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# Auxiliary fermion linearization

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**Abstract.** We present a novel mean-field-like scheme for $\frac{1}{2}$-spin fermions on a lattice in arbitrary dimension, generalizing the fermionic linearization approach. It describes the interaction of each lattice site with its neighbours by means of auxiliary fermions, living on the same site, dynamically coupled with the physical ones. This leads to a single-site picture in an enlarged 16-dimensional space given by the tensor square of the fermionic single-site Hilbert space. The general approach is applied to the extended Hubbard Hamiltonian and to the ferromagnetic Heisenberg model. The spectrum and the self-consistency equations can be determined in a straightforward way thanks to the factorization of the linearized dynamical algebra in $u(n)$ components with $n = 4$ at most. The self-consistency is formulated as a fixed-point problem for a map in the space of coupling constants.

## 1. Introduction

Model Hamiltonians for systems of strongly correlated electrons over a lattice have, in the past few years, been the object of intense study. This is mainly due to the role that they are supposed to play in a microscopic account of high-$T_c$ superconductivity. The predecessor of these models is the celebrated Hubbard model [2] which put in competition the itinerant character of the lattice electrons with the on-site correlation due to the Coulomb repulsion favouring localization. Despite its apparent simplicity the Hubbard model has been exactly solved only in the one-dimensional case by means of the Bethe ansatz (BA) [3]. For the two- (or three-) dimensional case one mainly relies on strong numerical computations both of exact-diagonalization [7] and quantum Monte Carlo [7]. It is also possible to formulate exact statements based on symmetry considerations. The Hubbard model at half-filling has a $SO(4)$ symmetry which has been used to show that it admits a class of excited eigenstates, the so-called $\eta$-paired states, with 'off-diagonal long-range order' (ODLRO) which implies superconductivity [5], and to prove the completeness of the BA eigenstates [6]. The extended Hubbard models contain additional nearest-neighbour terms describing spin–spin and charge–charge interactions as well as pair hopping processes. Rigorous results in various regions of the space of the parameters weighting the different couplings can be obtained [8, 16]; in particular it has been shown that non-vanishing pair-hopping for sufficiently negative on-site interaction leads to a $\eta$-paired ground state in the sector with zero magnetization [4]. In the one-dimensional case *ad hoc* choices of the model parameters allow integrable Hamiltonians [9–11] to be obtained. Supersymmetry plays an important role in the exact solvabilty of these models. Another approach consists of adopting approximation schemes to handle the electronic interactions, typically by means of mean-field-like treatments. To this class of theories belongs the fermionic linearization

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scheme (FLS) [12] (and references therein), in which one linearizes the hopping term—that is less important in a strong on-site coupling regime—with Grassmann-like coefficients representing averages of fermionic operators over a state (both in the quantum-mechanical and thermodynamical sense) to be determined by imposing self-consistency. This strategy can be used to map two-dimensional problems onto effective one-dimensional exactly solvable ones [14, 15]. In [14], linearizing the hopping between adjacent chains of the two-dimensional Hubbard model, the study of the Mott–Hubbard transition is performed by exploiting the BA solution of a (renormalized) one-dimensional Hubbard model. This idea has been generalized in [15] where all the inter-chain interactions of the two-dimensional extended Hubbard model are linearized and the resulting one-dimensional Hamiltonian is shown to be unitarily equivalent to the $u(2|2)$-supersymmetric model of Essler *et al* [11]. The FLS in its Clifford variables form preserves the algebraic structure of the exact problem in that expectation values of the electron operators are assumed proportional to the generators of a fermionic (super) algebra $u(1|1)$. In the case of the Falicov–Kimball model [13] the proportionality coefficient turns out to be an order parameter for the metal–insulator transition. At $T = 0$ one finds the Gutwiller results for the Hubbard model. In this paper we propose an extension of this approach to the general fermion lattice Hamiltonian (in arbitrary dimension) with two-centre interactions. Such a Hamiltonian can be expressed as a quadratic form in the generators of the local super-algebras. Adopting a single-site point of view, such a quadratic form is linearized by mapping all the algebras coupled to that associated with a given lattice site $j$ onto a single $u(2|2)$ algebra. The latter describes in some averaged way the lattice background of $j$. It is built by means of auxiliary fermionic operators anti-commuting with the physical ones, the coupling constants of the original model being rescaled by a factor that has to be determined imposing self-consistency conditions. The local Hilbert space becomes a tensor product of two four-dimensional factors. The linearized Hamiltonian leaves the eigenspaces of the total (physical plus auxiliary) fermion number invariant and *modulo* diagonal terms treat symmetrically auxiliary and physical fermions. The extended Hubbard model and the ferromagnetic Heisenberg model are considered in order to show how the scheme works. The spectrum and self-consistent equations are explicitly derived in a straightforward way thanks to the simple structure of the linearized dynamical algebras that turns out to be $\mathcal{A}_\ell = 4u(1) \oplus 6u(2) \oplus u(4)$. The case of the Hubbard model with correlated hopping conserving the number of doubly occupied sites is also discussed. The self-consistency equations assume the form of a fixed-point problem for a nonlinear map in the manifold of the rescaling factors; nonlinearity makes a careful classification and the physical interpretation of the results non-trivial. This work is devoted to the illustration of the conceptual features of the linearization scheme and therefore a systematic numerical analysis will be reserved for a future publication; only simple analytical results for the Heisenberg model are discussed.

## 2. The method

Let $\Lambda$ be a $d$-dimensional lattice of $L$ sites. Without loss of generality $\Lambda$ will be assumed hyper-cubic. $\mathcal{N}(i)$ denotes the set of the $z = 2d$ nearest neighbours of $i \in \Lambda$. A spin-$\frac{1}{2}$ fermionic field $\{a_{i\sigma}\}_{i\in\Lambda,\sigma=\uparrow,\downarrow}$ is defined over $\Lambda$. The global Hilbert space is built as the $L$-fold graded tensor product $\mathcal{H}_\Lambda = \mathcal{H} \otimes \cdots \otimes \mathcal{H}$, where $\mathcal{H}$ is the Fock space generated by the vectors

$$|0\rangle, |\uparrow\rangle \equiv a_\uparrow^\dagger|0\rangle \qquad |\downarrow\rangle \equiv a_\downarrow^\dagger|0\rangle \qquad |\ell\rangle \equiv a_\downarrow^\dagger a_\uparrow^\dagger|0\rangle. \tag{2.1}$$

$\mathcal{H}$ has a natural $\mathbb{Z}_2$-gradation, $\mathcal{H} = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)}$, $\mathcal{H}^{(\alpha)}$ denoting the even ($\alpha = 0$) and the odd ($\alpha = 1$) sector spanned by vectors corresponding to even and odd eigenvalues of the fermion number operators respectively. The algebra $\mathcal{A}$ of the linear maps of $\mathcal{H}$ onto itself inherits this graded structure; it is therefore a super-algebra isomorphic to $u(2|2)$. The superalgebra structure is defined by the graded commutators $[G^\alpha, G^\beta\} = K_\gamma^{\alpha\beta} G^\gamma$, where the symbol $[\bullet, \bullet\}$ denotes anticommutators if both the $G$'s are odd, commutators otherwise and $\{K_\gamma^{\alpha\beta}\}$ are the structure constants. We will denote the $\mathbb{Z}_2$-degree of a homogeneous element $G^\alpha$ by $|\alpha| \in \{0, 1\}$. For each $j \in \Lambda$ one introduces local operators acting in a non-trivial way only on the $j$th factor in $\mathcal{H}_\Lambda$, even (odd) operators sitting on different sites commute (anti-commute). A convenient basis for the corresponding local super-algebra $\mathcal{A}_j$ is given by

$$S_j = a_{j\downarrow}^\dagger a_{j\uparrow} \qquad S_j^\dagger = a_{j\uparrow}^\dagger a_{j\downarrow} \qquad S_j^z = \tfrac{1}{2}(n_{j\uparrow} - n_{j\downarrow}) \tag{2.2}$$

$$\eta_j = a_{j\uparrow} a_{j\downarrow} \qquad \eta_j^\dagger = a_{j\downarrow}^\dagger a_{j\uparrow}^\dagger \qquad \eta_j^z = \tfrac{1}{2}(1 - n_{j\uparrow} - n_{j\downarrow}) \tag{2.3}$$

$$X_j = (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}) \qquad \mathbb{I} \in \text{centre} \tag{2.4}$$

for the even (bosonic) sector $\mathcal{A}_j^{(0)}$,

$$Q_{j\uparrow} = (1 - n_{j\downarrow}) a_{j\uparrow} \qquad Q_{j\downarrow} = (1 - n_{j\uparrow}) a_{j\downarrow} \tag{2.5}$$

$$\tilde{Q}_{j\uparrow} = n_{j\downarrow} a_{j\uparrow} \qquad \tilde{Q}_{j\downarrow} = n_{j\uparrow} a_{j\downarrow} \tag{2.6}$$

for the odd (fermionic) sector $\mathcal{A}_j^{(1)}$. Here $n_{i\sigma} \equiv a_{j\sigma}^\dagger a_{j\sigma}$, $(j \in \Lambda, \sigma = \uparrow, \downarrow)$ is the local fermion number operator. These operators (with their Hermitian conjugates) are often referred to as the Hubbard operators. The Cartan sub-algebra $\mathcal{C}_j$ of $\mathcal{A}_j$ is spanned by the number operators

$$N_{i\sigma} \equiv (1 - n_{j-\sigma}) n_{i\sigma}, (\sigma = \uparrow, \downarrow) \qquad N_{i\ell} \equiv n_{i\uparrow} n_{i\downarrow}.$$

