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RKKY interaction in graphene at finite temperature

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In our publication from 8 years ago[?] we calculated RKKY interaction between two magnetic impurities in graphene. The consideration was based on the perturbation theory for the thermodynamic potential in the imaginary time representation and direct evaluation of real space spin susceptibility. Only the case of zero temperature was considered. We show in this short notice that the approach can be easily generalized to the case of finite temperature.

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Since graphene was first isolated experimentally[?] , it is in the focus of attention of both theorists and experimentalists. Many physical phenomena, well studied in "traditional" solid state physics look quite different in graphene. In this paper we will talk about the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction, first studied (in a normal metal) more than 60 years ago[? ? ?] . This interaction is the effective exchange between two magnetic impurities in a non–magnetic host, obtained as the second order perturbation with respect to exchange interaction between the magnetic impurity and the itinerant electrons of the host.

Quite a few theoretical papers published recently considered RKKY interaction in graphene[? ?] . Though analysis of the RKKY interaction is simple in principle, calculation of the integrals defining the interaction (whether analytical or numerical) can pose some problems. However, substantial progress was achieved in the field.

Our interest in the RKKY interaction in graphene started from learning that previously, while the interaction was calculated analytically in the approximation of the linear dispersion law for the electrons, the integrals obtained in both papers turned out to be divergent, and the complicated (and to some extent arbitrary) cut-off procedure was implemented to obtain from these integrals the finite results. So we started to look for the procedure which will allow to eliminate this problem. it turned out that when one uses Matsubara formalism and calculates the Green's functions in the coordinate-imaginary time representation the calculations are completely free from any diverging integrals[?] .

Though Matsubara formalism is quite appropriate for finate temperature calculations (it was invented for that purpose) in our previous publications[? ?] we studied RKKY interaction only at zero temperature. The present short note is intended to generalize the result obtained previously to the case of finite temperature.

We consider two magnetic impurities sitting on top of carbon atoms in graphene lattice at the sites i and j and assume a contact exchange interaction between the electrons and the magnetic impurities. Thus the total Hamiltonian of the system is

$$H_T = H + H_{int} = H - J\mathbf{S}_i\cdot\mathbf{s}_i - J\mathbf{S}_j\cdot\mathbf{s}_j, \qquad (1)$$

where H is the Hamiltonian of the electron system, $\mathbf{S}_i$ is the spins of the impurity and $\mathbf{s}_i$ is the spin of itinerant electrons at site i.

Our consideration is based on the perturbation theory for the thermodynamic potential[?] . The correction to the thermodynamic potential due to interaction is

$$\Delta\Omega = -T\ln\langle S\rangle \equiv -T\ln\mathrm{tr}\left\{S\cdot e^{-H/T}/Z\right\}, \qquad (2)$$

where the S–matrix is given by the equation

$$S = \exp\left\{-\int_0^{1/T} H_{int}(\tau)d\tau\right\}. \qquad (3)$$

Writing down $\mathbf{s}_i$ in the second quantization representation

$$\mathbf{s}_i = \frac{1}{2}c^\dagger_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}, \qquad (4)$$

the second order term of the expansion with respect to the interaction is

$$\Delta\Omega = \frac{J^2T}{4}\sum_{\alpha\beta\gamma\delta}\mathbf{S}_i\cdot\sigma_{\alpha\beta}\mathbf{S}_j\cdot\sigma_{\gamma\delta} \qquad (5)$$
$$\int_0^{1/T}\int_0^{1/T} d\tau_1 d\tau_2\left\langle T_\tau\left\{c^\dagger_{i\alpha}(\tau_1)c_{i\beta}(\tau_1)c^\dagger_{j\gamma}(\tau_2)c_{j\delta}(\tau_2)\right\}\right\rangle.$$

Notice that we have ignored the terms proportional to $\mathbf{S}_i^2$ and $\mathbf{S}_j^2$, because they are irrelevant for our calculation of the effective interaction between the adatoms spins.

