December 1994

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T. Toyoda
Tokai University, Japan

Y. Takahashi
University of Alberta, Canada

C. Zhang
University of Wollongong, czhang@uow.edu.au

PHYSICAL REVIEW B VOLUME 50, NUMBER 24 15 DECEMBER 1994-II

Exact formula for nondiagonal Green's functions in condensed-matter physics

Tadashi Toyoda
Department of Physics, Tokai University, 1117 Kitakaname, Hiratsuka, Kanagawa, 259-12 Japan

Yasushi Takahashi
Theoretical Physics Institute, University of Alberta, Edmonton, Alberta, Canada T6G 2J1

Chao Zhang
Department of Physics, University of Wollongong, New South Wales 2522, Australia
(Received 18 August 1994)

An exact formula for the nondiagonal part of the one-particle temperature Green's function is obtained within the framework of the nonperturbative canonical formulation of the finite-temperature generalized Ward-Takahashi relation. It is shown that the Landau-level Green's function for two-dimensional electrons has a nonvanishing nondiagonal part if the electron-electron interaction is included.

One of the most successful and most commonly used methods in studying many-particle systems is the Green's function formalism. A many-body Green's function contains most important physical information such as the ground-state energy and other thermodynamic functions, the energy and lifetime of excited states, and the linear response to external perturbations. In the past decade, the use of the Green's function has been developed further and generalized to systems of low-dimensionality, for example, many-electron systems in semiconductor heterostructures and quantum wells. These low-dimensional electronic systems manifest many interesting phenomena related to many-body effects, especially at low temperatures and under a strong magnetic field.[1] Most of these many-body phenomena (e.g., collective excitation, magnetotransport, etc.) can be studied by employing the Green's function method. In this report, we shall pay special attention to the nondiagonal part of the many-body Green's function. The result will be used to examine the Green's function of a two-dimensional electron gas in a magnetic field.

In quantum many-body theory, the one-particle Green's function

$$G_{\alpha_1\alpha_2}(\tau_1,\tau_2) \equiv -\langle T_\tau\{c_{\alpha_1}(\tau_1)c^\dagger_{\alpha_2}(\tau_2)\}\rangle,$$

where $c^\dagger_\alpha(\tau)$ is the creation operator of a particle with the quantum number α in the τ-Heisenberg picture,[2] is generally not diagonal with respect to α_1 and α_2. Nevertheless, approximations assuming $G_{\alpha_1\alpha_2} \propto \delta_{\alpha_1\alpha_2}$ are often adopted in order to simplify many-body calculations.[3–6] A typical example is the Landau level Green's function for a two-dimensional electron gas in a magnetic field. We shall derive an exact formula for the nondiagonal part of the Green's function on the basis of the nonperturbative canonical formulation of the finite-temperature generalized Ward-Takahashi relations (FTGWTR).[2] Using the formula we can straightforwardly check if the nondiagonal part vanishes. If the nondiagonal part exists, its magnitude can also be estimated using the formula.

We consider a many-boson (fermion) system described in terms of the second-quantized Schrödinger field $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$ satisfying the equal-time (anti-)commutation relation

$$\psi(\mathbf{r})\psi^\dagger(\mathbf{r}') \pm \psi^\dagger(\mathbf{r}')\psi(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}'), \tag{1}$$

where the upper plus sign is for fermions and the lower minus sign is for bosons. For simplicity the spin variables are omitted. We assume the Hamiltonian of the system is given as

$$H = H_0 + H_{\rm int}. \tag{2}$$

The free Hamiltonian H_0 contains the chemical potential term. We define the field operators in the τ-Heisenberg picture,[2]

$$\Omega(\mathbf{r},\tau) = e^{\frac{1}{\hbar}H\tau}\Omega(\mathbf{r})e^{-\frac{1}{\hbar}H\tau}, \tag{3}$$

where $\Omega(\mathbf{r})$ is any field operator in the Schrödinger picture. Introducing a set of eigenfunctions $u_p(\mathbf{r})$, we expand the field operators,

$$\psi(\mathbf{r},\tau) = \sum_p c_p(\tau)u_p(\mathbf{r}) \tag{4}$$

and

$$\psi^\dagger(\mathbf{r},\tau) = \sum_p c^\dagger_p(\tau)u^*_p(\mathbf{r}). \tag{5}$$