We now consider a lattice Hamiltonian over $\Lambda$ given by $H = H_0 + H_1$, where $H_0$ and $H_1$ are the inter-site and on-site interaction respectively. The local part $H_1$ has the form

$$H_1 = \sum_{i \in \Lambda} H_i \qquad H_i \in \mathcal{C}_i$$

hence it is diagonal in the (direct space) Fock representation. When interested in a strong coupling limit where the local Coulomb repulsion plays a major role, one may consider approximate treatments only of the non-local part $H_0$ of the lattice Hamiltonian. Assuming, for simplicity, nearest-neighbour interactions, the general expression for such an operator is given by the quadratic form in the Hubbard operators $\{G^\alpha\}_{\alpha=1}^{16}$

$$H_0 = \sum_{\langle ij \rangle} \sum_{\alpha\beta} C^{\alpha\beta} G_i^\alpha G_j^\beta \tag{2.7}$$

where $\langle ij \rangle$ denotes nearest-neighbour pairs in $\Lambda$. Isotropy and translational invariance are assumed as well. $H_0$ can be rewritten in the formally single-site form $H_0 = \frac{1}{2} z \sum_{j,\alpha} \Theta_j^\alpha G_j^\alpha$, where

$$\Theta_j^\alpha = \frac{1}{z} \sum_{i \in \mathcal{N}(j), \beta} C^{\beta\alpha} G_i^\beta. \tag{2.8}$$

These non-local operators describe the degrees of freedom of the lattice coupled, in the interaction channel associated with the generator $G^\alpha$, with those living at the site $j$. Notice that, since for a number-conserving Hamiltonian $H_0$ one has $C^{\alpha\beta} = 0$ unless $|\alpha| = |\beta|$,

the $\Theta_j^\alpha$'s carry a $\mathbb{Z}_2$-degree also. If $\mathcal{N}_{jk} \equiv \mathcal{N}(j) \bigcap \mathcal{N}(k) = \emptyset$ then $[\Theta_j^\alpha, \Theta_k^\beta\} = 0$ and if $k \notin \mathcal{N}(j)$ then $[\Theta_j^\alpha, G_k^\delta\} = 0$, otherwise

$$[\Theta_j^\alpha, \Theta_k^\beta\} = \frac{1}{z^2} \sum_{i \in \mathcal{N}_{jk}} C^{\alpha\gamma} C^{\beta\delta} K_\tau^{\gamma\delta} G_i^\tau \qquad [\Theta_j^\alpha, G_k^\delta\} = \frac{1}{z} C^{\alpha\gamma} K_\tau^{\gamma\delta} G_k^\tau. \tag{2.9}$$

These commutation rules describe how the lattice background dynamics couples with the local degrees of freedom in $j \in \Lambda$. In order to get a single-site picture one usually assumes that operators $\Theta_j^\alpha$ can be replaced by their averages $\langle \Theta_j^\alpha \rangle$ over a suitable equilibrium state to be determined self-consistently. In this way one neglects both correlations and fluctuations and violates statistics, having now a $c$-number field that obviously has trivial commutation rules. The auxiliary fermion linearization scheme consists in the transformation

$$\Theta_j^\alpha \to (\Theta_j^\alpha)^\phi \equiv \sum_\beta C^{\alpha\beta} p_\beta (G_j^\beta)^\phi \tag{2.10}$$

where $\{(G_j^\beta)^\phi\}$ are a set of operators spanning an algebra $\mathcal{A}^\phi \cong u(2|2)$, satisfying the further condition $[(G_i^\alpha)^\phi, G_j^\beta\} = 0$, and the $\{p_\alpha\}$'s are variational parameters. The $\{G_j^\beta\}$'s act on an auxiliary Hilbert space $\mathcal{H}^\phi$ ($\phi$-sector) attached to the site $j$ and may be thought of as realized in terms of auxiliary fermionic operators $\{a^\phi\}_{j\sigma}$ in the same way as the Hubbard operators $G_i$ are realized in terms of the physical ones. The transformation (2.10) assumes translational invariance in that all the algebras $\{\mathcal{A}_j\}$, $j \in \mathcal{N}(i)$ are replaced by the algebra $\mathcal{A}_i^\phi$ and moreover the parameters $\{p^\alpha\}$ do not depend upon the site label $j$. This procedure is a sort of dimerization of the dynamics over $\Lambda$ in which the two sites of each dimer play an asymmetric role: in one site there are physical fermions $\{a_{j\sigma}\}_{\sigma=\uparrow,\downarrow}$ whose local interactions (contained in $H_1$) are treated exactly, in the other site there are auxiliary fermions $\{a_{j\sigma}^\phi\}_{\sigma=\uparrow,\downarrow}$ representing the remainder of the lattice in an averaged way. The parameters $\{p_\alpha\}$ are to be determined by self-consistency conditions that will be discussed in section 3. The linearized Hamiltonian is then

$$H_0^\ell = \sum_j H_j^\ell \qquad H_j^\ell = \frac{z}{2} \sum_{\alpha,\beta} C^{\alpha\beta} p_\beta (G_j^\beta)^\phi G_j^\alpha \tag{2.11}$$

from which it follows that the $\{p_\alpha\}$'s play the role of coupling constants between the physical and auxiliary fermions. Since for $i \neq j$ one has $[H_i^\ell, H_j^\ell] = 0$ the approximation scheme has indeed led to a single-site picture, suited to describing phases with unbroken translational symmetry. The local Hilbert space is extended to $\tilde{\mathcal{H}} = \mathcal{H} \otimes \mathcal{H}^\phi$. This implies that the global dynamical algebra of the linearized system is $\mathcal{A}_\Lambda^\ell = \oplus_{j\in\Lambda} \mathcal{A}_j^\ell$, the local dynamical algebras $\mathcal{A}_j^\ell$ being given by sub-algebras of $u(2|2)_j \otimes u(2|2)_j$. The linearized Hamiltonian $H_0^\ell$ is invariant under the exchange of physical fermions with the auxiliary ones and conserves the total number of fermions $n_\mathrm{F} \equiv n_\mathrm{Phys} + n_\phi$ if $H_0$ does so. The local (non-linearized) interaction breaks the first symmetry only. Therefore we have the decomposition

$$\tilde{\mathcal{H}} = \bigoplus_{n_\mathrm{F}=0}^{4} \tilde{\mathcal{H}}^{(n_\mathrm{F})}$$

of the local enlarged Hilbert space as a direct sum of invariant sub-spaces with a fixed number $n_\mathrm{F}$ of fermions. This implies that $\mathcal{A}_j^\ell = \oplus_{n=0}^4 u(d_n)$, where $d_n \equiv \dim(\tilde{\mathcal{H}}^{(n)}) = \binom{4}{n}$. From the physical point of view this factorization corresponds to the different elementary processes that can occur between a site and its first neighbours: fermions hop from a singly (doubly) occupied site to an empty (singly occupied) one in $\mathcal{H}^{(1)}$ ($\mathcal{H}^{(3)}$), spin-flip (pair hopping), spin–spin (charge–charge) interactions in $\mathcal{H}^{(2)}$. The hopping from a doubly

occupied site to a single occupied one is in $\mathcal{H}^{(2)}$ also. The case $n_{\rm F}=0$ ($n_{\rm F}=4$) corresponds to an empty (fully occupied) lattice and has a trivial dynamics. The linearization scheme outlined above becomes simpler for the case of models in which a kinematical constraint is imposed on the local Hilbert space $\mathcal{H}\to\mathcal{H}'\subset\mathcal{H}$, as for the $t$–$J$ model (no doubly occupied sites) and the Heisenberg model (only spin degrees of freedom). The pertinent local algebra becomes $\mathcal{A}'\equiv\mathrm{End}(\mathcal{H}')\subset\mathcal{A}$ and the whole procedure can be performed as in the general case by simply replacing $\mathcal{H}$ ($\mathcal{A}$) with $\mathcal{H}'(\mathcal{A}')$. The approach described is supposed to improve the $c$-number-based single-site approach in that, on the one hand, it allows fluctuations of the background (accommodated in $\tilde{\mathcal{H}}$), on the other hand, by conserving some of the commutation rules, it takes into account the graded (i.e. statistical) nature of the involved objects. In this respect it is worth pointing out that the neglected commutators, compared with the ones assumed to be non-vanishing, are scaled by a factor $z^{-1}=(2d)^{-1}$. This suggests that the approximation should improve in high dimensions (indeed be exact for $d\to\infty$).

## 3. Extended Hubbard model

The extended Hubbard model in the presence of an external magnetic field $h$ is described by the grand-canonical Hamiltonian

$$\begin{aligned}H=&-t\sum_{\langle ij\rangle}\sum_{\sigma}(a^{\dagger}_{i\sigma}a_{j\sigma}+a^{\dagger}_{j\sigma}a_{i\sigma})+U\sum_{i}n_{i,\uparrow}n_{i\downarrow}\\&+V\sum_{\langle ij\rangle}\sum_{\sigma\sigma'}a^{\dagger}_{i\sigma}a_{j\sigma'}+X\sum_{\langle ij\rangle}\sum_{\sigma}(a^{\dagger}_{i\sigma}a_{j\sigma}+a^{\dagger}_{j\sigma}a_{i\sigma})(n_{i-\sigma}+n_{j-\sigma})\\&+J\sum_{\langle ij\rangle}\sum_{\sigma\sigma'}a^{\dagger}_{i\sigma}a^{\dagger}_{j\sigma'}a_{i\sigma'}a_{j\sigma}+J'\sum_{\langle ij\rangle}(a^{\dagger}_{i\uparrow}a^{\dagger}_{i\downarrow}a_{j\downarrow}a_{j\uparrow}+a^{\dagger}_{j\uparrow}a^{\dagger}_{j\downarrow}a_{i\downarrow}a_{i\uparrow})\\&+h\sum_{i}\tfrac{1}{2}(n_{i\uparrow}-n_{i\downarrow})-\mu\sum_{i\sigma}n_{i\sigma}.\end{aligned}\tag{3.1}$$

