1. *Владимирский А.А., Владимирский И.А., Криворучко И.П., Криворот А.А., Савчук Н.П.*. Разработка методов, аппаратных и программных средств контроля параметров подъемно-транспортного оборудования. Збірник доповідей 7-ї Національної науково-технічної конференції ”Неруйнівний контроль та технічна діагностика – UkrNDT-2012”. Київ: УТ НКТД, 2012. –с.383-386.
2. *Владимирский А.А., Владимирский И.А., Иващенко А.П.* Разработка автоматизированной виброкалибровочной установки АВКУ-2. Збірник наукових праць. Інститут проблем моделювання в енергетиці НАН України. Вип.42, Київ, 2007р.-с.23-27.

Поступила 11.02.2013р.

УДК 85.75.-d,72,25.

A. Korostil, I. Korostil, Ju. Korostil, B. Durnyak

NONEQUILIBRIUM MAGNETIC DYNAMICS IN HUBBARD MODEL

The spin dynamics of the magnetic system is considered in the multiband Hubbard model under noneuilibrium conditions simulating the impact of pulsed laser radiation. The laser-induced spin dynamics is decribed in tems of nonequilibrium Green functions in the Keldysh formalism which are determined by the Kadanov-Baym equations. Togather with a time-dependent dynamical meanfield method, the proposed approach permites to describe features of the laser-induced ultrafast spin dynamics and a magnetization reversal effect.

1. Introduction

The laser-induced ultrafast magnetization reversal belong to one of the most urgent issues of magnetism physics [1-6]. As it turned out [4-8], ultrashort optical laser pulses can occur magnetic phenomena on subpicosecond time scales. That represents the novel field of ultrafast spin dynamics including the inverse Faraday effect and all-optical helicity-dependent magnetization switching [8], and reversal of lattice magnetization in ferrimagnets via a transient ferromagnetic state [7,8]. These researches have played the important role for fundamental understanding of the pulse laser excitation of magnetic nanostructures.

The study of magnetization in a realistic solid-state system is a challenging problem. Magnetic interactions in magnetic metals and semiconductors is not Heisenberg because of a dependence of magnetization and exchange parameters on the magnetic configuration and temperature. In the case of equilibrium, the expressions for computing exchange parameters have been given, either within the multiple-scattering formalism in density functional theory [9] and in terms of electronic Green functions and self-energies within the Matsubara scheme, for a multiband Hubbard model (see [10]).

In the case of equilibrium states a spin dynamics can be derived in the Heisenberg model. In the nonequilibrium case, specifically for ultrafast magnetic processes such the model is not enough for the description of spin dynamics and magnetization. The nonequilibrium ultrafast spin dynamics characterized by nonadiabaticity of the external perturbation, which for the laser-induced magnetization dynamics related to small pulse durations of the laser radiation compared with character times of the exchange interactions (10 – 100 fs).

Within the LDA++ approach, the first-principles electronic structure is mapped to the multiband Hubbard model. A multiband Hubbard model, with realistic tight-binding and interaction parameters, is likely to be general and flexible enough to describe many strongly correlated systems relevant for ultrafast magnetism. In order to include a time-dependent optical excitation, we allow the hopping parameters to depend on time. The main approximation we can take advantage of consists in the fact that spin dynamics is known to be much slower than electron dynamics in relevant systems [3-8]. This means that an effective atomistic model can be derived, with time-dependent parameters accounting for the magnetic interactions mediated by the fast electronic dynamics, which can be computed from first principles. Technically, we need to separate the spin degrees of freedom from the electronic ones, and derive an effective action for the spin variables, after integrating on the electronic variables.

The above mentioned problem resolves with the help of nonequilibrium Green function formalism [11–13], which neglects initial (equilibrium) correlations. The Schwinger-Keldysh formulation has been applied to the study of spin dynamics, e.g. for a single spin in a Josephson junction, or in a junction between ferromagnets, or combined with the mean field approximation for the treatment of magnetic interaction [14]. In this paper a first-principle study of an extended and strongly correlated system out of equilibrium, such as a fermionic multi-band Hubbard model is considered in the framework of the Kadanov-Baym formalism.

The advantage of this approach is that it does not need any assumption on the time dependence of the external field, so there is no restriction on time scales, which allows to study the role of non-adiabatic and non-Heisenberg effects in magnetization dynamics. It is also suitable to make a first-principle formulation of quantum noise, whose time scale may be comparable to that of the ultrafast pulse.

In present paper we have considered the laser-induced magnetization dynamics in the multiband Hubbard model. In Section 2 the Kadanoff-Baym formalism is described. In Section 3 we consider features of the multiband Hubbard model which is applied for description of the laser-induced spin dynamics. In Section 4 the expression for a partition function is obtained via the transition from the fermionic to a bosonic representation, where the bosons are related to the directions of the spin axes is shown. In Section 5 nonequilibrium Green's functions of the considered system are calculated.

2. Kadanoff-Baym approach to nonequilibrium systems

For the sake of completeness, we here review briefly the main concepts of the

Kadanoff-Baym approach to the study of non-equilibrium systems, which combines the approaches of Matsubara, Schwinger and Keldysh.

