Alternative approach to the gradient expansion of Green's functions of noninteracting particles

E. Engel, H. Müller, and R. M. Dreizler

Institut für Theoretische Physik, Universitat Frankfürt, D-6000 Frankfürt am Main, Federal Republic of Germany

(Received 28 November 1988)

We present a new technique for evaluating the gradient expansion of the one-particle Green's function of a system of noninteracting particles. The method is based on the fundamental differential equation for the Green's function and is applicable to relativistic systems as well as to nonrelativistic ones. Explicitly we derive the gradient expansion of the relativistic Green's function of a system of electrons in an arbitrary time-independent external four potential to second order.

The semiclassical expansion of Green's functions or density matrices for systems of noninteracting particles is used extensively for the derivation of explicit ground-state energy density functionals.[1-6] In this contribution we present a method for the evaluation of the gradient expansion of the one-particle propagator, which is more easily applied than the standard Kirzhnits formalism.[7-9] We demonstrate the technique for a system characterized by the relativistic Lagrangian (using units with $c=1$ and the Feynman convention $\bar{A}=A_\nu\gamma^\nu$) describing fermions in an external four-potential,

$$\mathcal{L}=\bar{\psi}(x)[i\hbar\bar{\partial}-m-\bar{V}(x)]\psi(x) , \tag{1}$$

The one-particle Green's function of a system characterized by this Lagrangian is defined by the differential equation

$$[i\hbar\bar{\partial}_x-m-\bar{V}(x)]G(x,y)=i\delta^{(4)}(x-y) . \tag{2}$$

The ansatz

$$G(x,y)=\sum_{n=0}^{\infty} G^{[n]}(x,y) , \tag{3}$$

where $G^{[n]}$ denotes the nth order gradient contribution to G, leads to a recursion relation which allows the representation of $G^{[n]}$ in terms of the semiclassical limit $G^{[0]}$.

This quantity is most readily obtained in the standard local-density approximation. For the case of stationary systems,

$$V_\nu(x)=V_\nu(\mathbf{x}) ,$$

to which we restrict further discussion, one calculates the Green's function of a homogeneous relativistic electron gas in a constant four-potential A_μ and uses this expression with the replacement

$$A_\mu\to V_\mu(\mathbf{x}) .$$

The result is

$$\begin{aligned} G^{[0]}(x,y)&=e^{-(i/\hbar)(x^\nu-y^\nu)V_\nu(\mathbf{x})}\int\frac{d^4p}{(2\pi\hbar)^4}e^{-(i/\hbar)p(x-y)}g^{[0]}(p,\mathbf{x}) ,\\ g^{[0]}(p,\mathbf{x})&=(\bar{p}+m)\left[\frac{i}{p^2-m^2+i\epsilon}-2\pi\frac{\delta(p^0-E)}{2E}\Theta(S-V^0(\mathbf{x})-p^0)\right] , \end{aligned} \tag{4}$$

where $E=(\mathbf{p}^2+m^2)^{1/2}$. The threshold energy S distinguishes between occupied and unoccupied states. The vacuum part and the real electron gas part with energies between m and $S-A_0$ for the homogeneous system and consequently m and $S-V_0(\mathbf{x})$ for the inhomogeneous system in local-density approximation have been separated. This propagator satisfies Eq. (2) in lowest order,

$$\begin{aligned} &[i\hbar\bar{\partial}_x-m-\bar{V}(\mathbf{x})]G^{[0]}(x,y)\\ &=e^{-(i/\hbar)(x^\nu-y^\nu)V_\nu(\mathbf{x})}\int\frac{d^4p}{(2\pi\hbar)^4}e^{-(i/\hbar)p(x-y)}\left[i\hbar\bar{\partial}_x+\bar{p}-m-i\hbar[\bar{\partial}V_\nu(\mathbf{x})]\frac{\partial}{\partial p_\nu}\right]g^{[0]}(p,\mathbf{x})\\ &=e^{-(i/\hbar)(x^\nu-y^\nu)V_\nu(\mathbf{x})}\int\frac{d^4p}{(2\pi\hbar)^4}e^{-(i/\hbar)p(x-y)}\left[\left[i\hbar\bar{\partial}_x-i\hbar[\bar{\partial}V_\nu(\mathbf{x})]\frac{\partial}{\partial p_\nu}\right]g^{[0]}(p,x)\right.\\ &\qquad\left.+i-2\pi(p^2-m^2)\frac{\delta(p^0-E)}{2E}\Theta(S-V^0(\mathbf{x})-p^0)\right]\\ &=ie^{-(i/\hbar)(x^\nu-y^\nu)V_\nu(\mathbf{x})}\delta^{(4)}(x-y)+O(\hbar) . \end{aligned}$$