In terms of the generators of $\mathcal{A}_i$ the Hamiltonian (3.1) can be rewritten as $H=-\sum_{\langle ik\rangle}H_{ik}+\sum_i H_i$ where the non-local contribution is given by

$$\begin{aligned}H_{ik}=&\sum_{\sigma=\uparrow,\downarrow}t(Q^{\dagger}_{j\sigma}Q_{k\sigma}+Q^{\dagger}_{k\sigma}Q_{j\sigma})+(t-2X)(\tilde{Q}^{\dagger}_{j\sigma}\tilde{Q}_{k\sigma}+\tilde{Q}^{\dagger}_{k\sigma}\tilde{Q}_{j\sigma})\\&+(t-X)(\tilde{Q}^{\dagger}_{j\sigma}Q_{k\sigma}+Q^{\dagger}_{k\sigma}\tilde{Q}_{j\sigma})+(t-X)(Q^{\dagger}_{j\sigma}\tilde{Q}_{k\sigma}+\tilde{Q}^{\dagger}_{k\sigma}Q_{j\sigma})\\&+J(2S^{z}_{j}S^{z}_{k}+S^{\dagger}_{j}S_{k}+S^{\dagger}_{k}S_{j})+2(J-2V)\eta^{z}_{j}\eta^{z}_{k}-J'(\eta^{\dagger}_{j}\eta_{k}+\eta^{\dagger}_{k}\eta_{j})\end{aligned}\tag{3.2}$$

and the local terms by

$$H_i=-\tilde{\mu}(2N_{i\ell}+N_{i\uparrow}+N_{i\downarrow})+\frac{h}{2}(N_{i\uparrow}-N_{i\downarrow})+UN_{i\ell}+C.\tag{3.3}$$

Here we have introduced the modified chemical potential $\tilde{\mu}=\mu-\frac{1}{2}z(2V-J)$, and $C=\frac{1}{4}zL(2V-J)$ gives a shifting of the spectrum, since its contribution is immaterial, it will be neglected from now on. Performing the linearization of the two-site term $H_{ik}$ according to the general scheme of section 1, we get a single extended-site term which can be expressed, up to an overall $\frac{1}{2}z$ factor, as

$$\begin{aligned}H_{\ell}=&\sum_{\sigma=\uparrow,\downarrow}(-tq_{\sigma}Q^{\dagger}_{\sigma}Q^{\phi}_{\sigma}+(2X-t)\tilde{q}_{\sigma}\tilde{Q}^{\dagger}_{\sigma}\tilde{Q}^{\phi}_{\sigma}+\delta(q_{\sigma}\tilde{Q}^{\dagger}_{\sigma}Q^{\phi}_{\sigma}+\tilde{q}_{\sigma}Q^{\dagger}_{\sigma}\tilde{Q}^{\phi}_{\sigma}))\\&+(2V-J)e^{z}\eta^{z}\eta^{z\phi}+J'e^{-}\eta^{\dagger}\eta^{\phi}-J(s^{z}S^{z}S^{z\phi}+s^{-}S^{\dagger}S^{\phi})+\mathrm{HC}\end{aligned}\tag{3.4}$$

where $s^z, e^z \in \mathbb{R}, q_\sigma, \tilde{q}_\sigma, s^-, e^- \in \mathbb{C}$ are the variational parameters $\{p^\alpha\}$, and $\delta \equiv X - t$. In order to simplify the notation we perform a rescaling of some of the $\{p^\alpha\}$

$$\begin{aligned} &\tilde{q}_\sigma \mapsto (2X - t)\tilde{q}_\sigma \qquad (\sigma = \uparrow, \downarrow) \\ &e^z \mapsto e^z(2V - J) \qquad e^\pm \mapsto J' e^\pm \qquad (e^- \equiv (e^+)^*) \\ &s^\alpha \mapsto s^\alpha J \qquad (\alpha = \pm, z). \end{aligned} \tag{3.5}$$

This allows us to give explicit expressions for the projections of the linearized Hamiltonian into the subspaces $\tilde{\mathcal{H}}^{(i)} \subset \tilde{\mathcal{H}}$, $(i = 0, \ldots, 4)$ in terms of the basis vectors listed in appendix A.

$$\begin{aligned} H^{(0)} &= \frac{e^z}{2} |1\rangle_0 \langle 1|_0 \\ H_\ell^{(1)} &= \mathrm{diag}\left(0, 0, -\mu - \frac{h}{2}, -\mu + \frac{h}{2}\right) - t\left(q_\uparrow |4\rangle_1 \langle 1|_1 + q_\downarrow |3\rangle_1 \langle 2|_1 + \mathrm{HC}\right) \\ H_\ell^{(2)} &= -\tfrac{1}{4}\,\mathrm{diag}(e^z, -s^z + h + 2\mu, s^z - h + 2\mu, s^z + h + 2\mu, -h - s^z + 2\mu, \\ &\qquad -2U + e^z + 4\mu) - s^+ |5\rangle_2 \langle 2|_2 + e^+ |6\rangle_2 \langle 1|_2 \\ &\qquad -\delta(q_\uparrow |6\rangle_2 \langle 2|_2 - q_\downarrow |6\rangle_2 \langle 5|_2) + \delta(\tilde{q}_\uparrow |5\rangle_2 \langle 1|_2 - \tilde{q}_\downarrow |2\rangle_2 \langle 1|_2) + \mathrm{HC} \\ H_\ell^{(3)} &= \frac{1}{2}\,\mathrm{diag}\left(-\mu - \frac{h}{2}, U - 2\mu, -\mu + \frac{h}{2}, U - 2\mu\right) - (\tilde{q}_\uparrow |2\rangle_3 \langle 1|_3 + \tilde{q}_\downarrow |4\rangle_3 \langle 3|_3) + \mathrm{HC} \\ H_\ell^{(4)} &= \left(-2\mu + \frac{e^z}{2} + U\right) |1\rangle_4 \langle 1|_4. \end{aligned} \tag{3.6}$$

In the following we shall discuss the diagonalization of each of the non-trivial $H_\ell^{(i)}$, $(i = 1, 2, 3)$. For simplicity, since no ambiguity may arise, we shall drop the index $j$ from the vectors $|i\rangle_j$.

### *3.1. Spectrum of $H_\ell^{(1)}$*

The Hamiltonian for the one-particle sector $H^{(1)}$ has a twofold block-diagonal form, corresponding to the decoupling of the spin sectors. In terms of dynamical algebras this means that $\mathcal{A}^{(1)} = u(2) \oplus u(2)$ where the two $u(2)$'s are generated respectively by the operators ($u(2) \cong su(2) \oplus u(1)$):

$$\begin{aligned} &K_\uparrow^z \equiv \tfrac{1}{2}(|4\rangle\langle 4| - |1\rangle\langle 1|) \qquad K_\uparrow^+ \equiv \mathrm{e}^{\mathrm{i}\alpha_\uparrow} |4\rangle\langle 1| \qquad K_\uparrow^- \equiv (K_\uparrow^+)^\dagger \in su(2) \\ &K_\uparrow^0 = \tfrac{1}{2}(|1\rangle\langle 1| + |4\rangle\langle 4|) \in u(1) \\ &K_\downarrow^z \equiv \tfrac{1}{2}(|3\rangle\langle 3| - |2\rangle\langle 2|) \qquad K_\downarrow^+ \equiv \mathrm{e}^{\mathrm{i}\alpha_\downarrow} |3\rangle\langle 2| \qquad \tilde{K}_\downarrow^- \equiv (K_\downarrow^+)^\dagger \in su(2) \\ &K_\uparrow^0 = \tfrac{1}{2}(|2\rangle\langle 2| + |3\rangle\langle 3|) \in u(1) \end{aligned} \tag{3.7}$$

denoting $\alpha_\sigma$ the phase of $q_\sigma$. The central element $K_\sigma^0$ and $K_\sigma^z$ generate the Cartan subalgebras $\mathcal{C}_\sigma \subset u(2)$. By using these operators the Hamiltonian becomes

$$H^{(1)} = \sum_\sigma \left(\sigma \frac{h}{2} - \mu\right)(K_\sigma^0 - K_\sigma^z) - t|q_\sigma|(K_\sigma^+ + K_\sigma^-). \tag{3.8}$$

Diagonalization can be performed by the exponential of the adjoint action of the operator $Z = \mathrm{i}(\theta_\uparrow^{(1)} K_\uparrow^y + \theta_\downarrow^{(1)} K_\downarrow^y)$, where $K_\sigma^y = (2\mathrm{i})^{-1}(K_\sigma^+ - K_\sigma^-)$, with

$$\theta_\sigma^{(1)} = \tan^{-1}\left(\frac{2t|q_\sigma|}{\sigma h/2 - \mu}\right) \qquad (\sigma = \uparrow, \downarrow). \tag{3.9}$$

This means that if $U \equiv \exp(Z) \in U(2) \otimes U(2)$ then $U^{-1}H^{\ell}U \in \oplus_{\sigma}\mathcal{C}_{\sigma}$. Since in the representation (3.7) one has $(K^{y})^2 = \frac{1}{2}K_0 \equiv \frac{1}{2}\mathbb{I}$, the rotation $U$ can be straightforwardly calculated and its columns give the eigenvectors. The eigenvalues and the eigenvectors have the well known form $E^{(1)}_{\pm\sigma} = E^{(1)}_{0\sigma} \pm E^{(1)}_{1\sigma}$

$$E^{(1)}_{0\sigma} = \frac{\sigma h/2 - \mu}{2} \qquad E^{(1)}_{1\sigma} = \frac{1}{2}\sqrt{\left(\frac{\sigma h}{2} - \mu\right)^2 + 4t^2|q_{\sigma}|^2} \tag{3.10}$$

$$|\psi^{(1)}_{-\sigma}\rangle = \cos\frac{\theta^{(1)}_{\uparrow}}{2}|H\rangle^{(1)}_{\sigma} + \mathrm{e}^{-\mathrm{i}\alpha_{\uparrow}}\sin\frac{\theta^{(1)}_{\uparrow}}{2}|L\rangle^{(1)}_{\sigma}$$

$$|\psi^{(1)}_{+\sigma}\rangle = \sin\frac{\theta^{(1)}_{\uparrow}}{2}|H\rangle^{(1)}_{\sigma} - \mathrm{e}^{-\mathrm{i}\alpha}\cos\frac{\theta^{(1)}_{\uparrow}}{2}|L\rangle^{(1)}_{\sigma} \tag{3.11}$$

where the highest (lowest) $su(2)$ vectors $|H\rangle^{(1)}_{\sigma}$, ($|L\rangle^{(1)}_{\sigma}$) are respectively given by $|4\rangle$, ($|1\rangle$) in the up-sector and $|3\rangle$, ($|2\rangle$) in the down-sector.

