

# Exact Functional Integration of Radial and Complex Slave-boson Fields : Thermodynamics and Dynamics of the Two-site Extended Hubbard Model

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The functional integral formulation of the Hubbard model when treated in its Kotliar-Ruckenstein representation in the radial gauge involves fermionic, as well as complex and radial slave boson fields. In order to improve on the understanding of the interplay of the three types of fields, and on the nature of the latter, we perform a comprehensive investigation of an exactly solvable two-site cluster, as it entails all pitfalls embodied in this approach. It is first shown that the exact partition function is recovered, even when incorporating in the calculation the square root factors that are at the heart of the representation, when suitably regularized. We show that using radial slave boson fields allows to overcome all hurdles following from the normal ordering procedure. We then demonstrate that this applies to the Green's function as well, and to the correlation functions of physical interest, thereby answering the criticisms raised by Schönhammer [K. Schönhammer, Phys. Rev. B **1990** 42, 2591]. In addition, the investigation generalizes the calculations to the Hubbard model extended by a non-local Coulomb interaction.

## 1 Introduction

Strongly correlated electrons on a lattice, as encountered in transition-metal oxides, occupy a prominent place among the most interesting and challenging topics of contemporary theoretical physics. This interest is largely fueled by the functionality-oriented properties these systems harbor, such as high- $T_c$  superconductivity (see, e.g., [1–3]), colossal magnetoresistance (see, e.g., [4–7]), transparent conducting oxides (see, e.g., [8]), high capacitance heterostructures [9] or large thermopower (see, e.g., [10–16]), to quote a few. Furthermore, strongly correlated transition-metal oxides comprise rare-earth free per-

manent magnets [17], materials for batteries [18–21], and multiferroics [22–24]. Moreover, a broad diversity of further interesting properties are exhibited by these systems. They involve correlation-driven metal-to-insulator transition at the first place, for instance in vanadium sesquioxide [25–27] or in hole-doped titanates [28], as well as a rich palette of ordered phases of, e.g., magnetic, charge, stripes, nematic and, above all, superconducting nature.

The Hubbard model is the simplest model Hamiltonian entailing a genuine competition between the kinetic energy of electrons hopping on a lattice and the Coulomb interaction energy simplified to its sole local component. Initially introduced, *inter alia*, to describe metallic magnetism [29–31], it regained an immense popularity after Anderson's proposal that the Hubbard model on the square lattice entails the key ingredients to high- $T_c$  superconductivity [32], which  $d$ -wave symmetry may hardly be grasped in a simple one-electron picture. As of today, considering longer-ranged interaction is receiving increasing attention [33–50] (see also [51] and references therein for a more complete list).

Strongly correlated electron systems pose challenges that have been tackled using slave-boson approaches in a number of fashions. They mostly back on Barnes' [52, 53] and Kotliar and Ruckenstein's (KR) [54] representations, as well as on their multiband and rotation invariant generalizations [55–60]. They all exhibit their own gauge symmetry group.

As regards Barnes' representation to the infinite- $U$  single-impurity Anderson model, it involves one doublet of fermions, one slave boson, and one time-independent constraint binding all three fields. It entails a  $U(1)$  gauge symmetry, that may be used to gauge away the phase of

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the slave boson. This, however, requires to introduce a time-dependent constraint field [61–63]. The argument was originally put forward in the continuum limit, but later, a path integral representation on discrete-time steps for the remaining radial slave boson together with the time-dependent constraint has been proposed by one of us [64]. It could be used to solve the Ising chain [64].

A deeper understanding of radial slave bosons was gained through an analysis of a toy model. It yielded the exact expectation value of the radial slave boson to be generically finite [65], as well as a way to exactly handle functional integrals involving constrained fermions and radial slave bosons. A further feature of radial slave bosons is related to the saddle-point approximation. When the latter is performed to a complex slave boson field, it is intimately tied to a Bose condensation, that is generally viewed as spurious. On the contrary, radial slave bosons are phase-stiff and do not Bose condense, as they are deprived of a phase degree of freedom. Accordingly, their saddle-point amplitude approximates their – generically finite – exact expectation value.

The KR representation [54], and related slave-boson representations [56–58], have first been set up to the investigation of the Hubbard model, and have then been extended to account for long-ranged density-density and spin-spin interactions [39]. Meanwhile, a whole range of valuable results have been obtained, primarily on the square lattice. More specifically, they have been applied to the Mott metal-to-insulator transition [66–68], then to the description of anti-ferromagnetic [69], spiral [70–73], striped [74–77] phases, and even to the competition between the latter two has been addressed [78]. In addition, spin-and-charge ordered phases of a half-filled extended Hubbard model, which may be suitable for resistive switching, were recently put forward [47]. Besides, it has been obtained that the spiral order continuously evolves to the ferromagnetic order in the large  $U$  regime ( $U \gtrsim 60t$ ) [73] so that it is unlikely to be realized experimentally. Consistently, in the two-band model, ferromagnetism was found as a possible groundstate in the doped Mott insulating regime [79], only. Yet, the ferromagnetic instability line may be brought down to the intermediate coupling regime in various ways. They involve adding a nearest-neighbor ferromagnetic exchange coupling [39] or a sufficiently large next-nearest-neighbor hopping amplitude [80], to quote a few. Going to the fcc lattice [81] results in the same effect.