In order to derive a recursion relation for $G^{[n]}$ we use the ansatz

$$G^{[n]}(x,y)=e^{-(i/\hbar)(x^\nu-y^\nu)V_\nu(\mathbf{x})}g^{[n]}(x,y) , \tag{5}$$

which does not affect the ordering of the gradient corrections. Inserting this ansatz into Eq. (2) one obtains

$$e^{-(i/\hbar)(x^{\nu}-y^{\nu})V_{\nu}(x)}\{(x^{\nu}-y^{\nu})[\bar{\partial}V_{\nu}(x)]+i\hbar\bar{\partial}_x-m\}\sum_{n=0}^{\infty}g^{[n]}(x,y)=i\delta^{(4)}(x-y)\ , \tag{6}$$

which is most readily resolved in momentum space. The partial Fourier transformation

$$g^{[n]}(x,y)=\int\frac{d^4p}{(2\pi\hbar)^4}e^{-(i/\hbar)p(x-y)}g^{[n]}(p,x) \tag{7}$$

leads directly to

$$g^{[n]}(p,x)=i\hbar\frac{(\bar{p}+m)}{p^2-m^2}\left[[\bar{\partial}V_{\nu}(\mathbf{x})]\frac{\partial}{\partial p_{\nu}}-\bar{\partial}\right]g^{[n-1]}(p,x),\quad n>0\ . \tag{8}$$

The final resolution of the recursion relation (8) is

$$g^{[n]}(p,x)=(i\hbar)^n\left[\frac{(\bar{p}+m)}{p^2-m^2}\left[[\bar{\partial}V_{\nu}(x)]\frac{\partial}{\partial p_{\nu}}-\bar{\partial}\right]\right]^n g^{[0]}(p,x)\ . \tag{9}$$

We note that the pole structure in $g^{[0]}(p,x)$ and the prefactor $(\bar{p}+m)/(p^2-m^2)$ has to be the same, as the separation of the states indicated by the alternative form

$$g^{[0]}(p,\mathbf{x})=i\left[\frac{(\bar{p}+m)}{p^2-m^2+i\epsilon}+\Theta(S-V^0(\mathbf{x})-p^0)\left[\frac{(\bar{p}+m)}{p^2-m^2-i\epsilon}-\frac{(\bar{p}+m)}{(p^0+i\epsilon)^2-E^2}\right]\right]\ , \tag{10}$$

[which is equivalent to Eq. (4) but avoids mathematical ambiguities] is not changed in higher-order gradient terms. This leads to

$$\begin{aligned}g^{[n]}(p,\mathbf{x})=&\ i(i\hbar)^n\left[\frac{(\bar{p}+m)}{p^2-m^2+i\epsilon}\left[[\bar{\partial}V_{\nu}(\mathbf{x})]\frac{\partial}{\partial p_{\nu}}-\bar{\partial}\right]\right]^n\frac{(\bar{p}+m)}{p^2-m^2+i\epsilon}\\&+i(i\hbar)^n\Theta(S-V^0(\mathbf{x})-p^0)\left[\frac{(\bar{p}+m)}{p^2-m^2-i\epsilon}\left[[\bar{\partial}V_{\nu}(\mathbf{x})]\frac{\partial}{\partial p_{\nu}}-\bar{\partial}\right]\right]^n\frac{(\bar{p}+m)}{p^2-m^2-i\epsilon}\\&-i(i\hbar)^n\Theta(S-V^0(\mathbf{x})-p^0)\left[\frac{(\bar{p}+m)}{(p^0+i\epsilon)^2-E^2}\left[[\bar{\partial}V_{\nu}(\mathbf{x})]\frac{\partial}{\partial p_{\nu}}-\bar{\partial}\right]\right]\frac{(\bar{p}+m)}{(p^0+i\epsilon)^2-E^2}\ .\end{aligned} \tag{11}$$

An alternative but more cumbersome derivation of this result can be carried out by expanding the Green's function in powers of $V_{\nu}(\mathbf{x})$, then in powers of $\hbar$, and finally resumming the series in the field strength.