Given a time-dependent Hamiltonian $H(t)$, the equation of motion for the density operator is $\partial\rho(t)/\partial t = -i\left[H(t),\rho(t)\right]$, which can be solved formally as $\rho(t) = U(t,t_0)\rho(t_0)U(t_0,t)$, where $\rho(t_0)$ is the (supposedly known) density operator at a reference time t_0, and the evolution operator is

$$U(t,t') = \theta(t-t')\vec{T}\exp\left(-i\int_{t'}^{t} dt_1 H(t_1)\right) + \theta(t'-t)\overleftarrow{T}\exp\left(-i\int_{t'}^{t} dt_1 H(t_1)\right) \qquad (1)$$

for $t \neq t'$, while $U(t,t) = 1$; the symbol $\theta(t)$ denotes the step function ($\theta(x>0) = 1$, $\theta(x<0) = 0$). The expectation value for the observable O at time t is:

$$O(t) = \frac{\mathrm{Tr}\left[O\rho(t)\right]}{\mathrm{Tr}\left[\rho(t)\right]} = \frac{\mathrm{Tr}\left[\rho_0(t)U(t_0,t)OU(t,,t_0)\right]}{\mathrm{Tr}\left[\rho(t_0)\right]} \quad , \qquad (2)$$

where the trace is evaluated over the complete many-body Hilbert space, and in the last passage the cyclic property of the trace and the identity $U(t,t')U(t',t) = U(t,t) = 1$ have been used. We choose the reference time t_0 in such a way that, for $t < t_0$, the Hamiltonian is independent of time and the system is in equilibrium. Therefore, we can use for $\rho(t_0)$ the grand-canonical equilibrium expression,

$$\rho(t_0) = \frac{\mathrm{e}^{-\beta(H_0-\mu N)}}{Tr\left[\mathrm{e}^{-\beta(H_0-\mu N)}\right]}, \qquad (3)$$

where $H_0 = H(t \le t_0)$, N is the number-of-particle operator and μ is the chemical potential. We assume $\left[H_0,N\right] = 0$. We extend the time domain to the complex plane, defining the complex time variable $\varsigma = t - i\tau$, with the understanding that $H(\varsigma) = H(t)$ depends only on the real part of time, and we define the evolution operator in imaginary time

$$\mathrm{e}^{-\beta(H_0-\mu N)} \equiv U_0(t_0 - i\beta, t_0), \qquad (4)$$

Thus, we can write Eq.(2) as:

$$\begin{aligned} O(t) &= \frac{Tr\left[U(t_0-i\beta,t_0)U(t_0,\infty t)U(\infty,t))U(t_0,t)OU(t,,t_0)\right]}{Tr\left[\mathrm{e}^{-\beta(H_0-\mu N)}\right]} \\ &= \frac{Tr\left[U(t_0-i\beta,t_0)U(t_0,t)OU(t,,\infty)U(\infty,t_0)\right]}{Tr\left[\mathrm{e}^{-\beta(H_0-\mu N)}\right]} \end{aligned} \qquad (5)$$

which shows that the evaluation of $O(t)$ requires that we let the system evolve along three time domains in the complex plane: a forward branch $\gamma_+(t_0,\infty)$, a backward branch $\gamma_-(\infty,t_0)$, and a segment on the imaginary (vertical) axis of time $\gamma_v = (t_0, t_0 - i\beta)$, which we call the vertical branch (see Fig.1). It must be noted that the time value which we have labelled as ∞ may actually be chosen as a completely arbitrary (finite) value. The total domain over which the system evolves is the Kadanoff-Baym contour

$$\Gamma \equiv \gamma_+ \cup \gamma_- \cup \gamma_v \equiv (t_0,\infty) \cup (\infty,t_0) \cup (t_0, t_0 - i\beta)\,. \tag{6}$$

We define the total evolution operator on Γ as:

$$U_\Gamma \equiv U_v(t_0 - i\beta, t_0)U(t_0,\infty)U(\infty,t_0)\,. \tag{7}$$

From Eq.(5), we see that the computation of $O(t)$ is realized by opening the contour Γ at the instant t either on the branch γ_+ or on the branch γ_-, inserting there the Schrödinger-represented operator O in U_Γ, and evaluating the trace of the resulting operator. The inclusion of the branch γ_v is required to treat systems where the inital correlations are not negligible, as it is the case in typical solid-state systems. In the cases where the initial correlations can be neglected, the initial density matrix is of the single-particle kind and there is no need to express it in a contour formulation: in such conditions, one can restrict the contour to $\gamma_+ \cup \gamma_-$, possibly with $t_0 \to -\infty$, which is the Schwinger-Keldysh contour. In equilibrium conditions, on the other hand, the Hamiltonian is time-independent and the contour is restricted to γv, which is the Matsubara contour. The Kadanoff-Baym formulation, therefore, unifies and generalizes the other approaches, and allows to treat the most general case of a system in non-equilibrium with initial correlations.

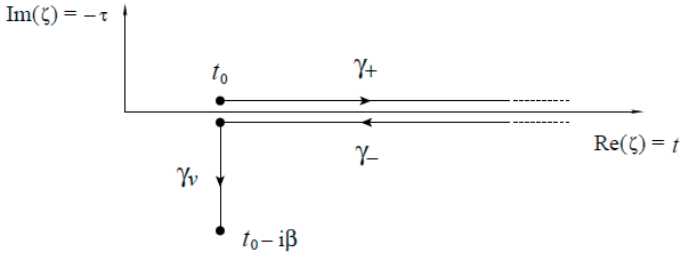

Fig..1. Schematic representation of the Kadanoff-Baym contour. Branches γ_+, γ_- are displaced for graphical convenience, but they both coincide with a portion of the real time axis, extending from t_0 to 1.