### *3.2. Spectrum of $H^{(2)}_{\ell}$*

In this sector, corresponding to $n_{\mathrm{F}} = 2$, the dynamical structure is more complex than in the former case due to the presence of the terms weighted by $\delta = X - t$. We split the Hamiltonian in $H^{(2)}_{\ell} = H^{(2)}_0 + \delta H^{(2)}_1$ where

$$H^{(2)}_1 = -q_{\uparrow}|6\rangle\langle 2| + q_{\downarrow}|6\rangle\langle 5| + \tilde{q}_{\uparrow}|5\rangle\langle 1| - \tilde{q}_{\downarrow}|2\rangle\langle 1| + \mathrm{HC} \tag{3.12}$$

and $H^{(2)}_0$ is the remainder. The dynamical algebra is given by $\mathcal{A}^{(2)} \cong u(4) \oplus u(2)$, if $\delta = 0$ we have the reduction $\mathcal{A}^{(2)} \to u(2) \oplus u(2) \oplus u(2)$, the three commuting $u(2)$ blocks, one of which is in diagonal form, will be labelled respectively by $\eta$, $S$, $D$. It is worth emphasizing that this drastic simplification that we find at the linearized level is reminiscent of the one occurring for the exact problem, where—providing an additional conserved quantity (i.e. the number of doubly occupied sites)—it is essential for the exact solvabilty of the one-dimensional Hubbard-like models. Of course in the present case the model remains also exactly solvable for $\delta \neq 0$, but the expressions for the eigenvalues and eigenvectors become much more complex, and therefore will not be reported in the following. The generators are

$$\begin{aligned}
&K^{z}_{\eta} \equiv \tfrac{1}{2}(|6\rangle\langle 6| - |1\rangle\langle 1|) \qquad K^{+}_{\eta} \equiv \mathrm{e}^{\mathrm{i}\alpha}|6\rangle\langle 1| \qquad K^{-}_{\eta} \equiv (K^{+}_{\eta})^{\dagger} \\
&K^{z}_{D} \equiv \tfrac{1}{2}(|3\rangle\langle 3| - |4\rangle\langle 4|) \qquad K^{+}_{D} \equiv |3\rangle\langle 4| \qquad \tilde{K}^{-}_{D} \equiv (K^{+}_{D})^{\dagger} \\
&K^{z}_{S} \equiv \tfrac{1}{2}(|5\rangle\langle 5| - |2\rangle\langle 2|) \qquad K^{+}_{S} \equiv \mathrm{e}^{\mathrm{i}\beta}|5\rangle\langle 2| \qquad \tilde{K}^{-}_{S} \equiv (K^{+}_{S})^{\dagger}
\end{aligned} \tag{3.13}$$

in which $\alpha$ ($\beta$) denotes the phase of $e^{-}$ ($s^{-}$), for the $su(2)$ components and by $K^{0}_{\alpha}$ ($\alpha = \eta, S, D$), built in the obvious way, for the $u(1)$ ones. $H^{(2)}_0$ can be rotated onto the Cartan subalgebra operating with the adjoint action of $U = U_{\eta}U_{S} \in U(2) \otimes U(2)$ where

$$\begin{aligned}
&U_{\eta,S} = \exp(\theta_{\eta,S}K^{y}_{\eta,S}) \qquad K^{y}_{\eta,S} = \frac{1}{2\mathrm{i}}(K^{+}_{\eta,S} - K^{-}_{\eta,S}) \\
&\theta_{\eta} = \tan^{-1}\left(\frac{2|e^{+}|}{U - 2\mu}\right) \qquad \theta_{S} = \tan^{-1}\left(\frac{2|s^{+}|}{h}\right).
\end{aligned} \tag{3.14}$$

The spectrum has the form $E^{\eta,S}_{\pm} = E^{\eta,S}_0 \pm E^{\eta,S}_1$ in which

$$\begin{aligned}
&E^{\eta}_0 = \tfrac{1}{2}(U - e^{z} - 2\mu) \qquad E^{\eta}_1 = \tfrac{1}{2}\sqrt{(U - 2\mu)^2 + 4|e^{+}|^2} \\
&E^{S}_0 = \tfrac{1}{2}(s^{z}/2 - \mu) \qquad E^{S}_1 = \tfrac{1}{2}\sqrt{h^2 + 4|s^{+}|^2}
\end{aligned} \tag{3.15}$$

and the eigenvectors

$$|\psi_+^\eta\rangle = \cos\frac{\theta^\eta}{2}|6\rangle + \mathrm{e}^{-\mathrm{i}\alpha}\sin\frac{\theta^\eta}{2}|1\rangle \qquad |\psi_-^\eta\rangle = \sin\frac{\theta^\eta}{2}|6\rangle - \mathrm{e}^{-\mathrm{i}\alpha}\cos\frac{\theta^\eta}{2}|1\rangle. \tag{3.16}$$

$|\psi_\pm^S\rangle$ are obtained by making the substitutions $|1\rangle \mapsto |2\rangle, |6\rangle \mapsto |5\rangle, \theta^\eta \mapsto \theta^S$. Besides these contributions we have

$$E_\pm^D = \frac{-s^z}{2} - \mu \pm \frac{h}{2} \qquad |\psi_{1,2}^D\rangle = |3,4\rangle. \tag{3.17}$$

The Hamiltonian $H_1^{(2)}$ couples the $\eta$ and $S$ sectors. Imposing $\delta = 0$ (i.e. $t = X$) the Hamiltonian has been diagonalized; if $\delta$ can be assumed to be a small parameter, one can resort to a perturbative expansion. Note that the first-order contribution is zero.

### *3.3. Spectrum of $H_\ell^{(3)}$*

In the three-particle case once more the dynamical algebra has the structure $\mathcal{A}^{(3)} = u(2) \oplus u(2)$. The generators are given by

$$\begin{aligned} &K_\uparrow^z \equiv \tfrac{1}{2}(|2\rangle\langle 2| - |1\rangle\langle 1|) \qquad K_\uparrow^+ \equiv \mathrm{e}^{\mathrm{i}\alpha_\uparrow}|2\rangle\langle 1| \qquad K_\uparrow^- \equiv (K_\uparrow^+)^\dagger \\ &K_\downarrow^z \equiv \tfrac{1}{2}(|3\rangle\langle 3| - |4\rangle\langle 4|) \qquad K_\downarrow^+ \equiv \mathrm{e}^{\mathrm{i}\alpha_\downarrow}|3\rangle\langle 4| \qquad \tilde{K}_\downarrow^- \equiv (K_\downarrow^+)^\dagger \end{aligned} \tag{3.18}$$

plus the central elements $K_\sigma^0$, $(\sigma = \uparrow, \downarrow)$ built as in the previous sections. Here $\alpha_\sigma$ denotes the phase of $\tilde{q}_\sigma$. Expressing $H_\ell^{(3)}$ in terms of these operators the spectrum can be obtained in the same way as in the previous case, the rotation angles now are

$$\theta_\sigma^{(3)} = \tan^{-1}\left(\frac{2|\tilde{q}_\sigma|}{\mu - U - \sigma h/2}\right) \qquad (\sigma = \uparrow, \downarrow) \tag{3.19}$$

and the eigenvalues $E_{\sigma\pm}^{(3)} = E_{0\sigma}^{(3)} \pm E_{1\sigma}^{(3)}$, where

$$E_{0\sigma}^{(3)} = \frac{U - 3\mu + \sigma h/2}{2} \qquad E_{1\sigma}^{(3)} = \frac{1}{2}\sqrt{\left(U - \mu + \frac{\sigma h}{2}\right)^2 + 4|\tilde{q}_\sigma|^2} \tag{3.20}$$

with eigenvectors

$$\begin{aligned} |\psi_{-\sigma}^{(3)}\rangle &= \cos\frac{\theta_\sigma^{(3)}}{2}|H\rangle_\sigma^{(3)} + \mathrm{e}^{-\mathrm{i}\alpha_\uparrow}\sin\frac{\theta_\sigma^{(3)}}{2}|L\rangle_\sigma^{(3)} \\ |\psi_{+\sigma}^{(3)}\rangle &= -\mathrm{e}^{-\mathrm{i}\alpha_\uparrow}\sin\frac{\theta_\sigma^{(3)}}{2}|H\rangle_\sigma^{(3)} + \mathrm{e}^{-\mathrm{i}\alpha_\uparrow}\cos\frac{\theta_\uparrow^{(3)}}{2}|L\rangle_\sigma^{(3)}. \end{aligned} \tag{3.21}$$

Now the highest (lowest) $u(2)$ vectors are given by $|2\rangle$ ($|1\rangle$) in the up-sector and $|4\rangle$ ($|3\rangle$) in the down-sector.