On the basis of Eq. (11) one can readily evaluate the low-order gradient terms, as demonstrated by the first- and second-order terms given below. Using standard Dirac matrix algebra and Lorentz gauge (a discussion of gauge questions is given in the appendix),

$$\partial^{\nu}V_{\nu}(\mathbf{x})=0\ ,$$

one finds

$$\begin{aligned}g^{[1]}(p,\mathbf{x})=\hbar[\partial_{\mu}V_{\nu}(\mathbf{x})]\Bigg\{&(\bar{p}+m)\left[-\frac{\gamma^{\mu}\gamma^{\nu}}{(p^2-m^2+i\epsilon)^2}+4\frac{p^{\nu}p^{\mu}}{(p^2-m^2+i\epsilon)^3}\right]-2\frac{\gamma^{\mu}p^{\nu}}{(p^2-m^2+i\epsilon)^2}\\&+2\pi i\Theta(S-V^0(\mathbf{x})-p^0)\left[(\bar{p}+m)\left[\frac{p^{\nu}p^{\mu}}{E[3(p^0)^2+E^2]}\delta''(p^0-E)+\frac{\gamma^{\mu}\gamma^{\nu}}{4p^0E}\delta'(p^0-E)\right]\right.\\&\left.+\frac{\gamma^{\mu}p^{\nu}}{2p^0E}\delta'(p^0-E)\right]\Bigg\}\ .\end{aligned} \tag{12}$$

and the more involved expression

$$\begin{aligned}g^{[2]}(p,\mathbf{x})=\hbar^2\{&[\partial_{\alpha}V_{\beta}(\mathbf{x})][\partial_{\mu}V_{\nu}(\mathbf{x})][iQ^{\alpha\beta\mu\nu}(p)+2\pi\Theta(S-V^0(\mathbf{x})-p^0)R^{\alpha\beta\mu\nu}(p,x)]\\&+[\partial_{\alpha}\partial_{\mu}V_{\nu}(\mathbf{x})][iS^{\alpha\mu\nu}(p)+2\pi\Theta(S-V^0(\mathbf{x})-p^0)T^{\alpha\mu\nu}(p,x)]\}\end{aligned} \tag{13a}$$

with

$$Q^{\alpha\beta\mu\nu}(p)=(\bar{p}+m)\left[-48\frac{p^\alpha p^\beta p^\mu p^\nu}{(p^2-m^2+i\epsilon)^5}-\frac{\gamma^\alpha\gamma^\beta\gamma^\mu\gamma^\nu+2g^{\alpha\mu}g^{\beta\nu}}{(p^2-m^2+i\epsilon)^3}+\frac{12p^\alpha p^\beta\gamma^\mu\gamma^\nu+8p^\alpha p^\mu g^{\beta\nu}+8p^\alpha p^\nu g^{\beta\mu}+8p^\beta p^\nu g^{\alpha\mu}}{(p^2-m^2+i\epsilon)^4}\right]$$
$$+24\frac{\gamma^\alpha p^\beta p^\mu p^\nu}{(p^2-m^2+i\epsilon)^4}-4\frac{\gamma^\alpha p^\beta\gamma^\mu\gamma^\nu+\gamma^\alpha p^\mu g^{\beta\nu}+\gamma^\alpha p^\nu g^{\beta\mu}}{(p^2-m^2+i\epsilon)^3}\ , \tag{13b}$$

$$R^{\alpha\beta\mu\nu}(p,\mathbf{x})=(\bar{p}+m)\left[\frac{p^\alpha p^\beta p^\mu p^\nu}{E[5(p^0)^4+10(p^0)^2E^2+E^4]}\delta''''(p^0-E)\right.$$
$$+\frac{3p^\alpha p^\beta\gamma^\mu\gamma^\nu+2p^\alpha p^\mu g^{\beta\nu}+2p^\alpha p^\nu g^{\beta\mu}+2p^\beta p^\nu g^{\alpha\mu}}{12p^0E[(p^0)^2+E^2]}\delta'''(p^0-E)$$
$$\left.+\frac{\gamma^\alpha\gamma^\beta\gamma^\mu\gamma^\nu+2g^{\alpha\mu}g^{\beta\nu}}{4E[3(p^0)^2+E^2]}\delta''(p^0-E)\right]$$
$$+\frac{\gamma^\alpha p^\beta p^\mu p^\nu}{2p^0E[(p^0)^2+E^2]}\delta'''(p^0-E)+\frac{\gamma^\alpha p^\beta\gamma^\mu\gamma^\nu+\gamma^\alpha p^\mu g^{\beta\nu}+\gamma^\alpha p^\nu g^{\beta\mu}}{E[3(p^0)^2+E^2]}\delta''(p^0-E)\ , \tag{13c}$$