The quantum number p can be either discrete or continuous. If p is continuous, the notation $\sum_p$ means an integral. We define a global operator $F(\tau)$,

$$F(\tau) \equiv \sum_p \xi_p c^\dagger_p(\tau)c_p(\tau)\ , \tag{6}$$

where ξ_p is a c-number function of p. This $F(\tau)$ can be H_0, the total momentum of the system, the total angular momentum of the system, etc., depending on the choice of $u_p(\mathbf{r})$ and ξ_p. Now we follow the nonperturbative canonical formulation of FTGWTR given in Ref. 2. We start with the identity,

$$\frac{\partial}{\partial\tau}\langle T_\tau\{F(\tau)c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\}\rangle$$

$$\begin{aligned}
&=\delta(\tau-\tau_1)\langle T_\tau\{[F(\tau),c_{p_1}(\tau_1)]c_{p_2}(\tau_2)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\}\rangle\\
&\quad+\delta(\tau-\tau_2)\langle T_\tau\{c_{p_1}(\tau_1)[F(\tau),c_{p_2}(\tau_2)]c_{p_3}(\tau_3)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\}\rangle+\cdots\\
&\quad+\delta(\tau-\tau_{2n})\langle T_\tau\{c_{p_1}(\tau_1)c_{p_2}(\tau_2)c_{p_3}(\tau_3)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots[F(\tau),c^\dagger_{p_{2n}}(\tau_{2n})]\}\rangle\\
&\quad+\left\langle T_\tau\left\{\frac{\partial F(\tau)}{\partial\tau}c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\right\}\right\rangle, \qquad (7)
\end{aligned}$$

where $\langle\cdots\rangle$ is the average over the grand canonical ensemble.[2] Integrating the both sides from 0 to $\beta\hbar$, where $\beta=1/k_BT$, with respect to τ and taking into account the cyclic invariance of the trace,[2] we obtain

$$\{\xi_{p_1}+\cdots+\xi_{p_n}-\xi_{p_{n+1}}-\cdots-\xi_{p_{2n}}\}\langle T_\tau\{c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\}\rangle$$

$$=\int_0^{\beta\hbar}d\tau\left\langle T_\tau\left\{\frac{\partial F(\tau)}{\partial\tau}c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\right\}\right\rangle, \qquad (8)$$

where we have used $[F(\tau),c_p(\tau)]=-\xi_pc_p(\tau)$ and $[F(\tau),c^\dagger_p(\tau)]=\xi_pc^\dagger_p(\tau)$. Now we rewrite (8) in terms of the n-particle Green's function,

$$G_{p_1,\ldots,p_n;p_{n+1},\ldots,p_{2n}}(\tau_1,\ldots,\tau_n;\tau_{n+1},\ldots,\tau_{2n})\equiv(-1)^n\langle T_\tau\{c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\}\rangle, \qquad (9)$$

to get the FTGWTR,[2]

$$\{\xi_{p_1}+\cdots+\xi_{p_n}-\xi_{p_{n+1}}-\cdots\xi_{p_{2n}}\}G_{p_1,\ldots,p_n;p_{n+1},\ldots,p_{2n}}(\tau_1,\ldots,\tau_n;\tau_{n+1},\ldots,\tau_{2n})$$

$$=(-1)^n\int_0^{\beta\hbar}d\tau\left\langle T_\tau\left\{\frac{\partial F(\tau)}{\partial\tau}c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)c^\dagger_{p_{n+1}}(\tau_{n+1})\cdots c^\dagger_{p_{2n}}(\tau_{2n})\right\}\right\rangle. \qquad (10)$$

If $F(\tau)$ commutes with the Hamiltonian,

$$\frac{\partial F(\tau)}{\partial\tau}=\frac{1}{\hbar}[H,F(\tau)]=0, \qquad (11)$$

then (10) yields

$$\{\xi_{p_1}+\cdots+\xi_{p_n}-\xi_{p_{n+1}}-\cdots-\xi_{p_{2n}}\}$$

$$\times G_{p_1,\ldots,p_n;p_{n+1},\ldots,p_{2n}}(\tau_1,\ldots,\tau_n;\tau_{n+1},\ldots,\tau_{2n})=0. \qquad (12)$$