## 4. Self-consistency

The self-consistency of the linearization procedure is implemented by means of the constraints

$$p_i = \frac{\langle G_i^\dagger G_i^\phi\rangle}{\langle G_i^{\phi\dagger} G_i^\phi\rangle} \equiv \Xi_i(\{p_j\}) \qquad (i, j = 1, \ldots, 8) \tag{4.1}$$

where $G_i$ denotes a generator of $u(2|2)$ and $p_i$ the corresponding variational parameter

$$\begin{aligned} &(G_i)_{i=1}^8 = (S^z, S, \eta^z, \eta, Q_\uparrow, Q_\downarrow, \tilde{Q}_\uparrow, \tilde{Q}_\downarrow) \\ &(p_i)_{i=1}^8 = (s^z, s^+, e^z, e^+, q_\uparrow, q_\downarrow, \tilde{q}_\uparrow, \tilde{q}_\downarrow) \in \mathbb{R}^2 \times \mathbb{C}^6. \end{aligned} \tag{4.2}$$

The ensemble averages $\langle\bullet\rangle$ are obtained by tracing over the physical as well as the auxiliary degrees of freedom. Explicit computations show that, for $\delta = 0$, in equation (4.1) the phases cancel out so that the effective parameters space $\mathcal{M}$ turns out to be $\mathbb{R}^2 \times (\mathbb{R}_0^+)^6$. These equations shed light onto the physical meaning of the $p_i$'s: they measure the correlation between the physical and the auxiliary fermions in each of the interaction channels associated with the generators of $u(2|2)$, in other words they determine the relative weight of the different couplings between the local degrees of freedom and those of the remainder of the lattice. The right-hand side of (4.1) defines a nonlinear map $\Xi$ of $\mathcal{M}$ onto itself, parametrized by the interaction strengths of the extended Hubbard Hamiltonian (3.1) and depending upon temperature. The self-consistency requirement can be viewed as a fixed-point problem for $\Xi$ constrained by the filling condition $n \equiv \langle N\rangle$ which allows the determination of the chemical potential $\mu$. Of course if we set the external magnetic field to zero, restoring the spin symmetry, $\mathcal{M}$ becomes smaller due to merging of the variational parameters associated to different spin sectors. Since this problem, although finite-dimensional, has quite a rich structure and has to be dealt with numerically, it is worthwhile to begin analysing some relevant subcases from the physical point of view. As mentioned in the previous section assuming $t = X$ the explicit expression for $\Xi$ (that is reported in appendix A) turns out to be particularly simple. The corresponding grand-canonical partition function is

$$\begin{aligned} Z &= \sum_{i=0}^{4} \zeta^{(i)} \qquad \text{where } \zeta^{(i)} = \mathrm{Tr}_{\mathcal{H}^{(i)}} \exp(-\beta H_\ell^{(i)}) \qquad (i = 0, \ldots, 4) \\ \zeta^{(i)} &= \mathrm{e}^{-\beta E^{(i)}} \qquad (i = 0, 4) \\ \zeta^{(i)} &= 2 \sum_{\sigma=\uparrow,\downarrow} \mathrm{e}^{-\beta E_{0\sigma}^{(i)}} \cosh(\beta E_{1\sigma}^{(i)}) \qquad (i = 1, 3) \\ \zeta^{(2)} &= 2 \sum_{\alpha=\eta,S,D} \mathrm{e}^{-\beta E_0^{(\alpha)}} \cosh(\beta E_1^{(\alpha)}). \end{aligned} \tag{4.3}$$

The explicit form of the eigenvalues $\{E\}$ was given in the previous section. Equations (4.3) describe the subcase $\delta = 0$; this is the case of the supersymmetric EKS model, and, more generally, that of those Hubbard-like models in which the number of doubly occupied sites is conserved. Another interesting choice—mainly in view of comparison with exact results—is given by the Heisenberg model. Although it could be derived directly from the extended Hubbard model by imposing the obvious kinematical constraints, the Heisenberg model will be treated on its own, in order to show that the method does not require the local algebras $\{\mathcal{A}\}_{j\in\Lambda}$ to be explicitly realized in terms of bilinears of a *background* fermionic algebra. Even in this case diagonalization can be carried over in a simple algebraic-theoretic way, thanks to the breaking of the dynamical algebra in a direct sum of $u(2)$ terms, plus two trivial $u(1)$ contributions.

## 5. Ferromagnetic Heisenberg model

Let us consider the ferromagnetic Heisenberg model on a $d$-dimensional hyper-cubic lattice $\Lambda$ with an external magnetic field $h$:

$$H = -\frac{J}{2} \sum_{\langle ij\rangle} (S_i^z S_j^z + S_i^+ S_j^- + \mathrm{HC}) + h \sum_i S_i^z \qquad (J > 0). \tag{5.1}$$

After the auxiliary-fermion linearization the local contribution is given by

$$H^\ell = -\frac{zJ}{4} (s^z S^{z\phi} S^z + s^+ S^{+\phi} S^- + \mathrm{HC}) + h S^z \tag{5.2}$$

in which $s^z \in \mathbb{R}, s^+ = |s^+|e^{i\alpha} \in \mathbb{C}$ are the variational parameters, and $z = 2d$ is the lattice coordination number. The Hilbert space consists of the tensor product of two spin-$\frac{1}{2}$ representation spaces of $su(2)$, namely $\tilde{\mathcal{H}} \equiv \mathcal{H} \otimes \mathcal{H}$, where $\mathcal{H} = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}$ (the first factor is assumed to be the auxiliary-fermion sector on which the operators labelled with $\phi$ act in a non-trivial way). The basis vectors of $\tilde{\mathcal{H}}$ are enumerated as follows:

$$|1\rangle \equiv |\uparrow\rangle \otimes |\uparrow\rangle \qquad |2\rangle \equiv |\uparrow\rangle \otimes |\downarrow\rangle$$
$$|3\rangle \equiv |\downarrow\rangle \otimes |\uparrow\rangle \qquad |4\rangle \equiv |\downarrow\rangle \otimes |\downarrow\rangle. \tag{5.3}$$

In terms of these states the Hamiltonian (absorbing, for the time being, the overall factor $\frac{1}{4}zJ$ in the $s^\alpha$'s) (5.2) can be written as

$$H^\ell = \tfrac{1}{2}\,\text{diag}(-s^z + 2h, s^z - 2h, s^z + 2h, -s^z - 2h) - s^+|2\rangle\langle 3| - s^-|3\rangle\langle 2|. \tag{5.4}$$

From this expression it is clear that the dynamical algebra of the linearized model is given by the direct sum over the lattice sites of local algebras $\mathcal{A} = u(1) \oplus u(2) \oplus u(1)$, the two $u(1)$'s being, respectively, generated by the projectors over the fully polarized states $|1\rangle\langle 1|, |4\rangle\langle 4|$, whereas $u(2)$ is spanned by the operators

$$K^0 = \tfrac{1}{2}(|2\rangle\langle 2| + |3\rangle\langle 3|) \qquad K^+ \equiv e^{i\alpha}|2\rangle\langle 3|$$
$$K^- \equiv (K^+)^\dagger \qquad K^z \equiv \tfrac{1}{2}(|2\rangle\langle 2| - |3\rangle\langle 3|). \tag{5.5}$$

Since the $u(1)$ components are trivial, one has to diagonalize only the $u(2)$ contribution

$$H_{u(2)} = s^z K^0 - hK^z - |s^+|(K^+ + K^-). \tag{5.6}$$

This can be achieved, as in the previous section, with the rotation $U \equiv \exp(i\theta K^y) \in U(2)$, with angular parameter $\theta(|s^+|, h) = \tan^{-1}(2|s^+|/h)$. The spectrum and the eigenvectors are given by

$$E^D_\pm = -\frac{s^z}{2} \pm \frac{h}{2} \qquad E^S_\pm = \frac{s^z}{2} \pm \sqrt{|s^+|^2 + \frac{h^2}{4}} \tag{5.7}$$
$$|\psi^D_+\rangle = |1\rangle \qquad |\psi^D_-\rangle = |4\rangle$$
$$|\psi^S_+\rangle = -e^{i\alpha}\sin\frac{\theta}{2}|2\rangle + \cos\frac{\theta}{2}|3\rangle \qquad |\psi^S_-\rangle = \cos\frac{\theta}{2}|2\rangle + e^{-i\alpha}\sin\frac{\theta}{2}|3\rangle. \tag{5.8}$$

The self-consistency is implemented by means of the two constraints

$$\langle S^\dagger S^\phi\rangle = s^+\langle S^{\phi\dagger} S^\phi\rangle \qquad \langle S^z S^{z\phi}\rangle = s^z\langle S^{z\phi} S^{z\phi}\rangle \tag{5.9}$$

where

$$\langle\bullet\rangle \equiv \sum_{i=1}^{4} \frac{\langle\psi_i|\bullet|\psi_i\rangle}{\langle\psi_i|\psi_i\rangle} e^{\beta E^i}.$$

