rewritten by using (7).

From (8) we then find

$$\begin{aligned}G^{(\mathrm{r})}_{\alpha\beta}&(\boldsymbol{x}'', \boldsymbol{x}', s)\\ &=\delta_{\alpha\beta}G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}', s)-\sum_{\gamma=1}^{4}\int_\Omega \mathrm{d}^3x\{G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)\\ &\quad\times[H^{(0)}_{\alpha\gamma}(\boldsymbol{x})-s\delta_{\alpha\gamma}]G^{(\mathrm{r})}_{\gamma\beta}(\boldsymbol{x}, \boldsymbol{x}', s)\}\\ &\quad+\int \mathrm{d}^3x[(T(\boldsymbol{x})-s)G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)]G^{(\mathrm{r})}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s)\end{aligned} \tag{9}$$

where it will be seen that the terms with s multiplying $G^{(\mathrm{nr})}G^{(\mathrm{r})}$ cancel.

In what follows let us suppose that, for $\boldsymbol{x}'\neq\boldsymbol{x}''$,

$$\int_\Omega \mathrm{d}^3x[T(\boldsymbol{x})G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}, s)]G^{(\mathrm{r})}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s)=\int_\Omega \mathrm{d}^3x\,G^{(\mathrm{nr})}(\boldsymbol{x}'', \boldsymbol{x}', s)[T(\boldsymbol{x})G^{(\mathrm{r})}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s)]. \tag{10}$$

Usually, Gauss' theorem is proved under the condition that all functions involved are continuously differentiable twice on Ω. However, $G^{(\mathrm{nr})}(x'', x, s)$ is singular at $x = x''$ and $G^{(\mathrm{r})}_{\alpha\beta}(x, x', s)$ is singular at $x = x'$, so it is not self-evident that (10) is valid here. Furthermore, if $\Omega = \mathbb{R}^3$, integrals over the surface of the infinite sphere vanish only if the integrand falls off rapidly enough at infinity so that Gauss' theorem takes the form of (10).

However, Gauss' theorem can be applied under much less restrictive conditions on the smoothness of the integrand as will be demonstrated explicitly for the case of a free particle below (i.e. for $V(x) = 0\ \forall x$, $\Omega = \mathbb{R}^2$). This example will show also that surface integrals at infinity must vanish because the decay of the free-particle Green functions $G_0^{(\mathrm{nr})}$ and $G^{(\mathrm{r})}_{0,\alpha\beta}$ is faster than exponential as $|x| \to \infty$ (with x'' and x' held fixed) provided that $\mathrm{Im}(s^{1/2})$ and $\mathrm{Im}(s^2 - m^2c^4)^{1/2}$ are taken to be positive, respectively.

The non-relativistic Green function is given by [5]

$$G_0^{(\mathrm{nr})}(x, x', s) = \frac{m \exp[\mathrm{i}(2ms/\hbar^2)^{1/2}|x - x'|]}{2\pi\hbar^2|x - x'|} \tag{11}$$

and the components of the relativistic Green function for a free particle are [6]

$$G^{(\mathrm{r})}_{0,\alpha\beta}(x, x', s) = (H^{(0)}_{\alpha\beta}(x) + s\delta_{\alpha\beta})P(|x - x'|, s) \tag{12}$$

where

$$P(|x - x'|, s) = \frac{\exp[\mathrm{i}|x - x'|\sqrt{s^2 - m^2c^4}/(c\hbar)]}{4\pi c^2\hbar^2|x - x'|}. \tag{13}$$

Evidently, if the imaginary parts of the square roots in expressions (11) and (13) are positive, the Green functions fall off rapidly enough to guarantee vanishing surface integrals when applying Gauss' theorem.

For those components (α, β) for which $H^{(0)}_{\alpha\beta}$ (equation (2)) does not contain a momentum operator, the corresponding component $G^{(\mathrm{r})}_{0,\alpha\beta}$ has a singularity at $x' = x$ of the same strength as P has, namely $\sim|x' - x|^{-1}$. If, however, $H^{(0)}_{\alpha\beta}$ contains a momentum operator, the singularity of $G^{(\mathrm{r})}_{0,\alpha\beta}$ is stronger still. For instance, $G^{(\mathrm{r})}_{0,13}(x, x', s) = cp_zP(|x - x'|, s)$ behaves like $(z' - z)/|x - x'|^3$ as $x' \to x$.

To prove the validity of (10) for the free-particle case it is therefore sufficient to consider this relation for one component of $G_0(\mathrm{r})$ which has the stronger divergence mentioned. If (10) turns out to be valid for this case, it is satisfied also for the more harmless components. Let us consider e.g. $G^{(\mathrm{r})}_{0,13}$ and introduce

$$f_i(|u|) \equiv \frac{\mathrm{e}^{-q_i|u|}}{|u|} \tag{14}$$

with $\mathrm{Re}(q_i) > 0$, $i = 1, 2$. Apart from unimportant prefactors, verification of (10) then amounts to showing that

$$I_1 \equiv \int_{\mathbb{R}^3} [\nabla^2_{x'} f_1(|x - x'|)] \frac{\partial f_2(|x' - x''|)}{\partial z'}\, \mathrm{d}^3x' \tag{15a}$$

equals

$$I_2 \equiv \int_{\mathbb{R}^3} f_1(|x - x'|) \nabla^2_{x'} \frac{\partial f_2(|x' - x''|)}{\partial z'}\, \mathrm{d}^3x'. \tag{15b}$$