The Kadanoff-Baym partition function is defined as

$$Z = \mathrm{Tr}\left[U_\Gamma\right] / \mathrm{Tr}\left[\mathrm{e}\right]^{-\beta(H_0-\mu N)}, \tag{8}$$

where U_Γ is given in Eq.(7). Since $U(t_0,\infty)U(\infty,t_0)=1$, it follows that $Z=1$. Despite this apparent triviality, expressing Z by means of path integrals allows to derive a non-equilibrium action, from which it is possible to extract physical information. To do this, we start by denoting the Hamiltonian as $H\left[\phi^+,\phi;t\right]$ for $t > t_0$, where ϕ^+ and ϕ represent the sets of fermionic creation and annihilation operators, respectively. Instead, for $t \le t_0$ and on the branch γ_v the Hamiltonian is constant and we denote it as $H_0\left[\phi^+,\phi\right]$. We parameterize the branch γ_v by means of the real variable

$$\tau = -\mathrm{Im}(\varsigma), \tag{9}$$

which is equal to 0 for $\varsigma = t_0$ and to β for $\varsigma = t_0 - i\beta$. On the γ_v contour, $\varsigma = t_0 - i\,\mathrm{Im}(\varsigma) = t_0 - i\tau$. Then, standard manipulations lead to the expression

$$Z = \int D\left[\phi^+,\phi\right] \mathrm{e}^{iS[\phi^+,\phi]}, \tag{10}$$

where the effective action $S\left[\phi^+,\phi\right]$ written in terms of the Grassmann variables $\bar{\phi}$ and ϕ relative to the operators, is:

$$\begin{aligned} S\left[\bar{\phi},\phi\right] = & \int_{t_0+\varepsilon}^{\infty} dt \Big\{ i\bar{\phi}_+(t)\cdot\dot{\phi}_+(t-\varepsilon) - H\left[\bar{\phi}_+(t),\bar{\phi}_+(t-\varepsilon);t\right] \\ & - i\bar{\phi}_-(t-\varepsilon)\cdot\dot{\phi}_-(t-\varepsilon) - H\left[\bar{\phi}_-(t-\varepsilon),\bar{\phi}_-(t-\varepsilon);t\right] \Big\} \\ & + \int_{t_0+\varepsilon}^{\infty} dt \Big\{ i\bar{\phi}_v(\tau)\cdot\dot{\phi}_v(\tau-\varepsilon) - H\left[\bar{\phi}_v(\tau),\phi_v(\tau-\varepsilon);t\right], \end{aligned} \tag{11}$$

where $K = H_0 - \mu N$, and which requires some explanations. First, Eq.(11) is written, for convenience, in terms of real time variables t and τ, instead of contour variables. Therefore, since each value of t corresponds to two distinct points on the Kadanoff-Baym contour (one on γ_+ and one on γ_-), the timedependent Grassmann fields must be specified by the index $\pm$ if their argument is on the real-time axis, while we use the label v for the fields with the argument on the branch γ_v.

Then, we have introduced two infinitesimally small positive quantities, λ and ε, in order to emphasize a subtle technical point, namely the fact that any product of $\hat{\phi}$ and $\hat{\phi}$ fermionic operators appearing in the Hamiltonian transforms in the path integral formulation into a product of $\bar{\phi}$ and ϕ Grassmann fields in which the fields $\bar{\phi}$ are evaluated at an instant occurring infinitesimally before (in the contour sense) the instant when the $\bar{\phi}$ fields are evaluated. While this aspect is often neglected, on the basis that the fields are assumed to be continuous functions, for our purposes it will be important to keep explicitly track of this discrete structure because we will have to deal with discontinuous functions, such as the correlators (Green functions) originating from the Grassmann numbers ($\bar{\phi}, \phi$). In these cases, we will need to consider carefully the direction along which the independent variables approach the discontinuity point, which will be possible in our formulation. At the appropriate stage of the calculations, we will send $\varsigma \to 0$ and $\varepsilon \to 0$. On the other hand, whenever ς or ε appears inside the argument of a continuous function, we are allowed to send it to 0 immediately, as we already did implicitly in the case of the time-dependent external field. Finally, derivatives of fields are always meant to be taken from the right side, i.e.,

$$\varphi(t) = \lim_{\varsigma \to 0} \left(\phi(t+\varsigma) - \phi(t)\right) / \varsigma \,.$$

3. Multiband Hubbard model

In order to model an electronic system driven out of equilibrium by a timedependent external field (e.g. a laser pulse), we must consider a Hamiltonian of the form

$$H(t) = H_T(t) + H_v(t)\,, \tag{12}$$

where $H_T(t)$ is the single-particle Hamiltonian, including the time-dependent field, and $H_v(t)$ is the (time-independent) interaction potential between the electrons. We will treat a multi-band Hubbard model [15], therefore the electronic single-particle states are identified by three labels: the site index i, the orbital index λ and the spin index σ. We ignore spin-orbit coupling and assume that the external field is diagonal in spin indices (we are therefore excluding magnetic fields, but including purely electric fields which are relevant for modelling all-optical experiments). The single-particle Hamiltonian is then given by

$$\begin{aligned} H_T(t) &= \sum_{i_\alpha \lambda_\alpha} \sum_{i_b \lambda_b} T_{i_\alpha,\lambda_\alpha,i_b\lambda_b}(t) \sum_\sigma \hat{\phi}^+_{i_\alpha \lambda_\alpha \sigma} \hat{\phi}_{i_b \lambda_b \sigma} \\ \sum_a \sum_b T_{ab}(t) \sum_\sigma \hat{\phi}^+_{a\sigma} \hat{\phi}_{b\sigma} &= \sum_a \sum_b T_{ab}(t) \hat{\phi}^+_a \cdot \hat{\phi}_b \end{aligned}\,, \tag{13}$$

where we have grouped the site and orbital indexes according to $a = (i_\alpha, \lambda_a)$ and $b = (i_b, \lambda_b)$, and we have defined the spinor fermionic operators

$$\hat{\phi}^+{}_a = \left(\hat{\phi}^+{}_{a\uparrow} \quad \hat{\phi}^+{}_{a\downarrow} \right), \qquad \hat{\phi}_b = \begin{pmatrix} \hat{\phi}_{b\uparrow} \\ \hat{\phi}_{b\downarrow} \end{pmatrix} \tag{14}$$

