INTRODUCTION

RKKY interaction between two magnetic impurities in graphene was theoretically studied quite intensely during last several years. A terse but precise review of the issue one can find in the book by M. Katsnelson. One may ask, why the problem, which is in principle so simple (when being treated in the lowest order of perturbation theory, like it was done in all the papers referenced above), was the subject of so many publication, using different approaches? The answer to this question, as presented below, is connected with the fact that a simply written integral is not necessarily a simply calculated integral, and in the frame work of all zero temperature Green’s functions (ZTGF) the integrals defining the RKKY interaction in graphene turned out to be divergent. Different ZTGF approaches can be thus viewed as different ways to obtain finite results from the divergent integrals.

In our previous publication dealing with the subject we were using the approach based on Matsubara Green’s functions (MGF) in the coordinate – imaginary time representation. In this work we consider RKKY interaction in graphene in the framework of approach based on MGF in the coordinate – frequency representation. We claim that both approaches have an important advantage over those based on zero temperature Green’s functions (ZTGF), which are very briefly reviewed in the beginning of the present work. The MGF approaches, in distinction to the ZTGF approaches, operate only with the convergent integrals from the start to the end of the calculation. The coordinate – frequency representation for the MGF turns out to be as convenient as the coordinate – imaginary time representation and allows to easily consider the cases of doped and gapped graphene.

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While calculating RKKY interaction in graphene no theorist should do a cut-off without cause

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In our previous work (E. Kogan, Phys. Rev. B 84, 115119 (2011)) we presented calculation of RKKY interaction between two magnetic impurities in graphene based on Matsubara Green’s functions (MGF) in the coordinate – imaginary time representation. Now we present the calculation based on MGF in the coordinate – frequency representation. We claim that both approaches have an important advantage over those based on zero temperature Green’s functions (ZTGF), which are very briefly reviewed in the beginning of the present work. The MGF approaches, in distinction to the ZTGF approaches, operate only with the convergent integrals from the start to the end of the calculation. The coordinate – frequency representation for the MGF turns out to be as convenient as the coordinate – imaginary time representation and allows to easily consider the cases of doped and gapped graphene.

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APPROACHES BASED ON ZTGF

The approach, used in Refs. [1, 3, 4] is based on equation

\[ \chi(R) = \int \frac{d^2 q}{(2\pi)^2} \chi(\omega = 0, q) e^{i q \cdot R}, \]  

where

\[ \chi(\omega = 0, q) = 2 \int \frac{d^2 k}{(2\pi)^2} \frac{n_F(\xi_k) - n_F(\xi_{k+q})}{E_{k+q} - E_k}, \]  

\[ \xi_n = E_n - \mu \text{ and } n_F(\xi) = (e^{\beta \xi} + 1)^{-1} \] is the Fermi distribution function. This approach, though looking quite straightforward, brings with it a problem. In a model of infinite Dirac cones for \( \chi(\omega = 0, q) \) we obtain a diverging integral. To obtain finite values from these divergent integrals, as it was mentioned previously, one has to implement the complicated (and to some extent arbitrary) cut-off procedure [4].

The problem can be formulated in a different way. Being calculated in a realistic band model, with the bands...
of finite width, $\chi(\omega = 0, q)$ is not a universal quantity. It depends not only on infrared physics, but on the properties of electron spectrum and eigenfunctions in the whole Brillouin zone (even for small $q$).

Another approach, formulated in Ref. [2], starts from a well known equation for the susceptibility

$$\chi(R) = \frac{2i}{\pi} \int_{-\infty}^{\infty} G^2(R, E) dE,$$

where $G$ is the retarded green’s function. Here again the integral diverges on both limits of integration. However the authors changed the contour of integration, transforming the divergent integral into the convergent integral along the imaginary axis (see also Ref. [20]). The authors also considered KAKY interaction in gapped graphene, when the power law decrease of the interaction integral along the imaginary axis (see also Ref. [20]).

Also in this case, to obtain finite values from these divergent integrals one has to implement the complicated cut-off procedure. The approach, using formula

$$\chi(r, r') = \delta n(r) / \delta V(r'),$$

and, hence, calculating electron susceptibility on the basis of equation

$$\chi(R) = -\frac{2}{\pi} \int_{-\infty}^{E_F} \text{Im} \left[ G^2(R, E) \right] dE,$$

where $E_F$ is the Fermi energy, was first used, in application to graphene, to the best of our knowledge, in Ref. [11]. An advantage of this approach is that it allows to easily consider the case of doped graphene, the disadvantage is that the approach, like the one presented above, has to deal with the divergent integral (the integral with respect to $dE$ diverges at the lower limit of integration). Also in this case, to obtain finite values from these divergent integrals one has to implement the complicated (and to some extent arbitrary) cut-off procedure.

