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

Hiromi Otsuka

Department of Physics, Tokyo Metropolitan University, Tokyo 192-0397, Japan

Abstract

A stability of the bond spin-density-wave (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 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 (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 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 $j$th site $c_{j,s}$ and the number operator $n_{j,s}$, the model Hamiltonian treated here is

$$
H = - \sum_{j,s} t (c_{j,s}^\dagger c_{j+1,s} + \text{H.c.}) - \sum_j (-1)^j H z S_j^z + \sum_j (U n_{j,\uparrow} n_{j,\downarrow} + V n_{j,\downarrow} n_{j+1,\uparrow} - J S_j^x S_{j+1}^x),
$$

where electron charge and spin (z-component) are given by $n_j, 2S_j^z = n_{j,\uparrow} \pm n_{j,\downarrow}$ (the former refers to the upper sign). In case of $H_z = 0$, 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 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 $\theta_\nu$ and $\phi_\nu$ ($\nu = \rho, \sigma$) are introduced to rewrite electron operators: at the half-filling, it consists of three parts, i.e., $\mathcal{H} = \mathcal{H}_\rho + \mathcal{H}_\sigma + \mathcal{H}_z$ with

$$
\mathcal{H}_\rho = \int dx \frac{\nu_\rho}{2\pi} \left[ K_\rho (\partial_x \theta_\rho)^2 + \frac{1}{K_\rho} (\partial_x \phi_\rho)^2 \right] + \int dx \frac{2g_\rho}{(2\pi)^2} \cos \sqrt{8} \phi_\rho,
$$

$$
\mathcal{H}_\sigma = \int dx - \frac{H_z}{\pi \alpha} \sin \sqrt{2} \phi_\sigma \sin \sqrt{2} \phi_\rho,
$$

$$
\mathcal{H}_z = \int dx - \frac{H_z}{\pi \alpha} \sin \sqrt{2} \phi_\sigma \sin \sqrt{2} \phi_\rho.
$$

1 E-mail: otsuka@phys.metro-u.ac.jp
where $K_\nu$ and $v_\nu$ are the Gaussian couplings and the velocities of elementary excitations. Couplings $g_\nu$ and $g_\sigma$ 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 ($\rho$) and spin ($\sigma$) degrees of freedoms which are separated by the coulomb interactions. Thus, the structure in the charge part may affect a role of $H_x$ in the spin-liquid part.

Second, to analyze $\mathcal{H}_x$ 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 $\beta$-function is determined by their scaling dimensions and Wilson coefficients, we can straightforwardly obtain the RG equations: For the change of the cutoff $a \rightarrow a e^{d_l}$,

$$\frac{dK_\rho(\sigma)}{dt} = -\frac{1}{2} \left( y^2_{\phi,\rho(\sigma)} + h^2_{\phi,\rho(\sigma)} \right) K^2_\rho(\sigma),$$

$$\frac{dy_{\phi,\rho(\sigma)}}{dt} = -2 \left( K_\rho(\sigma) - 1 \right) y_{\phi,\rho(\sigma)} + h^2_{\phi,\rho(\sigma)},$$

$$\frac{dh_x}{dt} = F(K_\rho, K_\sigma, y_{\phi,\rho}, y_{\phi,\sigma}) h_x,$$

where $y_{\phi,\rho}(0) = g_\rho/\pi v$, $h_x(0) = -H_x a/\sqrt{2}v$ 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 $H_x = 0$, $\mathcal{H}_x$ is always massive unless it is located on the unstable Gaussian fixed line $y_{\phi,\rho} = 0$, $y_{\phi,\rho} < 0$ ($y_{\phi,\rho} = 2K_\rho - 2$), and thus electronic phases with the massless spin part are (i) the SDW with the renormalization $(K_\rho, y_{\phi,\rho}, K_\sigma, y_{\phi,\sigma}) \rightarrow (0, +\infty, K^*_x, 0)$ and a locking point of the phase variable $\langle \sqrt{8} \phi_\rho \rangle \sim \pi$, and (ii) the SDW with $(0, -\infty, K^*_x, 0)$ 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 $\beta$-function of Eq. (6), $h_x$ 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 SDW phase is subtle, i.e., if the coupling of the “attractive” Umklapp scattering is renormalized to take an enough large value ($y_{\phi,\rho} \rightarrow -\infty$), then the coefficient $F$ can take negative values, where $H_x$ becomes irrelevant. Therefore, there is a possibility that the 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 $\phi_\rho$ in the SDW $|\sin \sqrt{2} \phi_\rho| \simeq 0$. So, intuitively, $H_x$ may become irrelevant in the sense that it cannot couple with electron spins in the 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 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 SDW will be destroyed by $H_x$ greater than a certain critical value $H^*_x$, 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 $H^*_x(L)$. Then by extrapolating data to $L \rightarrow \infty$, 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 SDW and ferromagnetic phases. The $x$ and $y$-axis are $u = U/(U + 4)$ and $h = H^*_x/(H^*_x + 2)$, respectively. Dotted line is an expected one in the limit.](image)

In conclusion, we have clarified the stable region of the 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

5. For example, J. Cardy, Scaling and Renormalization in Statistical Physics (Cambridge University Press, 1996).