The matrix element $T_{ab}(t) = T^*{}_{ba}(t)$ of the single-particle Hamiltonian is written as

$$T_{ab}(t) = T_{ab} + f_{ab}(t), \tag{15}$$

where T_{ab} is the time-independent hopping parameter due to electronic structure, and $f_{ab}(t)$ is the time-dependent matrix element of the perturbing field. We denote as t0 the time at which the external field is switched on: $f_{ab}(t) = 0$ for $t \le t_0$. The interaction potential generating H_v is assumed to be on-site, i.e.,

$$H_V = \frac{1}{2} \sum_i \sum_{\lambda_1,\lambda_2,\lambda_3,\lambda_4} \sum_\sigma V_{\lambda_1\lambda_2\lambda_3\lambda_4} \hat{\phi}^+{}_{\lambda_1\sigma} \hat{\phi}^+{}_{i\lambda_2\sigma'} \hat{\phi}_{i\lambda_3\sigma'} \hat{\phi}_{i\lambda_4\sigma}. \tag{16}$$

Including magnetic fields and spin-orbit coupling complicates the analysis significantly, and will be left to future work. However, this model already allows to describe some interesting magnetic phenomena. For example, consider a system which contains both spin-up and spin-down electrons. The arrangement of the spins within each lattice site depends initially on the equilibrium magnetic interactions, mainly exchange. Applying a time dependent electrostatic field on a portion of the sample, as we shall show, may change the strength of the magnetic interactions. If in a certain region of the sample the coupling switches, e.g., from antiferromagnetic to ferromagnetic, then this might generate a re-arrangement of the total spin in each lattice site as a purely electronic phenomenon, due to the inter-site hopping. Hence, even without individual spin rotations, domains with an ordering which is different from the initial one may originate as a consequence of electronic transfer between atomic sites. 4. Rotation of the spin quantization axes

4. Rotation of the spin quantization axes

For each site, we define a rotation matrix, acting in the space of spinor fermionic operators, as:

$$R_i(z) = \begin{pmatrix} \sqrt{1-\backslash\xi_i(z)^2\backslash} & \xi_i^*(z) \\ \xi_i(z) & \sqrt{1-\backslash\xi_i(z)^2\backslash} \end{pmatrix}, \tag{17}$$

where z is a contour variable which parameterizes the Kadanoff-Baym contour. In Eq.(17) we have introduced the boson fields

$$\xi_i(z) = -e^{i\phi_i(z)} \sin(\theta_i(z)/2) \tag{18}$$

with $\theta_i \in [0,\pi]$, $\varphi_i \in [0,2\pi]$ being the polar angles that determine the spin axis on site i at time z; it holds that $R_i^+(z)R_i(z) = 1$.

We transform the Grassmann variables appearing in the action, Eq.(11), according to

$$\begin{aligned} &\bar{\phi}_{a\pm}(t) = \bar{\psi}_{a\pm}(t)\cdot R^+_{a\pm}(t), \;\; \bar{\phi}_{a\pm}(t) = R_{a\pm}(t)\,\psi_{a\pm}(t), \\ &\bar{\phi}_{av}(\tau) = \bar{\psi}_{av}(\tau)\cdot R^+_{av}(\tau), \;\; \psi_{av}(\tau) = R_{av}(\tau)\,\psi_{av}(\tau). \end{aligned} \tag{19}$$

To understand the meaning of the rotation that we have just introduced, the following considerations are in order. The local vector spin operator for siteorbital a, in the laboratory reference frame, is

$$\sigma_a = \hat{\phi}^+_a \cdot \sigma \cdot \hat{\phi}_a, \tag{20}$$

where σ is the vector of Pauli matrices. The expectation value of this operator on the state $\hat{\phi}^+_{i\sigma} \mid 0>$ is

$$< 0 \mid \hat{\phi}_{a\sigma}\sigma\hat{\phi}^+_{a\sigma} \mid >= \sigma u_z \tag{21}$$

where $\sigma \in \{\uparrow,\downarrow\} = \{+,-\}$. Instead, the expectation value of the spin operator on the state $\hat{\phi}_{a\sigma} \mid 0>$ is

$$< 0 \mid \hat{\phi}_{a\sigma}\sigma\hat{\phi}^+_{a\sigma} \mid >= \sigma e_a \tag{22}$$

where we have used Eqs.(18) and (19), and the unit vector e_a is given by

$$e_a = u_x \sin\theta_a \cos\phi_a - u_y \sin\theta a \sin\phi_a + u_z \cos\theta_a. \tag{23}$$

Therefore, e_a (which depends on time) has the meaning of the unit spin vector on site-orbital a, measured in the laboratory reference frame, if the site a hosts a $\psi_\uparrow$ electron. Expression (23) can also be written as

$$e_a = \sqrt{1-|\xi_a|^2}\left[-(\xi_a+\xi_a^*)u_x + i(\xi_a-\xi_a^*)u_y\right] + u_z(1-2\mid\xi_a\mid^2). \tag{24}$$

which shows that ξ and ξ^* are, effectively, nothing else than Holstein-Primakoff bosons.