Explicit calculations show that equation (5.9) can be cast in the fixed-point form

$$|s^+| = \frac{N^+_h(s^+, s^z)}{D^+_h(s^+, s^z)} \qquad s^z = \frac{N^z_h(s^+, s^z)}{D^z_h(s^+, s^z)} \tag{5.10}$$

where

$$N^+_h(s^+, s^z) \equiv \sin\theta \sinh\left(\beta\left(\frac{h^2}{4} + |s^+|^2\right)^{1/2}\right)$$
$$N^z_h(s^+, s^z) \equiv e^{\beta s^z}\cosh\left(\beta\frac{h}{2}\right) - \cosh\left(\beta\left(\frac{h^2}{4} + |s^+|^2\right)^{1/2}\right)$$

$$D_h^+(s^+, s^z) \equiv \exp\left(-\beta\frac{h}{2}\right)\exp(\beta s^z) + \sin^2\frac{\theta}{2}\exp\left[\beta\left(\frac{h^2}{4}+|s^+|^2\right)^{1/2}\right] + \cos^2\frac{\theta}{2}\exp\left[-\beta\left(\frac{h^2}{4}+|s^+|^2\right)^{1/2}\right]$$

$$D_h^z(s^+, s^z) \equiv \cosh\left(\beta\frac{h}{2}\right)\mathrm{e}^{\beta s^z} + \cosh\left(\beta\left(\frac{h^2}{4}+|s^+|^2\right)^{1/2}\right) \tag{5.11}$$

with $\theta = \theta(|s^+|, h)$ given by (V). In the case of a vanishing external field (i.e. $\theta(|s^+|, 0) = \pi/2$) these equations reduce to

$$N_0^+(s^+, s^z) \equiv \sinh(\beta|s^+|) \qquad N_0^z(s^+, s^z) = \mathrm{e}^{\beta s^z} - \cosh(\beta|s^+|)$$
$$D_0^+(s^+, s^z) = D_0^z(s^+, s^z) = \mathrm{e}^{\beta s^z} + \cosh(\beta|s^+|). \tag{5.12}$$

We discuss this case in some detail. It is clear that the self-consistency equations admit (at least) three kinds of non-trivial solutions: (i) isotropic $s^z = |s^+|$, (ii) Ising-like $s^z \neq 0$, $s^+ \equiv 0$, (iii) $s^z = -|s^+|$, respectively labelled by $i = 1, 2, 3$. The system (5.10) can be reduced to a one-dimensional problem $x = F_i(x, \beta)$, $(i = 1, 2, 3)$, where $x$ denotes $s^z$ $(|s^+|)$. The function $x = f_i(\beta)$, solution of the latter problem, has an order-parameter-like behaviour: it is identically zero up to a critical $\beta_{ic}$, above which it has non-vanishing values that saturate for $\beta \to \infty$. The critical inverse temperature can be analytically determined by imposing $f_i$ to be singular at $\beta = \beta_c$; from the implict function theorem it follows that a sufficient condition is given by $\partial F_i(0, \beta_{ic})/\partial x = 0$. Explicit computations show that $\beta_{ic} = 2/J'$, for all $i$, $J' \equiv zJ/4$. The $f^i$'s have quite different critical behaviour. Let us first discuss the solutions (i) and (ii). The functions $F_i$ are given for $i = 1, 2$ by

$$F_1(x, \beta) = \frac{\sinh(J'\beta x)}{\mathrm{e}^{J'\beta x} + \cosh(J'\beta x)} \qquad F_2(x, \beta) = \frac{\mathrm{e}^{J'\beta x} - 1}{\mathrm{e}^{J'\beta x} + 1}. \tag{5.13}$$

Notice that the second one corresponds to a mean-field Ising system. For $\beta \to \beta_c^+$ we have

$$x_1(\beta) = C_1(\beta - \beta_c) \qquad x_2(\beta) = C_2(\beta - \beta_c)^{1/2}. \tag{5.14}$$

In both cases the ground state $|\Psi_0^i\rangle (i = 1, 2)$ is degenerate: for the isotropic solution, $i = 1$ we have the triplet $|\Psi_0^1\rangle = \{|1\rangle, |2\rangle, |4\rangle\}$, whereas for the Ising-like case ($i = 2$) one finds $|\Psi_0^2\rangle = \{|1\rangle, |4\rangle\}$. The corresponding eigenvalues are given by $E_0^1 = -J'/6$, $E_0^2 = -J'/2$, showing that phase 2 is energetically favourite. In the isotropic solution the self-consistent Hamiltonian commutes with the total spin operator $S = S_{\mathrm{phys}} + S_\phi$, and describes a paramagnetic phase in which the total spin does not point in any preferred direction. This can also be seen from the zero-temperature limit $x_1(\beta) \sim_{\beta\to\infty} \frac{1}{3}(1 - 4/3\mathrm{e}^{-2/3J'\beta})$. In the Ising-like case ($i = 2$) the $SU(2)$ symmetry is spontaneously broken, since $s^+ \equiv 0$ we have no contributions from the transverse spin degrees of freedom and we are left with an effective Ising coupling between the $z$-component of the spins. The asymptotic behaviour is now given by $x_2(\beta) \sim_{\beta\to\infty} 1 - 2\mathrm{e}^{-J'\beta}$. It is worth pointing out that we always have $\langle S^z\rangle = 0$, $(\sigma = \uparrow, \downarrow)$ meaning that our linearization scheme does not describe the ordered phases in terms of these expectation values, but by means of the correlations between the local spins ($f$-sector) and the background ($\phi$-sector). The solution $i = 3$ has a discontinuity at $\beta_{3c} < \beta_{1,2c}$ that leads to unphysical jumps in the thermodynamical potentials. However it should be noted that, since $s^z < 0$, this case corresponds to an effective anti-ferromagnetic coupling between the physical fermions and the auxiliary ones. In this situation the single-site approach is not expected to work in that it is strongly based on the hypothesis of unbroken translational invariance, and therefore the solution space has

to be limited *a priori* to the case $s_z > 0$, corresponding to $i = 1, 2$. From the relation $E(\beta) \equiv \langle H^\ell(\beta)\rangle = -J'/2[(s^z)^2 + 2(s^+)^2]$ follows $x_i(\beta) \sim \sqrt{-\langle H^\ell\rangle}$; this shows that the parameters $\{s^\alpha\}$, $(\alpha = +, z)$ can, in a sense, be considered as the order parameter being related to the expectation value of the exchange energy.

## 6. Hubbard model with correlated hopping

Let us consider the Hamiltonian for the Hubbard model with correlated hopping

$$H = -t \sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + X \sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} (n_{i-\sigma} + n_{j-\sigma})(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{6.1}$$

Upon imposing $t = X$ and introducing the projected fermions $Q_{i\sigma} \equiv (1 - n_{i-\sigma})c_{i\sigma}$, $\tilde{Q}_{i\sigma} \equiv n_{i-\sigma} c_{i\sigma}$, the kinetic term becomes

$$H_{\rm hop} = -t \sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} (Q^\dagger_{i\sigma} Q_{j\sigma} - \tilde{Q}^\dagger_{i\sigma} \tilde{Q}_{j\sigma} + \text{HC}) \tag{6.2}$$

whereas after the linearization the local Hamiltonian reads

$$H_\ell = -\frac{tz}{2} \sum_\sigma (q\, Q^\dagger_\sigma Q^\phi_\sigma - \tilde{q}\, \tilde{Q}^\dagger_\sigma \tilde{Q}^\phi_\sigma + \text{HC}) + U N_\ell. \tag{6.3}$$

Here $q = |q|e^{i\alpha} \tilde{q} = |\tilde{q}|e^{i\beta} \in \mathbb{C}$ and $N_\ell \equiv n_\uparrow n_\downarrow$. For this model the relevant Hilbert space is given by the full 16-dimensional tensor product $\mathcal{H} \equiv \mathcal{H} \otimes \mathcal{H}^\phi$. The linearized Hamiltonian has non-vanishing projections over the sub-spaces $\tilde{\mathcal{H}}^{(i)} \subset \tilde{\mathcal{H}}$, $i = 1, 2, 3, 4$. The action of $H^\ell$ is reducible thanks to the decoupling of the spin sectors; furthermore $H^{(2)}_\ell = U N^{(2)}_\ell$ is diagonal spanning a $u(1)$ dynamical sub-algebra. The whole dynamical algebra turns out to be

$$\mathcal{A} = u(2) \oplus u(2) \oplus u(1) \oplus u(2) \oplus u(2) \cong 4su(2) \oplus 5u(1) \tag{6.4}$$

where two $su(2)$'s are generated by the operators $\{Q^\dagger_\sigma Q^\phi_\sigma\}_{\sigma=\uparrow,\downarrow}$, the other two by $\{\tilde{Q}^\dagger_\sigma \tilde{Q}^\phi_\sigma\}_{\sigma=\uparrow,\downarrow}$. Now we give the projected Hamiltonian written in terms of the Fock basis of the $\tilde{\mathcal{H}}^{(i)}$ spaces of appendix A.

$$\begin{aligned}
&H^{(0)}_{\rm l} = 0 \qquad H^{(4)} = U|1\rangle\langle 1| \\
&H^{(1)}_{\rm l} = -\frac{tqz}{2}\,(|4\rangle\langle 1| + |3\rangle\langle 2| + \text{HC}) \qquad H^{(2)}_{\rm l} = U|6\rangle\langle 6| \\
&H^{(3)}_{\rm l} = -\frac{t\tilde{q}z}{2}\,(|2\rangle\langle 1| + |4\rangle\langle 3| + \text{HC}) + U\,(|4\rangle\langle 4| + |2\rangle\langle 2|) \\
&H^{(0)}_{\rm l} = U|1\rangle\langle 1|.
\end{aligned} \tag{6.5}$$