This equation shows that the Green's function conserves the quantity ξ_p, that is,

$$G_{p_1,\ldots,p_n;p_{n+1},\ldots,p_{2n}}(\tau_1,\ldots,\tau_n;\tau_{n+1},\ldots,\tau_{2n})$$

$$\propto\delta(\xi_{p_1}+\cdots+\xi_{p_n}-\xi_{p_{n+1}}-\cdots-\xi_{p_{2n}}), \qquad (13)$$

where $\delta(\cdots)$ is either a Kronecker's δ or a δ function. In practical calculations, a linear ξ_p,

$$\xi_p=ap+c, \qquad (14)$$

where a and c are constant parameters, is the most useful. Then Eq. (13) simply gives the conservation of the quantum number p,

$$G_{p_1,\ldots,p_n;p_{n+1},\ldots,p_{2n}}(\tau_1,\ldots,\tau_n;\tau_{n+1},\ldots,\tau_{2n})$$

$$\propto\delta(p_1+\cdots+p_n-p_{n+1}-\cdots-p_{2n}). \qquad (15)$$

If we choose the total momentum

$$\mathbf{P}(\tau)=\int d\mathbf{r}\psi^\dagger(\mathbf{r},\tau)(-i\hbar\nabla)\psi(\mathbf{r},\tau) \qquad (16)$$

for $F(\tau)$, we get the well-known result for the Green's functions,

$$G_{\mathbf{p_1};\mathbf{p_2}}\propto\delta(\mathbf{p_1},\mathbf{p_2}) \qquad (17)$$

and

$$G_{\mathbf{p_1p_2};\mathbf{p_3p_4}}\propto\delta(\mathbf{p_1}+\mathbf{p_2},\mathbf{p_3}+\mathbf{p_4}), \qquad (18)$$

if the Hamiltonian commutes with $\mathbf{P}$.

Now we shall examine the right-hand side of (10), which is responsible for the nondiagonal parts of the Green's function. We consider particularly a two-dimensional electron gas in a magnetic field, whose Hamiltonian is assumed to be

$$H=H_0+H_{\rm int}=H_0+H_1+H_2 \qquad (19)$$

with

$$H_0=\int d\mathbf{r}\psi^\dagger(\mathbf{r},\tau)\left[\frac{1}{2m}(-i\hbar\nabla+e\mathbf{A}/c)^2-\mu\right]\psi(\mathbf{r},\tau), \qquad (20)$$

$$H_1=\int d\mathbf{r}V_{\rm imp}(\mathbf{r})\psi^\dagger(\mathbf{r},\tau)\psi(\mathbf{r},\tau), \qquad (21)$$

$$H_2 = \int d\mathbf{r}d\mathbf{r}'\psi^\dagger(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau)V_{\text{el-el}}(\mathbf{r}-\mathbf{r}') \times\psi(\mathbf{r}',\tau)\psi(\mathbf{r},\tau). \quad (22)$$

Adopting the Landau gauge, where the vector potential is given as $\mathbf{A} = (0, Bx, 0)$ with B the magnitude of the magnetic field, we can diagonalize H_0 in terms of the Landau level operators, c_{Nk} and $c^\dagger_{Nk}$ that correspond to the eigenfunctions

$$u_{Nk}(\mathbf{r}) = e^{iky}\phi_N(x - l_B^2 k), \quad (23)$$

where $l_B = (\hbar c/eB)^{1/2}$ is the magnetic length and

$$\phi_N(x) = \frac{1}{\pi^{1/4}(l_B 2^N N!)^{1/2}} e^{-x^2/2l_B^2} H_N(x/l_B). \quad (24)$$

The operators c_{Nk} and $c^\dagger_{Nk}$ satisfy

$$c_{Nk}c^\dagger_{N'k'} + c^\dagger_{N'k'}c_{Nk} = \delta_{NN'}\delta(k-k'). \quad (25)$$

The free Hamiltonian can be written as

$$H_0 = \sum_{N,k}\{(n+1/2)\hbar\omega_c - \mu\}\, c^\dagger_{Nk}c_{Nk}. \quad (26)$$

We assume this $H_0(\tau)$ for $F(\tau)$ in the FTGWTR given by (10). If we put $n = 1$ and $F(\tau) = H_0(\tau)$ in (10), we get

$$\hbar\omega_c(N-N')G_{NkN'k'}(\tau,\tau') = -\int_0^{\beta\hbar} d\tau \left\langle T_\tau\left\{\frac{\partial H_0(\tau)}{\partial\tau} c_{Nk}(\tau_1)c^\dagger_{N'k'}(\tau')\right\}\right\rangle . \quad (27)$$