$$S^{\alpha\mu\nu}(p)=(\bar{p}+m)\left[8\frac{p^\alpha p^\mu p^\nu}{(p^2-m^2+i\epsilon)^4}-2\frac{p^\alpha\gamma^\mu\gamma^\nu+p^\nu g^{\alpha\mu}}{(p^2-m^2+i\epsilon)^3}\right]-4\frac{\gamma^\alpha p^\mu p^\nu}{(p^2-m^2+i\epsilon)^3}+\frac{\gamma^\nu g^{\alpha\mu}}{(p^2-m^2+i\epsilon)^2}\ , \tag{13d}$$

$$T^{\alpha\mu\nu}(p,\mathbf{x})=(\bar{p}+m)\left[\frac{p^\alpha p^\mu p^\nu}{6p^0E[(p^0)^2+E^2]}\delta'''(p^0-E)+\frac{p^\alpha\gamma^\mu\gamma^\nu+p^\nu g^{\alpha\mu}}{2E[3(p^0)^2+E^2]}\delta''(p^0-E)\right]$$
$$+\frac{\gamma^\alpha p^\mu p^\nu}{E[3(p^0)^2+E^2]}\delta''(p^0-E)+\frac{\gamma^\nu g^{\alpha\mu}}{4p^0E}\delta'(p^0-E)\ . \tag{13e}$$

For this propagator one can directly prove gauge invariance (up to the order of the gradient expansion). A discussion of a manifestly gauge invariant scheme is given in the appendix. This propagator reduces to the Green's function, evaluated with the Kirzhnits formalism in Ref. 6, for the case of a pure electrostatic potential,

$$V_\nu(\mathbf{x})=(V(\mathbf{x}),\mathbf{0})\ .$$

With the representation of the electron propagator given above one can, e.g., readily extend the relativstic Thomas-Fermi-Dirac-Weizsäcker model[6] to the case of arbitrary four potentials.[10]

Two additional remarks are in order. We have, by basing the discussion on the form (2), obtained a gradient expansion of the Green's function which, in accordance with the standard practice, does not exhibit the usual symmetry properties with respect to the coordinates x and y. It is possible to remedy this situation at least partially. Secondly, one might imagine applying the same technique to the case of time-dependent potentials, with the aim of providing a hydrodynamical description of the noninteracting relativistic many particle system. In fact the only restriction to stationary systems is due to the explicit form of $g^{[0]}$. The recursion relation is also valid for time-dependent potentials. An extension in this direction is in progress.

The authors acknowledge support by the Deutsche Forschungsgemeinschaft.

APPENDIX

The recursion relation, Eq. (8), as well as the explicit results for the Green's function, Eqs. (12) and (13), are not manifestly gauge invariant. Although one can immediately show that these expressions are in fact invariant it would be more satisfying to have a manifestly gauge invariant formalism. The corresponding treatment of the recursion scheme is given below.

Under a general gauge transformation,

$$V_\nu(x)\rightarrow V_\nu(x)+\partial_\nu\Lambda(x)\ , \tag{A1}$$

the propagator of an abelian gauge theory transforms as

$$G(x,y)\rightarrow e^{-(i/\hbar)[\Lambda(x)-\Lambda(y)]}G(x,y)\ . \tag{A2}$$

This suggests that one separate a different phase from $G(x,y)$ than the one used in Eq. (5), namely,

$$G(x,y)=\exp\left[-\frac{i}{\hbar}\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}[\partial_{\nu_1}\cdots\partial_{\nu_k}V_\mu(x)](x-y)^{\nu_1}\cdots(x-y)^{\nu_k}(x-y)^\mu\right]\bar{g}(x,y)\ . \tag{A3}$$

The phase factor in Eq. (A3) transforms under the gauge transformation (A1) exactly as the full Green's function

$$\exp\left[-\frac{i}{\hbar}\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}[\partial_{\nu_1}\cdots\partial_{\nu_k}V_\mu(x)](x-y)^{\nu_1}\cdots(x-y)^{\nu_k}(x-y)^\mu\right]$$

$$\to\exp\left[-\frac{i}{\hbar}\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}[\partial_{\nu_1}\cdots\partial_{\nu_k}V_\mu(x)](x-y)^{\nu_1}\cdots(x-y)^{\nu_k}(x-y)^\mu\right]$$

$$\times\exp\left[\frac{i}{\hbar}\sum_{k=1}^{\infty}\frac{(-1)^k}{k!}[\partial_{\nu_1}\cdots\partial_{\nu_k}\Lambda(x)](x-y)^{\nu_1}\cdots(x-y)^{\nu_k}\right]$$

$$=\exp\left[-\frac{i}{\hbar}\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}[\partial_{\nu_1}\cdots\partial_{\nu_k}V_\mu(x)](x-y)^{\nu_1}\cdots(x-y)^{\nu_k}(x-y)^\mu\right]\exp\left[-\frac{i}{\hbar}[\Lambda(x)-\Lambda(y)]\right].$$