The present case can be obtained from the extended Hubbard model above, treated by imposing all the self-consistent parameters different from the $\{q_\sigma, \tilde{q}_\sigma\}_{\sigma=\uparrow,\downarrow}$ to be vanishing and the chemical potential and the magnetic field as well. The spectrum and the eigenvectors can therefore be immediately obtained from the results of section 3. Here we report only the form of the self-consistency equations (we set $zt/2 = 1$):

$$q = \frac{\langle Q^\dagger_\sigma Q^\phi_\sigma\rangle}{\langle Q^{\phi\dagger}_\sigma Q^\phi_\sigma\rangle} = \frac{N^q_U(q,\tilde{q})}{D^q_U(q,\tilde{q})} e^{i\alpha} \qquad \tilde{q} = \frac{\langle \tilde{Q}^\dagger_\sigma \tilde{Q}^\phi_\sigma\rangle}{\langle \tilde{Q}^{\phi\dagger}_\sigma \tilde{Q}^\phi_\sigma\rangle} = \frac{N^{\tilde{q}}_U(q,\tilde{q})}{D^{\tilde{q}}_U(q,\tilde{q})} e^{i\tilde{\alpha}} \tag{6.6}$$

where the following functions were defined:

$$N_U^q \equiv \sinh(\beta|q|) \qquad N_U^{\tilde{q}} = \mathrm{e}^{-\beta\frac{U}{2}} \sin\theta \sinh\left(\beta\left(|\tilde{q}|^2 + \frac{U^2}{4}\right)^{1/2}\right)$$

$$D_U^q \equiv 2 + \cosh(\beta|q|) + \mathrm{e}^{-\beta\frac{U}{2}}\left(\cos^2\frac{\theta}{2}\exp\left[\beta\left(|\tilde{q}|^2 + \frac{U^2}{4}\right)^{1/2}\right]\right.$$
$$\left. + \sin^2\frac{\theta}{2}\exp\left[-\beta\left(\frac{|\tilde{q}|^2 + U^2}{4}\right)^{1/2}\right]\right)$$

$$D_U^{\tilde{q}} \equiv 2\mathrm{e}^{-\beta U} + 2\exp[-\beta U/2]\left(\cos^2\frac{\theta}{2}\exp[\beta(|\tilde{q}|^2 + U^2/4)^{1/2}]\right.$$
$$\left. + \sin^2\frac{\theta}{2}\exp[-\beta(|\tilde{q}|^2 + U^2/4)^{1/2}]\right) \tag{6.7}$$

and $\theta \equiv \theta_\sigma^{(3)} = \tan^{-1}(2|\tilde{q}|/U)$. Following the same lines as in the case of the Heisenberg model one finds that for $U = 0$ ($\theta = \pi/2$) and half-filling, we have the solution $|q| = |\tilde{q}|$, with the Ising-like autoconsistency condition $|q| = \frac{1}{2}\tanh(\beta|q|/2)$ from whence it follows that $\beta_c = 4$ and the zero temperature limit $|q| \to \frac{1}{2}$. For the non-vanishing Hubbard parameter $U$ (or filling $n \neq 1$) the symmetry between the $\{q_\sigma\}$ and the $\{\tilde{q}_\sigma\}$, reflecting the hole–particle symmetry in $\tilde{\mathcal{H}}$ for $H_1$ is explictly broken.

## 7. Conclusions

In this paper we have proposed an approximate treatment for a general system of interacting spin-$\frac{1}{2}$ fermions over a $d$-dimensional lattice $\Lambda$. The point of view is that of strong on-site coupling in which the Coulomb repulsion has to be treated exactly. The non-local interactions are linearized with operator coefficients built as bilinears of an auxiliary local fermionic algebra representing, in an averaged way, the lattice neighbourhood of each site. The coupling constants between physical and auxilary fermions are the variational parameters of the theory. The local Hilbert space has to be extended in order to accommodate the auxiliary degrees of freedom, and the dynamics is confined in finite-dimensional sectors of such space. The extended Hubbard model has been used to exemplify our approach, since it contains all possible elementary number-conserving fermionic interactions. The dynamical algebra of the linearized model has the form $\mathcal{A}_\ell = 4u(1) \oplus 6u(2) \oplus u(4)$, each of the terms being associated with different classes of elementary processes. The spectrum can be determined in a simple algebraic way; moreover, if we impose the conservation of the number of doubly occupied sites, the $u(4)$ term splits into two $u(2)$ contributions associated with the spin and pseudo-spin interactions. Since this method allows a description of systems in which the nearest-neighbour Hamiltonian includes charge–charge, spin–spin and pair interactions, it extends, in a substantial way, the fermionic linearization scheme in its Clifford variables form, where only the pure electron hopping was considered. The self-consistency equations can be explicitly written down for $T \neq 0$. They have a fixed point form for a map $\Xi$ in an eight-dimensional manifold $\mathcal{M}$, parametrized by chemical potential, Hubbard repulsion, magnetic field and temperature. Strong nonlinearity and high dimensionality make the dynamical system defined by $\Xi$ unstable and careful numerical investigations are requested.

In conclusion we wish to emphasize the great generality of the method proposed. Our scheme is characterized by two main features: on the one hand, the Hilbert space of states

is doubled introducing auxiliary degrees of freedom in addition to the physical ones; on the other hand, the operators representing such new degrees of freedom are assumed to belong to an algebra isomorphic with that of the original dynamical variables. The latter construction, which has been adopted here and in [13–15] in a representation-dependent form, can be applied more generally to cases where the dynamics is given in terms of bilinears of the generators of some abstract algebra, without resorting explicitly to a background algebra of fermions or bosons. We therefore expect the method to be effective not only for local Lie–Hopf algebras but for deformed Hopf algebra ($q$-algebra) as well. Of course in these cases the linearized problem will typically lead to infinite-dimensional dynamical algebras for which the diagonalization is non-trivial. However the diagonalization is expected to be much simpler than in the original problem.

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## Appendix A

### *A.1 States*

We list hereafter the 16-dimensional basis of $\tilde{\mathcal{H}}$. $P_i^{(n_F)} \equiv |i\rangle_{n_F}\langle i|_{n_F}$ denotes the projector associated with the $i$th state of $\tilde{\mathcal{H}}^{(n_F)}$.

$n_F = 0$:

$$P_1^{(0)} = \prod_\sigma (1-n_\sigma)(1-n_\sigma^\phi). \tag{A1}$$

$n_F = 1$:

$$\begin{aligned}
P_1^{(1)} &= n_\uparrow^\phi (1-n_\downarrow^\phi)(1-n_\uparrow)(1-n_\downarrow)\\
P_2^{(1)} &= (1-n_\uparrow^\phi) n_\downarrow^\phi (1-n_\uparrow)(1-n_\downarrow)\\
P_3^{(1)} &= (1-n_\uparrow^\phi)(1-n_\downarrow^\phi) n_\downarrow (1-n_\uparrow)\\
P_4^{(1)} &= (1-n_\uparrow^\phi)(1-n_\downarrow^\phi)(1-n_\downarrow) n_\uparrow .
\end{aligned} \tag{A2}$$

$n_F = 2$:

$$\begin{aligned}
P_1^{(2)} &= n_\uparrow^\phi n_\downarrow^\phi (1-n_\uparrow)(1-n_\downarrow)\\
P_2^{(2)} &= n_\uparrow^\phi (1-n_\downarrow^\phi)(1-n_\uparrow) n_\downarrow\\
P_3^{(2)} &= n_\uparrow^\phi (1-n_\downarrow^\phi)(1-n_\downarrow) n_\uparrow\\
P_4^{(2)} &= (1-n_\uparrow^\phi) n_\downarrow^\phi n_\downarrow (1-n_\uparrow)\\
P_5^{(2)} &= (1-n_\uparrow^\phi) n_\downarrow^\phi (1-n_\downarrow) n_\uparrow\\
P_6^{(2)} &= (1-n_\uparrow^\phi)(1-n_\downarrow^\phi) n_\downarrow n_\uparrow .
\end{aligned} \tag{A3}$$

$n_F = 3$:

$$\begin{aligned}
P_1^{(3)} &= n_\uparrow^\phi n_\downarrow^\phi (1-n_\uparrow) n_\downarrow\\
P_2^{(3)} &= (1-n_\uparrow^\phi) n_\downarrow^\phi n_\uparrow n_\downarrow
\end{aligned}$$

$$P_3^{(3)} = n_\uparrow^\phi n_\downarrow^\phi (1-n_\downarrow) n_\uparrow$$
$$P_4^{(3)} = n_\uparrow^\phi (1-n_\downarrow^\phi) n_\downarrow n_\uparrow. \tag{A4}$$

$n_{\rm F} = 4$:

$$P_1^{(4)} = \prod_\sigma n_\sigma n_\sigma^\phi. \tag{A5}$$

Of course $\tilde{\mathcal{H}}^{(1)}$ and $\tilde{\mathcal{H}}^{(3)}$ are particle–hole conjugate ($\tilde{\mathcal{H}}^{(0)}$ and $\tilde{\mathcal{H}}^{(4)}$) whereas $\tilde{\mathcal{H}}^{(2)}$ is self-conjugate.