Noting

$$\frac{\partial H_0(\tau)}{\partial\tau} = \frac{1}{\hbar}[H(\tau), H_0(\tau)] = [H_0(\tau) + H_{\text{int}}(\tau), H_0(\tau)] = [H_{\text{int}}(\tau), H_0(\tau)] = [H_{\text{int}}(\tau), H_0(\tau) + H_{\text{int}}(\tau)] = -\frac{\partial H_{\text{int}}(\tau)}{\partial\tau}, \quad (28)$$

we can also write (27) as

$$\hbar\omega_c(N-N')G_{NkN'k'}(\tau,\tau') = \int_0^{\beta\hbar} d\tau \left\langle T_\tau\left\{\frac{\partial H_{\text{int}}(\tau)}{\partial\tau} c_{Nk}(\tau_1)c^\dagger_{N'k'}(\tau')\right\}\right\rangle . \quad (29)$$

Because $H_{\text{int}}(\tau)$ contains only the density operator $\rho(\mathbf{r},\tau) = \psi^\dagger(\mathbf{r},\tau)\psi(\mathbf{r},\tau)$, the second formula (29) is most convenient. For the nondiagonal parts Eq. (29) gives

$$G_{NkN'k'}(\tau,\tau') = \frac{1}{\hbar\omega_c(N-N')}\int_0^{\beta\hbar} d\tau \left\langle T_\tau\left\{\frac{\partial H_{\text{int}}(\tau)}{\partial\tau} \times c_{Nk}(\tau_1)c^\dagger_{N'k'}(\tau')\right\}\right\rangle \quad (N \neq N'). \quad (30)$$

To examine $\partial H_{\text{int}}(\tau)/\partial\tau$ we first rewrite $H_{\text{int}}(\tau)$ given by (21) and (22) in terms of $\rho(\mathbf{r},\tau)$

$$H_1 = \int d\mathbf{r}V_{\text{imp}}(\mathbf{r})\rho(\mathbf{r},\tau)\ , \quad (31)$$

$$H_2 = \int d\mathbf{r}d\mathbf{r}'V_{\text{el-el}}(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',\tau)\rho(\mathbf{r},\tau) - \frac{1}{2}\int d\mathbf{r}V(0)\rho(\mathbf{r},\tau). \quad (32)$$

Because the total Hamiltonian commutes with $\int d\mathbf{r}\rho(\mathbf{r},\tau)$, from $H_0(\tau)$ we can define the current density $\mathbf{J}(\mathbf{r},\tau)$ such that

$$\frac{\partial}{\partial\tau}\rho(\mathbf{r},\tau) = -\nabla\cdot\mathbf{J}(\mathbf{r},\tau). \quad (33)$$

By virtue of this "continuity equation," we get

$$\frac{\partial H_1(\tau)}{\partial\tau} = \int d\mathbf{r}[\nabla V_{\text{imp}}(\mathbf{r})]\cdot\mathbf{J}(\mathbf{r},\tau) \quad (34)$$

and

$$\frac{\partial H_2(\tau)}{\partial\tau} = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'V_{\text{el-el}}(\mathbf{r}-\mathbf{r}')[\{\nabla\cdot\mathbf{J}(\mathbf{r},\tau)\} \times\rho(\mathbf{r}',\tau) + \rho(\mathbf{r},\tau)\{\nabla'\cdot\mathbf{J}(\mathbf{r}',\tau)\}] \quad (35)$$

$$= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\nabla V_{\text{el-el}}(\mathbf{r}-\mathbf{r}')\cdot[\mathbf{J}(\mathbf{r},\tau)\rho(\mathbf{r}',\tau) + \rho(\mathbf{r},\tau)\mathbf{J}(\mathbf{r}',\tau)]. \quad (36)$$

The second term on the right-hand side of (32) does not contribute to $\partial H_2(\tau)/\partial\tau$.

Equations (34) and (36) show that the Green's function $G_{NkN'k'}$ will have nonvanishing nondiagonal parts if electron-impurity or electron-electron interactions are included in the Hamiltonian. The average over the random impurity configuration may restore the translational invariance and allows one to neglect the nondiagonal parts of the Green's function,[5] $G_{NkN'k'} \propto \delta_{NkN'k'}$. However, the effect of the electron-electron interaction is always present. A similar technique such as configuration averaging over the impurity distribution cannot be used to treat the electron-electron interaction, and, therefore, the Green's function for a magnetically quantized electron gas always has a nondiagonal part. Such an effect should become more important in samples with a weak electron-impurity interaction, and a lower electron density where the electron-electron interaction strength exceeds that of the electron-impurity interaction. In these systems, it is not sufficient to simply include the diagonal part of the self-energy correction to evaluate the mass shift and lifetime, but one must also include the contribution of the nondiagonal part of the Green's function and the self-energy.

This work is supported in part by the Australian Research Council (C.Z.) and by the Natural Science and Engineering Research Council of Canada (Y.T.).

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