Therefore $\tilde{g}$ must be gauge invariant. Of course the phase chosen contains all orders of $\hbar$. It thus leads to a reordering of the gradient corrections to the Green's function,

$$G(x,y)=\exp\left[-\frac{i}{\hbar}\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}[\partial_{\nu_1}\cdots\partial_{\nu_k}V_\mu(x)](x-y)^{\nu_1}\cdots(x-y)^{\nu_k}(x-y)^\mu\right]\sum_{n=0}^{\infty}\tilde{g}^{[n]}(x,y)\,, \tag{A4}$$

$$\tilde{g}^{[n]}(x,y)\neq g^{[n]}(x,y)\,. \tag{A5}$$

The gauge invariance of $\tilde{g}^n(x,y)$ becomes apparent if one evaluates the recursion formula corresponding to Eq. (8),

$$\tilde{g}^{[n]}(p,x)=\frac{\not{p}+m}{p^2-m^2}\gamma^\lambda\left[4\sum_{k=1}^{n}\frac{(i\hbar)^{k+1}}{(k+1)!}[\partial_{\nu_1}\cdots\partial_{\nu_{k-1}}F_{\lambda\nu_k}(x)]\frac{\partial}{\partial p_{\nu_1}}\cdots\frac{\partial}{\partial p_{\nu_k}}\tilde{g}^{[n-k]}(p,x)-i\hbar\partial_\lambda\tilde{g}^{[n-1]}(p,x)\right], \tag{A6}$$

where the gauge invariant field tensor $F_{\lambda\nu}(x)$ has been used. If

$$\tilde{g}^{[0]}(p,x)=g^{[0]}(p,x) \tag{A7}$$

is gauge invariant, all higher orders are also gauge invariant. For stationary problems where $g^{[0]}(p,x)$ is given by Eq. (10) only a very restricted class of gauge transformations is permitted, namely,

$$\Lambda(x)=ax^0+\lambda(\mathbf{x}),\quad a=\text{const},\quad \Delta\lambda(\mathbf{x})=0\,.$$

In order to describe the same physical system after the gauge transformation the integration contour of the Feynman propagator has to be changed. This corresponds to a shift of the threshold S to $S+a$ in Eq. (10) together with the gauge transformation

$$V^\nu(\mathbf{x})\to V^\nu(\mathbf{x})+\partial^\nu\Lambda(x)$$
$$=(V^0(\mathbf{x})+a,\mathbf{V}(\mathbf{x})-\nabla\lambda(\mathbf{x}))\,.$$

Thus the difference $S-V^0(\mathbf{x})$ which occurs in $g^{[0]}(p,\mathbf{x})$ remains unchanged.

The price of gauge covariance is a recursion formula which cannot be resolved as simply as Eq. (8). Furthermore, one has

$$\left[\partial_\mu-2F_{\mu\nu}(x)\frac{\partial}{\partial p_\nu}\right]\Theta(S-V^0(\mathbf{x})-p^0)\neq0\,,$$

which even makes the evaluation of low-order terms much more difficult.

[1]G. A. Baraff and S. Borowitz, Phys. Rev. **121**, 1704 (1961).

[2]R. Baltin, Z. Naturforsch. **27a**, 1176 (1972).

[3]M. Durand, M. Brack, and P. Schuck, Z. Phys. A **286**, 381 (1978).

[4]E. K. U. Gross and R. M. Dreizler, Phys. Lett. A **81**, 447 (1981).

[5]E. K. U. Gross and R. M. Dreizler in *Density Functional Methods in Physics*, Vol. 123 of *NATO Advanced Study Institute, Series B: Physics*, edited by R. M. Dreizler and J. da Providencia (Plenum, New York, 1985), p. 81–140.

[6]E. Engel and R. M. Dreizler, Phys. Rev. A **35**, 3607 (1987).

[7]A. S. Kompaneets and E. S. Pavlovskii, Zh. Eskp. Teor. Fiz. **31**, 427 (1956) [Sov. Phys.-JETP **4**, 328 (1957)].

[8]D. A. Kirzhnits, Zh. Eskp. Teor. Fiz. **32**, 115 (1957) Sov. Phys.-JETP **5**, 64 (1957).

[9]D. A. Kirzhnits, *Field Theoretical Methods in Many Body Systems*, (Pergamon, Oxford, 1967).

[10]H. Müller, E. Engel, and R. M. Dreizler (unpublished).