### *A.2 Operators*

We introduce the physical sector projectors

$$N_0^f = (1-n_\uparrow)(1-n_\downarrow) = P_1^{(0)} + P_1^{(1)} + P_2^{(1)} + P_1^{(2)}$$
$$N_\downarrow^f = (1-n_\uparrow) n_\downarrow = P_3^{(1)} + P_2^{(2)} + P_4^{(2)} + P_1^{(3)}$$
$$N_\uparrow^f = n_\uparrow (1-n_\downarrow) = P_4^{(1)} + P_3^{(2)} + P_5^{(2)} + P_3^{(3)}$$
$$N_\ell^f = n_\uparrow n_\downarrow = P_6^{(2)} + P_2^{(3)} + P_4^{(3)} + P_1^{(4)} \tag{A6}$$

and the operators $O_\alpha \in \mathrm{End}(\tilde{\mathcal{H}})$, $(\alpha = 1, \ldots, 12)$ acting in a non-trivial way on both the factors of the tensor product

$$O_{1,2} = Q_{\uparrow,\downarrow}^\dagger Q_{\uparrow,\downarrow}^\phi \qquad O_{3,4} = \tilde{Q}_{\uparrow,\downarrow}^\dagger \tilde{Q}_{\uparrow,\downarrow}^\phi$$
$$O_{5,6} = \tilde{Q}_{\uparrow,\downarrow}^\dagger Q_{\uparrow,\downarrow}^\phi \qquad O_{7,8} = Q_{\uparrow,\downarrow}^\dagger \tilde{Q}_{\uparrow,\downarrow}^\phi$$
$$O_9 = \eta^\dagger \eta^\phi \qquad O_{10} = S^\dagger S^\phi$$
$$O_{11} = \eta^z \eta^{z\phi} \qquad O_{12} = S^z S^{z\phi}. \tag{A7}$$

Projecting these operators $\tilde{\mathcal{H}}^{(n_{\rm F})}$ by means of the projectors $P^{(n_{\rm F})} = \sum_\alpha^{d_{\rm F}} P_\alpha^{(n_{\rm F})}$ (i.e. $O_j^{(n_{\rm F})} = P^{(n_{\rm F})} O_j P^{(n_{\rm F})}$), we get the non-vanishing components:

$$O_1^{(1)} = |4\rangle\langle 1| \qquad O_2^{(1)} = |3\rangle\langle 2|$$
$$O_3^{(3)} = -|2\rangle\langle 1| \qquad O_4^{(3)} = -|4\rangle\langle 3|$$
$$O_5^{(2)} = -|6\rangle\langle 2| \qquad O_6^{(2)} = |6\rangle\langle 5|$$
$$O_7^{(2)} = |5\rangle\langle 1| \qquad O_8^{(2)} = -|2\rangle\langle 1|$$
$$O_9^{(2)} = |6\rangle\langle 1| \qquad O_{10}^{(2)} = |5\rangle\langle 2|$$
$$O_{11}^{(0)} = \tfrac{1}{4}|1\rangle\langle 1| \qquad O_9^{(1)} = \tfrac{1}{4}|1\rangle\langle 1|$$
$$O_{11}^{(2)} = -\tfrac{1}{4}(|1\rangle\langle 1| + |6\rangle\langle 6|) \qquad O_{11}^{(4)} = \tfrac{1}{4}|1\rangle\langle 1|$$
$$O_{12}^{(2)} = \tfrac{1}{4}(|3\rangle\langle 3| + |4\rangle\langle 4| - |2\rangle\langle 2| - |5\rangle\langle 5|). \tag{A8}$$

We list the projectors on the auxiliary sector

$$N_\uparrow^\phi = P_1^{(1)} + P_2^{(2)} + P_3^{(2)} + P_4^{(3)}$$
$$N_\downarrow^\phi = P_2^{(1)} + P_4^{(2)} + P_5^{(2)} + P_2^{(3)}$$
$$N_\ell^\phi = P_1^{(2)} + P_1^{(3)} + P_1^{(4)} + P_3^{(3)}. \tag{A9}$$

The diagonal operators

$$(\eta^z)^2 = \tfrac{1}{4}(P_1^{(0)} + P_3^{(1)} + P_4^{(1)} + P_6^{(2)} + P_1^{(2)} + P_1^{(4)})$$
$$(S^z)^2 = \tfrac{1}{4}(P_1^{(1)} + P_2^{(1)} + P_2^{(2)} + P_3^{(2)} + P_4^{(2)} + P_5^{(2)} + P_3^{(3)} + P_4^{(3)}) \tag{A10}$$

are useful in the calculations.

**Appendix B**

The components of $\Xi\colon \mathbb{R}^8 \to \mathbb{R}^8$ are given by

$$\Xi_1 = \frac{\langle S^z S^{z\phi}\rangle}{\langle (S^{z\phi})^2\rangle} \qquad \Xi_2 = \frac{\langle S^\dagger S^\phi\rangle}{\langle N^\phi_\uparrow\rangle}$$
$$\Xi_3 = \frac{\langle \eta^z \eta^{z\phi}\rangle}{\langle (\eta^{z\phi})^2\rangle} \qquad \Xi_4 = \frac{\langle \eta^\dagger \eta^\phi\rangle}{\langle N^\phi_\ell\rangle}$$
$$\Xi_{5,6} = \frac{\langle Q_{\uparrow,\downarrow} Q^\phi_{\uparrow,\downarrow}\rangle}{\langle N^\phi_{\downarrow,\downarrow}\rangle} \qquad \Xi_{7,8} = \frac{\langle \tilde{Q}_{\uparrow,\downarrow} \tilde{Q}^\phi_{\uparrow,\downarrow}\rangle}{\langle N^\phi_\ell\rangle} \tag{B1}$$

where the quantities in brackets have the following explicit expressions ($\langle\bullet\rangle^{(i)}$ denotes $\mathrm{tr}\{\bullet\, \mathrm{e}^{-\beta H^{(i)}_\ell}\}$)

$$\langle N^\phi_\sigma\rangle^{(1)} = \cos^2\frac{\theta^{(1)}_\sigma}{2}\,\mathrm{e}^{-\beta E^{(1)}_{+\sigma}} + \sin^2\frac{\theta^{(1)}_\sigma}{2}\,\mathrm{e}^{-\beta E^{(1)}_{-\sigma}}$$
$$\langle N^\phi_\sigma\rangle^{(2)} = \cos^2\frac{\theta^{S}}{2}\,\mathrm{e}^{-\beta E^{S}_{+}} + \sin^2\frac{\theta^{S}}{2}\,\mathrm{e}^{-\beta E^{S}_{-}} + \mathrm{e}^{-\beta E^{D}_{\sigma}}$$
$$\langle N^\phi_\sigma\rangle^{(3)} = \cos^2\frac{\theta^{(3)}_{-\sigma}}{2}\,\mathrm{e}^{-\beta E^{(3)}_{-(-\sigma)}} + \sin^2\frac{\theta^{(3)}_{-\sigma}}{2}\,\mathrm{e}^{-\beta E^{(3)}_{+(-\sigma)}} \tag{B2}$$
$$\langle N^\phi_\ell\rangle = \langle N^\phi_\ell\rangle^{(2)} + \langle N^\phi_\ell\rangle^{(3)} + \langle N^\phi_\ell\rangle^{(4)}$$
$$\langle N^\phi_\ell\rangle^{(2)} = \cos^2\frac{\theta^{\eta}}{2}\,\mathrm{e}^{-\beta E^{\eta}_{+}} + \sin^2\frac{\theta^{\eta}}{2}\,\mathrm{e}^{-\beta E^{\eta}_{-}}$$
$$\langle N^\phi_\ell\rangle^{(3)} = \sum_\sigma \left(\cos^2\frac{\theta^{(3)}_\sigma}{2}\,\mathrm{e}^{-\beta E^{(3)}_{+\sigma}} + \sin^2\frac{\theta^{(3)}_\sigma}{2}\,\mathrm{e}^{-\beta E^{(3)}_{-\sigma}}\right)$$
$$\langle N^\phi_\ell\rangle^{(4)} = \mathrm{e}^{-\beta E^4} \tag{B3}$$

and (up to a phase factor)

$$\langle S^\dagger S^\phi\rangle^{(2)} = \sin\theta^S \mathrm{e}^{-\beta E^S_0}\sinh(\beta E^S_1)$$
$$\langle \eta^\dagger \eta^\phi\rangle^{(2)} = \sin\theta^\eta \mathrm{e}^{-\beta E^\eta_0}\sinh(\beta E^\eta_1)$$
$$\langle Q^\dagger_\sigma Q^\phi_\sigma\rangle^{(1)} = \sin\theta^{(1)}_\sigma \mathrm{e}^{-\beta E^{(1)}_{0\sigma}}\sinh(\beta E^{(1)}_{1\sigma})$$
$$\langle \tilde{Q}^\dagger_\sigma \tilde{Q}^\phi_\sigma\rangle^{(3)} = \sin\theta^{(3)}_\sigma \mathrm{e}^{-\beta E^{(3)}_{0\sigma}}\sinh(\beta E^{(3)}_{1\sigma}) \qquad (\sigma = \uparrow, \downarrow)$$
$$\langle S^z S^{z\phi}\rangle^{(2)} = \tfrac{1}{4}\left(\sum_\sigma \mathrm{e}^{-\beta E^D_\sigma} - \mathrm{e}^{-\beta E^S_+} - \mathrm{e}^{-\beta E^S_-}\right). \tag{B4}$$

Finally

$$\langle (\eta^{z\phi})^2\rangle^{(i)} = \langle \eta^z \eta^{z\phi}\rangle^{(0)} = \frac{\mathrm{e}^{-\beta E^{(i)}}}{4} \qquad (i = 0, 4)$$
$$\langle (\eta^{z\phi})^2\rangle^{(2)} = -\langle \eta^z \eta^{z\phi}\rangle^{(2)} = \tfrac{1}{4}\sum_{\alpha=\pm} \mathrm{e}^{-\beta E^\eta_\alpha}$$
$$\langle (\eta^{z\phi})^2\rangle^{(i)} = \langle (S^{z\phi})^2\rangle^{(i)} = \tfrac{1}{4}\sum_\sigma \left(\cos^2\frac{\theta^{(i)}}{2}\mathrm{e}^{-\beta E^{(i)}_{+\sigma}} + \sin^2\frac{\theta^{(i)}}{2}\mathrm{e}^{-\beta E^{(i)}_{-\sigma}}\right) \qquad (i = 1, 3)$$
$$\langle (S^{z\phi})^2\rangle^{(2)} = \tfrac{1}{4}\sum_{\alpha=\pm} \mathrm{e}^{-\beta E^S_a} + \tfrac{1}{4}\sum_\sigma \mathrm{e}^{-\beta E^D_\sigma}$$
$$\langle (\eta^{z\phi})^2\rangle^{(4)} = \langle \eta^z \eta^{z\phi}\rangle^{(4)} = \tfrac{1}{4}\mathrm{e}^{-\beta E^{(4)}}. \tag{B5}$$

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