Leaving aside the question about the spin structure of the two–particle Green's function standing in the r.h.s. of Eq. (??) (for interacting electrons), further on we assume that the electrons are non–interacting. This will allow us to use Wick theorem and present the correlator from Eq. (??) in the form

$$\left\langle T_\tau\left\{c^\dagger_{i\alpha}(\tau_1)c_{i\beta}(\tau_1)c^\dagger_{j\gamma}(\tau_2)c_{j\delta}(\tau_2)\right\}\right\rangle$$
$$= -\mathcal{G}_{\beta\gamma}(i,j;\tau_1-\tau_2)\mathcal{G}_{\delta\alpha}(j,i;\tau_2-\tau_1), \qquad (6)$$

where

$$\mathcal{G}_{\beta\gamma}(i,j,\tau_1-\tau_2) = -\left\langle T_\tau \left\{ c_{i\beta}(\tau_1) c^\dagger_{j\gamma}(\tau_2) \right\} \right\rangle \quad (7)$$

is the Matsubara Green's function[?] . We can connect $\mathcal{G}_{\beta\gamma}$ with the Green's function of spinless electron

$$\mathcal{G}_{\beta\gamma}(i,j,\tau_1-\tau_2) = -\delta_{\beta\gamma} \left\langle T_\tau \left\{ c_i(\tau_1) c^\dagger_j(\tau_2) \right\} \right\rangle . \quad (8)$$

Presence of delta-symbols allows to perform summation with respect to spin indices in Eq. (**??**)

$$\sum_{\alpha\beta} \mathbf{S}_i \cdot \sigma_{\alpha\beta} \mathbf{S}_j \cdot \sigma_{\beta\alpha} = \mathbf{S}_i \cdot \mathbf{S}_j, \quad (9)$$

which gives

$$\Delta\Omega = -J^2 \chi_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (10)$$

where

$$\chi_{ij} = -\frac{1}{4} \int_0^{1/T} \mathcal{G}(i,j;\tau)\mathcal{G}(j,i;-\tau) d\tau \quad (11)$$

is the free electrons static real space spin susceptibility[? ?] .

Thus we obtain

$$H_{RKKY} = -J^2 \chi_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (12)$$

The Green's function can be easily written down using representation of eigenvectors and eigenvalues of the operator H

$$(H - E_n)\, u_n = 0. \quad (13)$$

It is

$$\mathcal{G}(i,j;\tau) = \sum_n u_n^*(i) u_n(j) e^{-\xi_n \tau} \times \begin{cases} -\left(1 - n_F(\xi_n)\right), & \tau > 0 \\ n_F(\xi_n), & \tau < 0 \end{cases}, \quad (14)$$

where $\xi_n = E_n - \mu$, and $n_F(\xi) = \left(e^{\beta\xi} + 1\right)^{-1}$ is the Fermi distribution function.

In calculations of the RKKY interaction in graphene the $\sum_n$ in Eq. (**??**) turns into $\frac{a^2}{(2\pi)^2} \int d^2\mathbf{p}$, where a is the carbon–carbon distance. (Actually, there should appear a numerical multiplier, connecting the area of the elementary cell with a^2, but we decided to discard it, which is equivalent to some numerical renormalization of J.) Also

$$u_n(i) = e^{i\mathbf{p}\cdot\mathbf{R}_i} \psi_{\mathbf{p}}, \quad (15)$$

where $\psi_{\mathbf{p}}$ is the appropriate component of spinor electron wave-function (depending upon which sublattice the magnetic adatom belongs to) in momentum representation.

Further on the integration with respect to $d^2\mathbf{p}$ we'll treat as the integration in the vicinity of two Dirac points K, K' and present $\mathbf{p} = \mathbf{K}(\mathbf{K}') + \mathbf{k}$. The wave function for the momentum around Dirac points K and K' has respectively the form

$$\begin{aligned} \psi_{\nu,\mathbf{K}}(\mathbf{k}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta_{\mathbf{k}}/2} \\ \nu e^{i\theta_{\mathbf{k}}/2} \end{pmatrix} \\ \psi_{\nu,\mathbf{K}'}(\mathbf{k}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta_{\mathbf{k}}/2} \\ \nu e^{-i\theta_{\mathbf{k}}/2} \end{pmatrix}, \end{aligned} \quad (16)$$

where $\nu = \pm 1$ corresponds to electron and hole band[?] ; the upper line of the spinor refers to the sublattice A and the lower line refers to the sublattice B.