From

$$\nabla^2_{x'} f_i(|x - x'|) = -4\pi\delta(x - x') + q_i^2 f_i(|x - x'|) \tag{16}$$

it follows that

$$I_1 = -4\pi \frac{\partial f_2(|\boldsymbol{x}-\boldsymbol{x}''|)}{\partial z} + q_1^2 \int_{\mathbf{R}^3} f_1(|\boldsymbol{x}-\boldsymbol{x}'|) \frac{\partial f_2(|\boldsymbol{x}'-\boldsymbol{x}''|)}{\partial z'} \, \mathrm{d}^3x' \tag{17a}$$

and, analogously,

$$I_2 = 4\pi \frac{\partial f_1(|\boldsymbol{x}-\boldsymbol{x}''|)}{\partial z''} + q_2^2 \int_{\mathbf{R}^3} f_1(|\boldsymbol{x}-\boldsymbol{x}'|) \frac{\partial f_2(|\boldsymbol{x}'-\boldsymbol{x}''|)}{\partial z'} \, \mathrm{d}^3x'. \tag{17b}$$

Using

$$\frac{\partial f_2(|\boldsymbol{x}-\boldsymbol{x}''|)}{\partial z} = -\frac{\partial f_2(|\boldsymbol{x}-\boldsymbol{x}''|)}{\partial z''}$$

we obtain

$$I_1 - I_2 = 4\pi \frac{\partial}{\partial z''} [f_2(|\boldsymbol{x}-\boldsymbol{x}''|) - f_1(|\boldsymbol{x}-\boldsymbol{x}''|)] + (q_2^2 - q_1^2) \frac{\partial W}{\partial z''} \tag{18}$$

where the special form of the functions f_i (equation (14)) enables us to calculate

$$W \equiv \int_{\mathbf{R}^3} f_1(|\boldsymbol{x}-\boldsymbol{x}'|) f_2(|\boldsymbol{x}-\boldsymbol{x}''|) \, \mathrm{d}^3x' \tag{19}$$

explicitly, yielding

$$(q_2^2 - q_1^2) W = 4\pi \frac{\mathrm{e}^{-q_1|\boldsymbol{x}-\boldsymbol{x}''|} - \mathrm{e}^{-q_2|\boldsymbol{x}-\boldsymbol{x}''|}}{|\boldsymbol{x}-\boldsymbol{x}''|}. \tag{20}$$

When this expression is inserted into (18), it follows that $I_1 = I_2$, i.e. (10) is proved for the case of a free particle.

Going back to the general case of spatially variable potentials, it does not seem to be easy to characterise a general function space containing elements $G^{(\mathrm{nr})}$ and $G^{(\mathrm{r})}_{\alpha\beta}$ which become singular when their spatial arguments coincide and, at the same time, obey (10). However, the free-particle case shows that this space is certainly not empty. So, for the time being, let us suppose that (10) remains valid for reasonable variable potentials, at least for a certain domain of the complex s plane. Thus we arrive at

$$\begin{aligned} G^{(\mathrm{r})}_{\alpha\beta}&(\boldsymbol{x}, \boldsymbol{x}', s) \\ &= \delta_{\alpha\beta} G^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}', s) - \int_{\Omega} \mathrm{d}^3x_1 \, G^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}_1, s) \sum_{\gamma=1}^{4} [H^{(0)}_{\alpha\gamma}(\boldsymbol{x}_1) - T(\boldsymbol{x}_1)\delta_{\alpha\gamma}] \\ &\quad \times G^{(\mathrm{r})}_{\gamma\beta}(\boldsymbol{x}_1, \boldsymbol{x}', s). \end{aligned} \tag{21}$$

Here $\boldsymbol{x}$ has been written instead of $\boldsymbol{x}''$, and $\boldsymbol{x}_1$ instead of $\boldsymbol{x}$. One may cast this basic equation (21) into a more concise form as follows.

Define $\mathbb{G}^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}', s) \equiv$ non-relativistic Green's (4×4) matrix with components

$$G^{(\mathrm{nr})}_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}', s) \equiv \delta_{\alpha\beta} G^{(\mathrm{nr})}(\boldsymbol{x}, \boldsymbol{x}', s) \tag{22}$$

and $\mathbb{T}^{(\mathrm{nr})}(\boldsymbol{x}) \equiv$ non-relativistic kinetic energy operator matrix with components

$$T^{(\mathrm{nr})}_{\alpha\beta}(\boldsymbol{x}) \equiv \delta_{\alpha\beta} T(\boldsymbol{x}) = -\frac{\hbar}{2m} \delta_{\alpha\beta} \nabla_x^2. \tag{23}$$

It follows that

$$\mathbb{G}^{(r)}(x, x', s) = \mathbb{G}^{(nr)}(x, x', s) - \int_{\Omega} d^3x_1\, \mathbb{G}^{(nr)}(x, x_1, s)\mathbb{W}(x_1)\mathbb{G}^{(r)}(x_1, x', s) \tag{24}$$

where the 'perturbation' operator $\mathbb{W}$ is defined through

$$\mathbb{W}(x) \equiv \mathbb{H}^{(0)}(x) - \mathbb{T}^{(nr)}(x). \tag{25}$$

Equation (24) is the main result of the present letter. It can be seen that it is an integral equation for the determination of the relativistic Green function $\mathbb{G}^{(r)}$ given the non-relativistic result $\mathbb{G}^{(nr)}$ for the chosen external potential. The 'perturbation' operator $\mathbb{W}$ in (25) is, of course, known explicitly through (2) and (23).

Equation (24) provides a direct route to calculate the relativistic Green function from the non-relativistic result for independent particles moving in a chosen external potential. In the spirit of density functional theory, this external potential is here being characterised by the (assumed known) non-relativistic Green function. While (24) is an off-diagonal integral equation for $\mathbb{G}^{(r)}$, given $\mathbb{G}^{(nr)}$, we found [4] that, for a linear response theory, it can be reduced to an algebraic relation in Fourier space between diagonal electron densities with and without relativity.

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