**MGF in Frequency Representation**

Our approach will be based on equation [21]

$$\chi(R) = -\frac{1}{\pi} \int_{-\infty}^{\infty} G^2(R; \omega) d\omega,$$

where $G(R; \omega)$ is the MGF in frequency momentum representation. Dirac equation describing electrons is

$$H = v(\tau^x k_x + \tau^y k_y),$$

where the matrix $\tau$ acts in the space of two sublattices. From Eq. (9) we obtain

$$G(k, \omega) = \frac{1}{i \omega + \mu - v(\tau^x k_x + \tau^y k_y)},$$

where $\mu$ is a chemical potential. From Eq. (10) we obtain

$$G^{CC}(R, \omega) = -\frac{i(\omega - i\mu)}{(2\pi)^2} \int_{0}^{\infty} dk \frac{k^2}{(\omega - i\mu)^2 + v^2 k^2}$$

$$\cdot \int_{0}^{2\pi} e^{ikR \cos \theta} d\theta = -\frac{i(\omega - i\mu)}{2\pi} \int_{0}^{\infty} dk J_0(kR) \frac{k^2}{(\omega - i\mu)^2 + v^2 k^2}$$

$$= \frac{-i(\omega - i\mu)}{2\pi v^2} K_0 \left[ \text{sign}(\omega)(\omega - i\mu)R/v \right].$$

$$G^{AA}(R, \omega) = -\frac{v}{(2\pi)^2} \int_{0}^{\infty} dk \frac{k^2}{(\omega - i\mu)^2 + v^2 k^2}$$

$$\cdot \int_{0}^{2\pi} e^{ikR \cos \theta} d\theta = -\frac{v}{2\pi} \int_{0}^{\infty} dk J_1(kR) \frac{k^2}{(\omega - i\mu)^2 + v^2 k^2}$$

$$= \frac{-\text{sign}(\omega)(\omega - i\mu)}{2\pi v^2} K_1 \left[ \text{sign}(\omega)(\omega - i\mu)R/v \right].$$

(11)

(12)

**UNDOPED GRAPHENE**

Consider first the case of undoped graphene ($\mu = 0$).

**MGF in Frequency Representation**

Using another mathematical identity [23]

$$\int_{0}^{\infty} x^{\alpha-1} \frac{1}{(x^2 + z^2)^\rho} J_\nu(cx) dx = \frac{c^{\rho-1} z^{\nu-\rho-1}}{2^{\nu-1} \Gamma(\rho)} K_{\nu-\rho+1}(cz).$$

(13)

**MGF in Time Representation**

For completeness, we reproduce here the calculation of $\chi$ based on MGF in coordinate – imaginary time representation, presented in our previous paper [11]. The susceptibility was written as [1, 2, 11]

$$\chi(R) = -2 \int_{-\infty}^{\infty} G(R; \tau) G(R, -\tau) d\tau.$$
Transition from frequency to imaginary time representation yields the MGF

\[ g^{CC}(k, \tau) = \frac{\text{sign}(\tau)}{2} e^{-vk|\tau|}, \]

\[ g^{AB}(k, \tau) = \frac{1}{2} e^{-vk|\tau| + i\vartheta}. \]  

(17)

As a result we obtain \[ g^{CC}(R, \tau) = \frac{\text{sign}(\tau)}{8\pi^2} \int_0^\infty \int_0^{2\pi} dk dk R e^{-vk|\tau|} \int_0^{2\pi} d\theta e^{ikR \cos \theta - vk|\tau|}. \]

\[ g^{AB}(R, \tau) = \frac{1}{8\pi^2} \int_0^\infty \int_0^{2\pi} dk dk R e^{ikR \cos \theta + i\vartheta - vk|\tau|}. \]

(18)

Performing the angular integrations in Eq. (18) we get

\[ g^{CC}(R; \tau) = \frac{\text{sign}(\tau)}{4\pi} \int_0^\infty dk J_0(kR)e^{-vk|\tau|} \]

\[ g^{AB}(R; \tau) = \frac{1}{4\pi} \int_0^\infty dk k J_1(kR)e^{-vk|\tau|}. \]

(19)