Like in our previous publication[?] , here we consider for simplicity only the case of undoped graphene. The chemical potential is at the Dirac points; $E_+(\mathbf{k})$ and $E_-(\mathbf{k})$ would be electron and hole energy. Then Eq. (**??**) takes the form: for i and j belonging to the same sublattice

$$\mathcal{G}^{AA}(i,j;\tau>0) = -\frac{1}{2}\left[e^{i\mathbf{K}\cdot\mathbf{R}_{ij}} + e^{i\mathbf{K}'\cdot\mathbf{R}_{ij}}\right] \frac{a^2}{(2\pi)^2} \int d^2\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{R}_{ij} - E_+(\mathbf{k})\tau}, \quad (17)$$

and for i and j belonging to different sublattices

$$\mathcal{G}^{AB}(i,j;\tau>0) = \frac{1}{2}\frac{a^2}{(2\pi)^2} \int d^2\mathbf{k} e^{-E_+(\mathbf{k})\tau} \times \left[e^{i(\mathbf{K}+\mathbf{k})\cdot\mathbf{R}_{ij} - i\theta_k} - e^{i(\mathbf{K}'+\mathbf{k})\cdot\mathbf{R}_{ij} + i\theta_k}\right]. \quad (18)$$

For $\tau < 0$ we should change the sign of the Green's functions and substitute E_- for E_+.

For isotropic dispersion law $E(\mathbf{k}) = E(k)$ we can perform the angle integration in Eqs. (**??**) and (**??**) to get

$$\begin{aligned} \int d^2\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{R}_{ij} - E(k)\tau} &= \int_0^\infty dk k J_0(kR) e^{-E(k)\tau} \quad (19) \\ \int d^2\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{R}_{ij} \pm i\theta_k - E(k)\tau} &= e^{\pm i\theta_{\mathbf{R}}} \int_0^\infty dk k J_1(kR) e^{-E(k)\tau} \end{aligned}$$

(J_0 and J_1 are the Bessel function of zero and first order respectively, and $\theta_{\mathbf{R}}$ is the angle between the vectors $\mathbf{K} - \mathbf{K}'$ and $\mathbf{R}_{ij}$; $R = |\mathbf{R}_{ij}|$).

For the linear dispersion law

$$E_\pm(k) = \pm v_F k, \quad (20)$$

using mathematical identity[?]

$$\begin{aligned} &\int_0^\infty x^{n-1} e^{-px} J_\nu(cx) dx \quad (21) \\ &= (-1)^{n-1} c^{-\nu} \frac{\partial^{n-1}}{\partial p^{n-1}} \frac{\left(\sqrt{p^2+c^2} - p\right)^\nu}{\sqrt{p^2+c^2}}, \end{aligned}$$

we can explicitly calculate the Green's functions.

In our previous publication we considered only the case $T = 0$, which corresponded to infinite upper integration

limit in Eq. (??). However, consideration of finite temperature just modifies our previous results -

$$\chi^{AA}_{T=0}(\mathbf{R}_{ij}) = \frac{a^4}{256 v_F R^3}\left[1+\cos((\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}_{ij})\right] \quad (22)$$

$$\chi^{AB}_{T=0}(\mathbf{R}_{ij}) = -\frac{3a^4}{256 v_F R^3}\left[1-\cos((\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}_{ij}-2\theta_{\mathbf{R}})\right]. \quad (23)$$

- in a simple way. Instead of Eqs. (??), (??) we obtain

$$\chi^{AA}_{T}(\mathbf{R}_{ij}) = \chi^{AA}_{T=0}(\mathbf{R}_{ij})\frac{16}{\pi}\int_0^{v/RT}\frac{x^2dx}{(x^2+1)^3} \quad (24)$$

$$\chi^{AB}_{T}(\mathbf{R}_{ij}) = \chi^{AB}_{T=0}(\mathbf{R}_{ij})\frac{16}{3\pi}\int_0^{v/RT}\frac{dx}{(x^2+1)^3}. \quad (25)$$