We assume the rotation matrices $R(t)$ to be differentiable functions of t over the interval $[t_0+\varepsilon,\infty]$, and the rotation matrices $R(t)$ to be differentiable functions of τ over the interval $[\varepsilon,\beta]$. So, in the evaluation of Eq.(11) we can

already apply the replacements $R(t)+\varepsilon \to R(t)$. Instead, we need to keep finite ς and ε in the arguments of the fermionic fields ($\bar{\psi},\psi$). Since we are considering a on-site interaction, H_v is rotationally invariant, hence it is unaffacted by the transformation defined in Eq.(19), which means that $H_v(\bar{\phi},\phi) = H_v(\bar{\psi},\psi)$.

On the other hand, the single-particle Hamiltonian acquires a dependence on the bosonic fields, $H_T[\bar{\phi},\phi;t] = H_T[\bar{\psi},\psi,\xi^*,\xi;t]$.

The transformed action, depending on the fermionic (Grassmann) ψ fields and on the bosonic (complex) ξ fields, is written as:

$$S[\bar{\phi},\phi] = S[\bar{\psi},\psi,\xi^*,\xi] = S[\bar{\psi},\psi] + S'[\bar{\psi},\psi,\xi^*,\xi] \tag{25}$$

with $S[\bar{\psi},\psi]$ denoting the original expression of the action, with the $(\bar{\phi},\phi)$, fermions replaced by the $(\bar{\psi},\psi)$, ψfermions, and

$$\begin{aligned} S'[\bar{\psi},\psi,\xi^*,\xi] &= \int_{\varepsilon}^{\beta} d\tau \bar{\psi}_v(\tau)\cdot\Delta_v(\tau)\cdot\psi_v(\tau+\varepsilon) \\ &+ \int_{t_0+\varepsilon}^{\infty} dt\left[\bar{\psi}_+(t)\cdot\Delta_+(t)\cdot\psi_+(t-\varepsilon) - \bar{\psi}_+(t-\varepsilon)\cdot\Delta_-(t)\cdot\psi_-(t)\right] \end{aligned} \tag{26}$$

where the quantities Δ_v and $\Delta_\pm$ are matrices in both the spaces of Hubbard indexes and spin indexes, and they depend on the fields (ξ_v,ξ_v^*) and ($\xi_\pm,\xi_\pm^*$), respectively. Expressing explicitly their Hubbard-space structure,

$$\Delta_{ab\pm}(t) = iR^+_{a\pm}(t)R_{a\pm}(t)\delta_{ab} + T_{ab}(t)\left[R^+_{a\pm}(t)R_{b\pm}(t) - 1\right], \tag{27}$$

$$\text{with } \Delta_{abv}(\tau) = \Delta_{ab\pm}(t)\,|_{\pm\to v,\,\tau\to t}\,.$$

These are now matrices in spin space, which include diagonal and non-diagonal components. We separate the corresponding parts of the action:

$$S' = S^{(1)} + S^{(2)}, \tag{28}$$

with

$$\begin{aligned} S^{(1)} = \sum_{a,b,\sigma}\Bigg\{ &\int_{\varepsilon}^{\beta} d\tau \bar{\psi}^{\sigma}_{av}(\tau)\Delta^{\sigma\bar{\sigma}}_{abv}(\tau)\psi^{\sigma}_{bv}(\tau-\varepsilon) + \\ &+ \int_{t_0+\varepsilon}^{\infty} dt\left[\bar{\psi}^{\sigma}_{a+}(t)\Delta^{\sigma\bar{\sigma}}_{ab+}(t)\psi^{\sigma}_{b+}(t-\varepsilon) - \bar{\psi}^{\sigma}_{a-}(t-\varepsilon)\Delta^{\sigma\bar{\sigma}}_{ab-}(t)\psi^{\sigma}_{b-}(t)\right] \end{aligned} \tag{29}$$

and $S^{(2)} = S^{(1)}\big|_{\bar{\sigma}\to\sigma}$, where $\bar{\sigma} = -\sigma$.

The partition function is written in terms of the rotated fields as:

$$Z = \int D[\bar{\psi},\psi] e^{iS[\bar{\psi},\psi]} \int D[\theta,\varphi] e^{iS'[\bar{\psi},\psi,\xi^*(\theta,\varphi),\xi(\theta,\varphi)]}, \tag{30}$$

where the symbol

$$\int D[\theta,\varphi] = \prod_{\alpha} [d\theta_\alpha \sin\theta_\alpha \int_0^{2\pi} d\varphi_\alpha]. \tag{31}$$

means integration over all possible orientations $(\theta_\alpha, \varphi_\alpha)$ at all lattice sites. The dependence of the fields $(\xi_\alpha^*, \xi_\alpha)$ on the angles $(\theta_\alpha, \varphi_\alpha)$ is given by Eq.(18). It can be shown that integrating over the angles $(\theta_\alpha, \varphi_\alpha)$ ensures that the partition function as written in Eq.(30) is equal to Eq.(10), i.e., Eq.(30) is an identity. Since φ is the phase of the complex number $-\xi$, while $\sin\theta/2$ is its modulus, we see that