\( J_0 \) and \( J_1 \) are the Bessel function of zero and first order respectively. Using mathematical identity \[ \int_0^\infty x^{n-1} e^{-p x} J_\nu(cx) dx \]

\[ = (-1)^n c^{-\nu} \frac{\partial^{n-1}}{\partial p^{n-1}} \left( \sqrt{p^2 + c^2} - p \right)^\nu, \]

integrals in the RHS of Eq. (19) can be calculated exactly, giving a well known result \[ g^{CC}(R; \tau) = \frac{1}{4\pi} \left( \frac{v\tau}{(v^2 \tau^2 + R^2)^{3/2}} \right) \]

\[ g^{AB}(R; \tau) = \frac{1}{4\pi} \left( \frac{R}{(v^2 \tau^2 + R^2)^{3/2}} \right). \]

(21)

The remaining integration in Eq. (19) is trivial; as a result we recover Eq. (15).

**DOPED GRAPHENE**

In the case of doped graphene the susceptibility \[ \chi_{\mu}^{CC}(R) = \frac{1}{v} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta^2 + (\omega^2 + \frac{\omega R}{v})^2} \]

\[ \chi_{\mu}^{AB}(R) = \frac{1}{v} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta^2 + (\omega^2 + \frac{\omega R}{v})^2} \]

Taking into account the identity \[ \frac{d\omega}{\Delta^2 + (\omega^2 + \frac{\omega R}{v})^2} = \frac{1}{2} i \left[ J_{\alpha+1}(\omega x) + iY_{\alpha}(\omega x) \right] \]

we get \[ \chi_{\mu}^{CC}(R) = \frac{1}{v} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta^2 + (\omega^2 + \frac{\omega R}{v})^2} \]

\[ \chi_{\mu}^{AB}(R) = \frac{1}{v} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta^2 + (\omega^2 + \frac{\omega R}{v})^2} \]

(24)

where \( k_F = \mu/v \). The integrals in Eq. (25) can be presented in terms of Meijer functions \[ \text{I send the reader to Reference for the details).} \]

It is interesting to compare the RKKY exchange in doped graphene, with its two sublattices and linear dispersion law, with that in ordinary two-dimensional electron gas. For the latter the Green’s function is

\[ G(k, \omega) = \frac{1}{i\omega + \mu - k^2/2m}. \]

(26)

Hence the susceptibility turns out to be \[ \chi(R) \sim \frac{1}{R^2} \int_0^{\infty} dzz J_0(z) Y_0(z). \]

(27)

Amusing, that the authors of Ref. (24) were affiliated with the same University, as the author of the present paper.

**GAPPED GRAPHENE**

Consider now graphene with the gap in electron spectrum described by Dirac Hamiltonian

\[ H = \nu(\tau^x k_x + \tau^y k_y) + \Delta \tau^z. \]

(28)

The Green’s function is

\[ G(k, \omega) = \frac{-i\omega - \Delta \tau^z - \nu(\tau^x k_x + \tau^y k_y)}{\omega^2 + \Delta^2 + v^2 k^2}. \]

(29)

**MGF in frequency representation**

From Eq. (29) we obtain

\[ g^{CC}(R, \omega) = \frac{-i\omega \pm \Delta}{2\pi} \int_0^\infty \frac{k J_0(kR)dk}{\omega^2 + \Delta^2 + v^2 k^2} \]

\[ = \frac{-i\omega \pm \Delta}{2\pi v^2} K_0 \left( \sqrt{\omega^2 + \Delta^2 R/v} \right). \]

(30)

\[ g^{AB}(R, \omega) = \frac{-v}{2\pi} \int_0^\infty \frac{k^2 J_1(kR)dk}{\omega^2 + \Delta^2 + v^2 k^2} \]

\[ = \frac{-\sqrt{\omega^2 + \Delta^2}}{2\pi v^2} K_1 \left( \sqrt{\omega^2 + \Delta^2 R/v} \right). \]

(31)
In Eq. (30) minus corresponds to $AA$ and plus to $BB$. Substituting into Eq. (3) we obtain

$$
\chi^{CC}(R) = \frac{1}{4\pi^3 v^4} \int_{-\infty}^{\infty} (\omega^2 - \Delta^2) K_0^2 \left( \sqrt{\omega^2 + \Delta^2 R/v} \right) d\omega. \tag{32}
$$

$$
\chi^{AB}(R) = -\frac{1}{4\pi^3 v^4} \int_{-\infty}^{\infty} (\omega^2 + \Delta^2) K_1^2 \left( \sqrt{\omega^2 + \Delta^2 R/v} \right) d\omega. \tag{33}
$$

The remaining integrations can be performed analytically in two limiting cases.