Integrals in Eqs. (??), (??) can be easily calculated, but we'll restrict ourselves only by analyzing the limiting cases. For $T \ll v/R$ we obtain the previous ($T=0$) results, in the opposite limiting case $T \gg v/R$ we get

$$\chi^{AA}_{T}(\mathbf{R}_{ij}) = \chi^{AA}_{T=0}(\mathbf{R}_{ij})\frac{16}{\pi}\left(\frac{v}{RT}\right)^3 \quad (26)$$

$$\chi^{AB}_{T}(\mathbf{R}_{ij}) = \chi^{AB}_{T=0}(\mathbf{R}_{ij})\frac{16}{3\pi}\frac{v}{RT}. \quad (27)$$

We must mention that comparing our results with those obtained earlier for the case of doped graphene[?] , one should be aware of the fact that the exponential decrease of the RKKY interaction with the distance at high temperatures obtained in Ref. [?] , was obtained for $k_F R \gg 1$ (in our case $k_F = 0$).

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1 E. Kogan, Phys. Rev. B **84**, 115119 (2011).
2 K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, Science **306**, 5696 (2004)
3 M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954).
4 T. Kasuya, Prog. Theor. Phys. **16**, 45 (1956).
5 K. Yosida, Phys. Rev. **106**, 893 (1957).
6 M. A. H. Vozmediano, M. P. Lopez-Sancho, T. Stauber and F. Guinea, Phys. Rev. B **72**, 155121 (2005).
7 V. K. Dugaev, V. I. Litvinov and J. Barnas, Phys. Rev. B **74**, 224438 (2006).
8 L. Brey, H. A. Fertig and S. D. Sarma, Phys. Rev. Let. **99**, 116802 (2007).
9 S. Saremi, Phys. Rev. B **76**, 184430 (2007).
10 A. M. Black–Schaffer, Phys. Rev. B **81**, 205416 (2010).
11 M. Sherafati and S. Satpathy, Phys. Rev. B **83**, 165425 (2011).
12 B. Uchoa, T. G. Rappoport, and A. H. Castro Neto, Phys. Rev. Lett. **106**, 016801 (2011).
13 S. R. Power, F. S. M. Guimaraes, A. T. Costa, R. B. Muniz, and M. S. Ferreira, Phys. Rev. B **85**, 195411 (2012).
14 P. N. Patrone and T. L. Einstein Phys. Rev. B **85**, 045429 (2012).
15 P. D. Gorman, J. M. Duffy, M. S. Ferreira, and S. R. Power Phys. Rev. B **88**, 085405 (2013).
16 P. Stano, J. Klinovaja, A. Yacoby, and D. Loss Phys. Rev. B **8**, 045441 (2013).
17 K. Szalowski Journal of Physics: Condensed Matter **25**, 166001 (2013).
18 O. Roslyak, G. Gumbs, and D. Huang, J. of Appl. Phys. **1**, 123702 (2013).
19 X. Xiao, Yu Liu and W. Wen, Journal of Physics: Condensed Matter **26**, 266001 (2014).
20 T. Shirakawa and S. Yunoki Phys. Rev. B **9**, 195109 (2014).
21 M. V. Hosseini and M. Askari Phys. Rev. B **92**, 224435 (2015).
22 M. Zare, F. Parhizgar, and R. Asgari Phys. Rev. B **94**, 045443 (2016).
23 J. Fransson, A. M. Black-Schaffer, and A. V. Balatsky, Phys. Rev. B **94**, 075401 (2016).
24 H. Rezania and F. Azizi,JMMM **417**, 272 (2016).
25 M. Agarwal and E. G. Mishchenko, Phys. Rev. B **95**, 075411 (2017).
26 F. J. Sousa, B. Amorim, E. V. Castro, arXiv:1901.08614.
27 E. Kogan, Graphene **2**, N 1, 8 (2013).
28 A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyloshinski, *Methods of Quantum Field Theory in Statistical Physics*, (Pergamon Press, 1965).
29 V. V. Cheianov, O. Syljuasen, B. L. Altshuler, and V. Fal'ko, Phys. Rev. B **80**, 233409 (2009).
30 A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009).
31 A. P. Prudnikov, Yu. A. Brychkov and O. I. Marichev, *Integrals and Series* Vol. 2 (Gordon and Breach Science Publishers, 1986).
32 N. Klier, S. Shallcross, S. Sharma, and O. Pankratov, Phys. Rev. B **92**, 205414 (2015).