Bond spin-density-wave phase in the staggered magnetic field

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Abstract

A stability of the bond spin-density-wave ($\overline{\mathrm{SDW}}$) phase observed in the one-dimensional half-filled anisotropic extended Hubbard model is discussed in the staggered magnetic field. A renormalization group (RG) analysis using the effective Hamiltonian implies that, due to the charge distribution in the $\overline{\mathrm{SDW}}$, the staggered magnetic field is irrelevant to its spin-liquid part, so it may survive in the weak field region. To determine its stable region, we employ a numerical procedure based upon the level-spectroscopy method and confirm our RG argument.

So far, investigations on the effects of the alternating perturbations including the staggered magnetic field on the one-dimensional (1D) correlated electrons have been intensively performed. As a model for the ferroelectricity observed in $BaTiO_3$, the standard Hubbard model with the alternating energy levels for cation and oxygen sites has been employed to describe a competition between electron correlations and alternating potential effects [1,2]. The lattice dimerization effects have been also discussed in the linear conjugated polymers and the inorganic spin-Peierls material $CuGeO_3$, where the alternating energy for the "bond" charge has been treated [3]. In this research, we shall discuss effects of the staggered magnetic field in the so-called bond spin-density-wave ($\overline{\mathrm{SDW}}$) phase which is realized as the one of ground states in an extended Hubbard chain [4]. Although, generally, the staggered magnetic field has a small energy scale and it may be relevant in the ordinary SDW phase, we shall show its irrelevancy in the $\overline{\mathrm{SDW}}$ on the basis of the renormalization group (RG) argument and further determine the stable region using a numerical method. Naturally, this can be also viewed as a consequence of the above-mentioned competition, and further, these alternating perturbation problems share a same background. So, we expect that our research contributes to its understandings.

Using the annihilation operator of a s-spin electron on the jth site $c_{j,s}$ and the number operator $n_{j,s}$, the model Hamiltonian treated here is

$$H = -\sum_{j,s} t\left(c^{\dagger}_{j,s}c_{j+1,s} + \mathrm{H.c.}\right) - \sum_{j}(-1)^j H_\pi S^z_j + \sum_j \left(U n_{j,+}n_{j,-} + V n_j n_{j+1} - J S^z_j S^z_{j+1}\right), \qquad (1)$$

where electron charge and spin (z-component) are given by $n_j, 2S^z_j = n_{j,+} \pm n_{j,-}$ (the former refers to the upper sign). In case of $H_\pi = 0$, Eq. (1) expresses the extended Hubbard model with the U(1) exchange coupling, which introduces the easy plain/axis anisotropy to the spin space depending on the sign of J, so we refer to this as the anisotropic extended Hubbard model (AEHM). In fact, the ground-state phase diagram of this model which possesses the $\overline{\mathrm{SDW}}$ (we define it below) has been precisely obtained [4]. Thus, when necessary, we shall utilize the knowledges in the following.

First, we extract an effective Hamiltonian of H using the bosonization method, where the fields θ_ν and ϕ_ν ($\nu = \rho, \sigma$) are introduced to rewrite electron operators: at the half-filling, it consists of three parts, i.e., $\mathcal{H} = \mathcal{H}_\rho + \mathcal{H}_\sigma + \mathcal{H}_\pi$ with

$$\mathcal{H}_\nu = \int \mathrm{d}x\ \frac{v_\nu}{2\pi}\left[K_\nu\left(\partial_x\theta_\nu\right)^2 + \frac{1}{K_\nu}\left(\partial_x\phi_\nu\right)^2\right] + \int \mathrm{d}x\ \frac{2g_\nu}{(2\pi\alpha)^2}\cos\sqrt{8}\phi_\nu, \qquad (2)$$

$$\mathcal{H}_\pi = \int \mathrm{d}x\ -\frac{H_\pi}{\pi\alpha}\sin\sqrt{2}\phi_\rho\sin\sqrt{2}\phi_\sigma, \qquad (3)$$

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where K_ν and v_ν are the Gaussian couplings and the velocities of elementary excitations. Couplings g_ρ and g_σ stand for the Umklapp and the backward scattering, respectively; they may take the system out of the Tomonaga-Luttinger liquid universality class. Here, it is worthy of noticing that the staggered magnetic field brings about a coupling term of the charge (ρ) and spin (σ) degrees of freedoms which are separated by the coulomb interactions. Thus, the structure in the charge part may affect a role of H_π in the spin-liquid part.