Consider first the case $\Delta R/v \ll 1$. Here it is appropriate to mention the relation between the toy model, we are using, and real graphene. The existence of two Dirac points in graphene leads to additional angular dependent factor in the formula for the RKKY interaction. It was thoroughly studied previously and does not interfere with the physics we are discussing in this work. More interesting is the condition of the applicability of the approximation of linear dispersion law is applicable, provided $R \gg a$, where $a$ is the graphene lattice constant. Now we realize, that the case $\Delta R/v \ll 1$ can be described in the framework of the model if $\Delta \ll av$, or in simple terms, if the gap is narrow in comparison with the graphene band width, which is certainly true in most cases of gapped graphene. So finally, in the case of a narrow gap and relatively small distances we can go to the limit $\Delta \to 0$ in Eqs. (32) and (33), and recover the results of the gapless case.

The other limiting case $\Delta R/v \gg 1$ is more interesting. In this case we may use asymptotic expression for modified Bessel functions

$$
K_{\nu}(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z}. \tag{34}
$$

After calculating the resulting integrals in Eq. (33) using the Laplace method, we obtain the same result both for inter-sublattice and intra-sublattice susceptibility

$$
\chi = -\frac{1}{8v} \left( \frac{\Delta}{\pi v R} \right)^{3/2} e^{-2R\Delta/v}. \tag{35}
$$

It is worth paying attention to the fact that Eq. (35) seems to contradict rigorously proved theorem stating that for any bipartite lattice at half filling, the RKKY interaction is antiferromagnetic between impurities sitting on top of atoms belonging to opposite sublattices (i.e., $A$ and $B$ sublattices in graphene), and is ferromagnetic between impurities sitting on top of atoms belonging to the same sublattice [1, 11, 20]. However, the theorem is not applicable to Hamiltonian (28), with its last term meaning that if we rewrite the Hamiltonian in the tight-binding representation, the intra-sublattice hopping will appear, hence the lattice is no longer bipartite. More specifically, the spectrum still has the symmetry of that in bipartite lattice, but the wave functions do not.

The MGF in time representation

Here we’ll restrict ourselves with the calculation of $\chi^{AB}$. Transition from frequency to imaginary time representation yields the MGF

$$
G^{AB}(k, \tau) = \frac{v k}{2 \sqrt{\Delta^2 + v^2 k^2}} e^{-\sqrt{\Delta^2 + v^2 k^2} \tau} + i\theta. \tag{36}
$$

Hence instead of Eq. (19) we obtain

$$
J_0(kR) e^{-\sqrt{\Delta^2 + v^2 k^2} \tau}. \tag{37}
$$

Using mathematical identity [23]

$$
\int_0^{\infty} \frac{x^{n+1} e^{-\frac{a}{2} \sqrt{x^2 + z^2}}}{\sqrt{x^2 + z^2}} J_\nu(cx) dx = B_\nu, \tag{39}
$$

where

$$
B_1 = c \left( 1 + z \sqrt{p^2 + c^2} \right) \frac{e^{-\frac{a}{2} \sqrt{p^2 + c^2}}}{(p^2 + c^2)^{3/2}},
$$

we obtain

$$
G^{AB}(R; \tau) = \frac{R}{4\pi} \left( 1 + \sqrt{v^2 \tau^2 + R^2 \Delta/v} \right) \frac{e^{-\sqrt{v^2 \tau^2 + R^2 \Delta/v}}}{(v^2 \tau^2 + R^2)^{3/2}}. \tag{40}
$$

Thus we obtain

$$
\chi^{AB}(R) = -\frac{R^2}{8\pi^3} \int_{-\infty}^{\infty} \left( 1 + \sqrt{v^2 \tau^2 + R^2 \Delta/v} \right)^2 \frac{e^{-2\sqrt{v^2 \tau^2 + R^2 \Delta/v}}}{(v^2 \tau^2 + R^2)^{3/2}} d\tau. \tag{41}
$$

In the case $\Delta R/v \gg 1$ we can calculate integral in Eq. (41) using the Laplace method, to recover Eq. (35).

**CONCLUSIONS**

In the end we would like to mention again that though we were considering the case of $T = 0$, we have found, that, as it is not infrequently happens, the MGF have advantages over ZTGF. In particular, using the former one have to operate only with the convergent integrals, in distinction to what happens when one uses the latter.
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