$$\begin{aligned} &\int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\varphi f\left[-\sin(\theta/2)e^{i\varphi}, -\sin(\theta/2)e^{-i\varphi}\right] \\ &= 4\iint_{C_1} d\,\mathrm{Re}(\xi) d\,\mathrm{Im}(\xi) f[\xi, \xi^*]. \end{aligned} \tag{32}$$

where the integration domain C_1 is the circle of radius equal to 1 in the complex plane, centered on 0, i.e., $|\xi|/2 < 1$, which is described by $\varphi \in [0, 2\pi]$ and $\theta \in [0, \pi]$. We therefore change the path variables from (θ, φ) to (ξ^*, ξ), by introducing the notation

$$\int D[\theta,\varphi] = \prod_{\alpha} \left[\frac{1}{\pi} \iint_{C_1} d\,\mathrm{Re}(\xi_\alpha)\, \mathrm{d}\,\mathrm{Im}(\xi_\alpha)\right] = \int D[\xi^*,\xi], \tag{33}$$

so that

$$Z = D[\bar{\psi},\psi] e^{iS[\bar{\psi},\psi]} \int D[\xi^*,\xi] e^{iS[\bar{\psi},\psi,\xi^*,\xi]}. \tag{34}$$

The introduction of the Holstein-Primakoff bosons allows to decouple the dynamics of electronic and spin degrees of freedom. Now suppose that the equilibrium spin configuration is collinear (ferro-, antiferro-, or ferri- magnetic), with uz being the initial direction of atomic spin alignment. Our goal is to derive a theory for the low-energy excitations on the top of the equilibrium configuration. Such excitations corrispond to small deviations of the atomic spins from the direction of u_z, i.e., we can assume that the polar angles θi be small. We can therefore approximate

$$R_i \approx \begin{pmatrix} 1 - \frac{|\xi_i|^2}{2} & \xi_i^* \\ -\xi_i & 1 - \frac{|\xi_i|^2}{2} \end{pmatrix}. \tag{35}$$

Now the unitarity of the transformation (19) holds but for corrections of the order of $|\xi|^4$. Under this approximation,

$$R^{+}_{as}\dot{R}as \approx \begin{pmatrix} \dfrac{\dot{\xi}_{as}\xi^{*}_{as}-\xi_{as}\dot{\xi}^{*}_{as}}{2} & \dot{\xi}^{*}_{as} \\ -\dot{\xi}_{as} & \dfrac{\dot{\xi}_{as}\xi^{*}_{as}-\xi_{as}\dot{\xi}^{*}_{as}}{2} \end{pmatrix} \tag{36}$$

and

$$R^{+}_{as}R_{as}-1 \approx \begin{pmatrix} \xi^{*}_{as}\xi_{bs}-\dfrac{|\xi_{as}|^2+|\xi_{bs}|^2}{2} & \xi^{*}_{bs}-\xi^{*}_{as} \\ \xi_{as}-\xi_{bs} & \xi_{as}\xi^{*}_{bs}-\dfrac{|\xi_{as}|^2+|\xi_{bs}|^2}{2} \end{pmatrix} \tag{37}$$

This procedure is justified if we limit ourselves to the description of small rotations of the spins with respect to the direction of the initial quantization axis. For future convenience, we define permutation operators P_{ab}, which substitute

a with b and b with a in the expressions they act upon, where a and b are Hubbard indexes. Moreover, in order to adopt a compact notation, we will sometimes put arrows $\rightarrow,\leftarrow$ over the permutation and derivative operators to indicate the direction along which they act. The Δ matrices are written as:

$$\Delta^{\uparrow\downarrow}_{ab,\eta}(t_\eta)=\left(\delta_{ab}i\frac{\vec{\partial}}{\partial t_\eta}+T_{ab\eta}(t_\eta)\left(1-\vec{P}_{ab}\right)\right)\xi^{*}_{a}(t_\eta), \tag{38}$$

$$\Delta^{\downarrow\uparrow}_{ab,\eta}(t_\eta)=\left(\delta_{ab}i\frac{\vec{\partial}}{\partial t_\eta}+T_{ab\eta}(t_\eta)\left(1-\vec{P}_{ab}\right)\right)\xi_{a}(t_\eta) \tag{39}$$

$$\begin{aligned}\Delta^{\uparrow\uparrow}_{ab\eta}(t_\eta) &= \delta_{ab}\xi_{a\eta}(t_\eta)\frac{i}{2}\left(\frac{\overrightarrow{\partial}}{\partial t_\eta}-\frac{\overleftarrow{\partial}}{\partial t_\eta}\right)\xi^{*}_{a\eta}(t_\eta) \\ &+ T_{ab_\eta}(t_\eta)\left[\frac{|\xi_{a\eta}(t_\eta)|^2+|\xi_{b\eta}(t_\eta)|^2}{2}-\xi^{*}_{a\eta}(t_\eta)\xi_{b\eta}(t_\eta)\right],\end{aligned} \tag{40}$$

$$\begin{aligned}\Delta^{\downarrow\downarrow}_{ab\eta}(t_\eta) &= \delta_{ab}\xi^{*}_{a\eta}(t_\eta)\frac{i}{2}\left(\frac{\overrightarrow{\partial}}{\partial t_\eta}-\frac{\overleftarrow{\partial}}{\partial t_\eta}\right)\xi_{a\eta}(t_\eta) \\ &+ T_{ab_\eta}(t_\eta)\left[\frac{|\xi_{a\eta}(t_\eta)|^2+|\xi_{b\eta}(t_\eta)|^2}{2}-\xi_{a\eta}(t_\eta)\xi^{*}_{b\eta}(t_\eta)\right],\end{aligned} \tag{41}$$