Second, to analyze $\mathcal{H}$, we employ the perturbative RG method [5]. For simplicity, we put excitation velocities equal ($v = v_\rho = v_\sigma$), then the corresponding Euclidean action can be expressed as the 2D Gaussian model perturbed by operators. Since the β-function is determined by their scaling dimensions and Wilson coefficients, we can straightforwardly obtain the RG equations: For the change of the cutoff $a \to a e^{\mathrm{d}l}$,

$$\frac{\mathrm{d}K_{\rho(\sigma)}}{\mathrm{d}l} = -\frac{1}{2}\left(y_{\phi,\rho(\sigma)}^2 + h_\pi^2\right) K_{\rho(\sigma)}^2, \tag{4}$$

$$\frac{\mathrm{d}y_{\phi,\rho(\sigma)}}{\mathrm{d}l} = -2\left(K_{\rho(\sigma)} - 1\right) y_{\phi,\rho(\sigma)} + h_\pi^2, \tag{5}$$

$$\frac{\mathrm{d}h_\pi}{\mathrm{d}l} = F(K_\rho, K_\sigma, y_{\phi,\rho}, y_{\phi,\sigma}) h_\pi, \tag{6}$$

where $y_{\phi,\nu}(0) = g_\nu/\pi v$, $h_\pi(0) = -H_\pi a/\sqrt{2}v$ and $F = 2 - (K_\rho + K_\sigma - y_{\phi,\rho} - y_{\phi,\sigma})/2$. These equations are basically the same as those derived in Ref. [2], but important differences are visible in the signs of some coefficients, which depend on the trigonometric functions in nonlinear terms. For repulsive interactions at $H_\pi = 0$, $\mathcal{H}_\rho$ is always massive unless it is located on the unstable Gaussian fixed line $y_{\phi,\rho} = 0,\ y_{0,\rho} < 0$ ($y_{0,\rho} = 2K_\rho - 2$), and thus electronic phases with the massless spin part are (i) the SDW with the renormalization $(K_\rho, y_{\phi,\rho}, K_\sigma, y_{\phi,\sigma}) \to (0, +\infty, K_\sigma^*, 0)$ and a locking point of the phase variable $\langle\sqrt{8}\phi_\rho\rangle \sim \pi$, and (ii) the $\overline{\mathrm{SDW}}$ with $(0, -\infty, K_\sigma'^*, 0)$ and $\langle\sqrt{8}\phi_\rho\rangle \sim 0$.

Now, we shall deduce a role of the staggered magnetic field in these phases. From the β-function of Eq. (6), h_π is relevant (irrelevant) for $F > 0$ ($F < 0$). In the SDW phase there is almost no chance to take a negative value of F. On the other side, its role in the $\overline{\mathrm{SDW}}$ phase is subtle, i.e., if the coupling of the "attractive" Umklapp scattering is renormalized to take an enough large value ($y_{\phi,\rho} \to -\infty$), then the coefficient F can take negative values, where H_π becomes irrelevant. Therefore, there is a possibility that the $\overline{\mathrm{SDW}}$ phase survives against the staggered magnetic field. These predictions may become more convincing by noticing that the staggered component of spins defined on sites, $\sin\sqrt{2}\phi_\rho \sin\sqrt{2}\phi_\sigma$, is considerably reduced on the locking point of ϕ_ρ in the $\overline{\mathrm{SDW}}$ [$\langle\sin\sqrt{2}\phi_\rho\rangle \simeq 0$]. So, intuitively, H_π may become irrelevant in the sense that it cannot couple with electron spins in the $\overline{\mathrm{SDW}}$ phase.

In order to check the above prediction, we numerically investigate the half-filled AEHM at $J/4V = 0.5$ along the $2V = U$ line, where the $\overline{\mathrm{SDW}}$ and ferromagnetic phases are realized as the zero field ground states [see Fig. 7(b) in Ref. [4]]. Since details of our numerical treatment will be presented elsewhere, here we just summarize our main consequences. The spin-liquid part in the $\overline{\mathrm{SDW}}$ will be destroyed by H_π greater than a certain critical value H_π^*, whose indication can be detected as the degeneracy condition of the spin excitation spectrum observed in finite size systems. Therefore, according to the so-called level-spectroscopy method [6], we numerically treat up to $L = 18$ sites systems using the Lanczos algorithm to analyze the level structure in specified subspaces and estimate $H_\pi^*(L)$. Then by extrapolating data to $L \to \infty$, the phase boundary is evaluated; Figure 1 exhibits the stable region and the inset shows its magnification (ferromagnetic phase boundary has been also given).

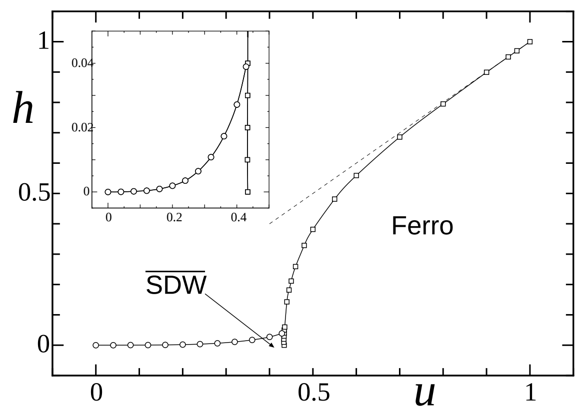

Fig. 1. Stable regions of the $\overline{\mathrm{SDW}}$ and ferromagnetic phases. The x and y-axis are $u = U/(U+4)$ and $h = H_\pi^*/(H_\pi^* + 2)$, respectively. Dotted line is an expected one in the limit.

In conclusion, we have clarified the stable region of the $\overline{\mathrm{SDW}}$ in the staggered magnetic field; its presence has been predicted in the RG argument, and for its stability the charge distribution plays a crucial role.

References

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