where $t_\eta=\begin{pmatrix} t,\eta=\pm \\ \tau,\ \eta=v \end{pmatrix}$ and $T_{ab\eta}(t_\eta)=\begin{pmatrix} T_{ab\pm}(t),\eta=\pm \\ -iT_{ab},\ \eta=v \end{pmatrix}$. It is seen that the $\Delta^{\sigma\sigma'}_{ab}$ are

linear, while the $\Delta_{ab}^{\sigma\sigma'}$ are quadratic, in the bosonic fields (ξ^*, ξ). To be consistent with the small ϑ's approximation, we must expand the partition function in series of the bosonic fields and retain only up to quadratic terms. We obtain

$$Z = \int D[\overline{\psi},\psi,\xi^*,\xi] e^{i\left\{S[\overline{\psi},\psi]-S'[\overline{\psi},\psi,\xi^*,\xi]\right\}} \approx \int D[\overline{\psi},\psi,\xi^*,\xi] e^{S[\overline{\psi},\psi]} \times \left\{\left\{1+iS'[\overline{\psi},\psi,\xi^*,\xi]-\frac{1}{2}\left(S^{(1)}[\overline{\psi},\psi,\xi^*,\xi]\right)\right\}\right\} = Z^{(0)} + Z^{(1)} + Z^{(2)}. \quad (42)$$

where

$$Z^{(0)} = \int D[\overline{\psi},\psi,\xi^*,\xi] e^{iS[\overline{\psi},\psi]} = \int D[\xi^*,\xi],$$

$$Z^{(1)} = \int D[\overline{\psi},\psi,\xi^*,\xi] e^{iS[\overline{\psi},\psi]} \left\{iS^{(1)}[\overline{\psi},\psi,\xi^*,\xi]-\frac{1}{2}\left(S^{(1)}[\overline{\psi},\psi,\xi^*,\xi]\right)^2\right\},$$

$$Z^{(2)} = \int D[\overline{\psi},\psi,\xi^*,\xi] iS^{(2)}[\overline{\psi},\psi,\xi^*,\xi].$$

5. Fermionic correlators

Now we will integrate out the fermionic fields, by exploiting the expression for the single-particle Green function (for $s \in [+,-,v]$, and $z = t$ or $z = \tau$, accordingly),

$$\int D[\overline{\psi},\psi,\xi^*,\xi] e^{iS[\overline{\psi},\psi]} \overline{\psi}_{as'}^{\sigma'}(z')\psi_{bs}^{\sigma}(z) = G_{ba,ss'}^{\sigma\sigma'}(z,z'). \quad (44)$$

Since the Hamiltonian is spin-independent (i.e., the hopping is diagonal in spin space), the Green functions with $\sigma \neq \sigma''$ are zero in our system. Therefore,

$$Z^{(1)} = \int D[\overline{\psi},\psi,\xi^*,\xi] e^{iS[\overline{\psi},\psi]} \left\{-\frac{1}{2}\left(S^{(1)}[\overline{\psi},\psi,\xi^*,\xi]\right)^2\right\} \quad (45)$$

As a consequence, the action will contain no terms linear in the bosonic fields, which is due to the fact that we are not including spin-orbit coupling. Therefore, our model will not include Dzyaloshinskii-Moriya interactions [18]. Since we will need only spin-diagonal single-particle Green functions, we will label them with just one spin index. We also need the expression for the following two-particle Green function,

$$-\int D[\overline{\psi},\psi] e^{iS[\overline{\psi},\psi]} \overline{\psi}_{as}^{\sigma}(z)\psi_{bs}^{\sigma}(z)\overline{\psi}_{a's'}^{\sigma}(z')\psi_{b's'}^{\sigma}(z') = \lambda_{bab'a',sss's'}^{\sigma\sigma\sigma\sigma}(z,z,z',z'). \quad (46)$$

We adopt the approximation

$$\lambda_{bab'a',sss's'}^{\sigma\sigma\sigma\sigma}(z,z,z',z') \approx G_{ba',ss'}^{\sigma}(z,z')G_{b'a,s's}^{\sigma}(z',z), \quad (47)$$

which corresponds to neglecting the vertex in the two-particle Dyson equation, and where we have already taken into account the fact that correlators $G^{\sigma\sigma}$ are zero in our system. It must be noted that Eq.(47) is the only approximation that we adopt on the many-body level.

All quantities will then be written in terms of single-particle Green functions. The correlators can be classified according to the positions of their time arguments on the Kadanoff-Baym contour, and put in correspondence with nonequilibrium Green functions written in terms of the field operators, as follows:

$$G^{\sigma}_{ba,\eta\eta'}(t_1,t_2) \equiv G^{\eta\eta'\sigma}_{ba}(t_1,t_2) == -i\left\langle T^{\eta\eta'}_{t}[\psi^{\sigma}_{b}(t_1)\psi^{+\sigma}_{a}(t_2)]\right\rangle, \qquad (48)$$

where $\eta,\eta' = (+,-,>,<,M,|^{-},{}^{-}|)$ take values denoting an integration contour. Here

$$G^{<\sigma}_{ba}(t_1,t_2) = \left\langle T^{+-}_{t}[\psi^{\sigma}_{b}(t_1)\psi^{+\sigma}_{a}(t_2)]\right\rangle = \left\langle \psi^{+\sigma}_{a}(t_2)\psi^{\sigma}_{b}(t_1)\right\rangle,$$

$$G^{>\sigma}_{ba}(t_1,t_2) = \left\langle T^{-+}_{t}[\psi^{\sigma}_{b}(t_1)\psi^{+\sigma}_{a}(t_2)]\right\rangle = \left\langle \psi^{\sigma}_{b}(t_1)\psi^{+\sigma}_{a}(t_2)\right\rangle,$$

An index M denotes integration on the imagenary temporal contour (Fig.1), the subscript ${}^{-}|$ implies integration over a real and then an imagenary temporal contours; the subscript $|^{-}$ implies integration over an imagenary and then a real temporal contour. Besides we have used the notation

$$\left\langle O(z_1,z_2)\right\rangle = \mathrm{Tr}\left\{e^{-\beta(H_0-\mu N)}O(z_1,z_2)\right\} / \mathrm{Tr}\left\{e^{-\beta(H_0-\mu N)}\right\}, \qquad (49)$$

and

$$\psi(t) = U_{\nu}(t_0,t)\psi U_{\nu}(t,t_0),\ \ \psi(\tau) = U_{\nu}(t_0,t_0-i\tau)\psi U_{\nu}(t_0,t_0+i\tau), \qquad (50)$$

where the identity $U_{\nu}(t_0,t_0-i\tau) = e^{\tau(H_0-\mu N)}$ follows from the fact that the Hamiltonian is constant (equal to H_0) on the vertical branch of the Kadanoff-Baym contour. The correlators $G^{<\sigma}_{ba}(t_1,t_2)$ and $G^{>\sigma}_{ba}(t_1,t_2)$ are continuous functions of their time arguments (t_1,t_2), while $G^{\eta\eta\sigma}_{ba}(t_1,t_2)$. Such nonequilibrium Green's function allow to described the spin dynamics in the framework of the multiband Hubbard model.

1. *Kirilyuk A., Kimel A. V., Rasing* Th. Rev. Mod. Phys. **82** 2731 (2010).
2. *Tudosa I., Stamm C., Kashuba A. B., King F., Siegmann H. C., Stöhr J., Ju G., Lu B., and Weller D*. Nature, **428** 831 (2004).
3. *Kimel A. V., Kirilyuk A., Usachev P. A., Pisarev R. V., Balbashov A. M., and Rasing Th*., Nature, **435** 655 (2005).
4. *Stanciu C. D., Hansteen F., Kimel A. V., Kirilyuk A., Tsukamoto A., Itoh A., and Rasing Th*. Phys. Rev. Lett., **99** 047601 (2007).
5. *Vahaplar K., Kalashnikova A. M., Kimel A.V., et al*. Phys. Rev. Lett., **103** 117201 (2009).

6. *Radu I., Vahaplar K., Stamm C.*, et al., Nature, **472** 205 (2011).
7. *Vahaplar K.* Ultrafast Path for Magnetization Reversal in Ferrimagnetic GdFeCo Films //Doctoral thesis, (2011) .
8. *Ostler T.A., Barker J., Evans R.F.L., et al*. //Nature Communications, **3**, 1 (2012).
9. *Liechtenstein A. I.0, Katsnelson M. I., Antropov V. P., Gubanov V. A., J. Magn*. Magn. Mater. **67** 65 (1987).
10. *Katsnelson M. I., Lichtenstein A. I.*, Phys. Rev. B **61** 8906 (2000).
11. *Kadanoff L. P. and Baym G*., Quantum Statistical Mechanics, W. A. Benjamin, Inc., New York, 1962.
12. *Schwinger J.,* J. Math. Phys. **2** 407 (1961).
13. *Keldysh L*. V., Zh. Eksp. Teor. Fiz. **47** 1515 (1964) .
14. *Fransson J*, Phys. Rev. B **82** 180411(R) (2010).
15. *Feng Q. and Oppeneer P. M*., Phys. Rev. B **86** 035107 (2012).

Поступила 11.02.2013р.

УДК 519.6 : 504.064

В.О. Артемчук, м. Київ

ПЕРСПЕКТИВИ ВИКОРИСТАННЯ БЕЗПРОВІДНИХ СЕНСОРНИХ МЕРЕЖ

Abstract. The article describes the main types of wireless sensor networks. Identified and analyzed prospects of wireless sensor networks in Ukraine.

Вступ. З підвищенням технічного потенціалу людства моніторинг та попередження забруднення атмосферного повітря стали обов'язковою частиною природоохоронної діяльності всіх розвинених держав.

В рамках 7-ї Рамкової програми розробляються заходи щодо формування комплексних мереж моніторингу стану атмосферного повітря (МСАП) з використанням інформаційних можливостей наземних і космічних систем спостереження, результатів моделювання переносу атмосферних домішок, координованої роботи станцій спостережень в глобальному масштабі.

В останні роки з'явилася низка публікацій, присвячених створенню систем МСАП на основі безпровідних сенсорних мереж, які складаються з мініатюрних обчислювальних пристроїв – мотів, оснащених сенсорами, що можуть фіксувати як метеодані, так і концентрацій забруднюючих домішок, та надавати отриману інформації в режимі реального часу.

Аналіз світового досвіду свідчить про ефективність та перспективність сенсорних мереж як аналізаторів якості повітряного середовища. Значний інтерес при побудові бездротових сенсорних мереж МСАП в Україні