The KR representation implies six auxiliary particles [54]. Two of them form a doublet of fermions, the remaining ones are bosons, and they are “enslaved” by three time-independent constraints. Ending a long-standing debate [69, 82–84], a consensus that the gauge symmetry

group reads  $U(1) \times U(1) \times U(1)$  has been reached [57, 85, 86]. Accordingly, the phase of three of the four slave bosons can be gauged away, with the counterpart that all three constraints become time-dependent constraint fields. Therefore one bosonic field remains as a complex one. It may be chosen to be the  $d$  field, which accounts for doubly occupied sites, or the  $e$  field, which accounts for empty sites. These two fields are at the first place associated with charge fluctuations, and one might wonder whether the charge fluctuation spectrum depends on this asymmetry, but it could be shown that this is not the case, at least when it is computed to one-loop order around the paramagnetic saddle-point [67, 87]. In this context this one-loop calculation was believed to coincide with the time-dependent Gutzwiller approximation (TDGA) until discrepancies between the two were put forward [67]. This motivated an extension of the TDGA to achieve agreement with the one-loop calculation [88].

A whole series of functional integral representations has been formulated for various correlated systems. They quite systematically make use of coherent states [89]. This also applies to the current auxiliary fermionic and complex bosonic fields, but not to the radial slave bosons for which the functional integral representation under study is established from the outset. By now, the received attention has been limited to the atomic limit [90], and the purpose of this work is to establish the handling of the delocalization of the electrons due to hopping. To that aim, we compute in this context the partition function and dynamical quantities of the extended Hubbard model on the two-site cluster, and we show that the exact results are recovered for all densities. Eventually, we furthermore demonstrate that the so-called Kotliar roots entering the kinetic energy may equally well be included in the calculation, provided a new regularization scheme is enforced, with the same result. We thereby generalize earlier works where all relevant slave-boson fields entered as radial fields [64, 65, 91].

The paper is organized as follows. In Section 2 we present the model and its representation in terms of KR slave bosons in the radial gauge. The functional integration of the latter is further detailed in Section 3. In order to validate the procedure and to illustrate the key features of the computation, the paper presents the evaluation of the partition function, of the physical electron Green's function, and of several thermal averages of quantities represented by radial slave bosons. The fermionic fields are integrated out in Section 4, where  $N$ -time products are introduced. The integration over the complex bosonic field is performed in Section 5, and the remaining ones in Section 6. The agreement between the so-computed thermal averages and the expressions derived from the

physical electron Hamiltonian is established in Section 7. Section 8 summarizes our work. The calculation of the pseudofermion Green's function is extensively presented in Appendix A, while the irregular contributions to the traces involved in the computation of thermal averages are explicitly handled in Appendix B.

## 2 The model and its Kotliar and Ruckenstein representation

We investigate the extended Hubbard model in an exactly soluble case, which is the two-site cluster. It reads

$$\mathcal{H} = \sum_{\sigma} \sum_{i=1}^2 \left( \varepsilon c_{\sigma,i}^{\dagger} c_{\sigma,i} - t c_{\sigma,i}^{\dagger} c_{\sigma,i-1} \right) + U \sum_{i=1}^2 c_{\uparrow,i}^{\dagger} c_{\uparrow,i} c_{\downarrow,i}^{\dagger} c_{\downarrow,i} + V \prod_{i=1}^2 \left( c_{\uparrow,i}^{\dagger} c_{\uparrow,i} + c_{\downarrow,i}^{\dagger} c_{\downarrow,i} \right), \quad (1)$$

and is made of the single-electron Hamiltonians for each of the spin projections ( $\sigma = \uparrow, \downarrow$ ), supplemented by the Coulomb interaction terms, with amplitude  $U$  on each site  $i$ , and  $V$  on the bond. The factor  $\varepsilon$  is the difference in energy between the orbital level and the chemical potential. In the hopping terms with amplitude  $t$ , we use the periodic boundary condition in order to shorten the notation.

The Kotliar and Ruckenstein (KR) representation [54] of this model involves one doublet of fermionic fields  $\{f_{\uparrow}, f_{\downarrow}\}$  and four bosonic fields  $\{e, p_{\uparrow}, p_{\downarrow}, d\}$ . The latter are tied to an empty site, single occupancy of the site with spin projection up or down, and double occupancy, respectively. This implies redundant degrees of freedom which have to be discarded. This is achieved by imposing the three constraints

$$e^{\dagger} e + \sum_{\sigma} p_{\sigma}^{\dagger} p_{\sigma} + d^{\dagger} d = 1 \quad (2a)$$

$$p_{\sigma}^{\dagger} p_{\sigma} + d^{\dagger} d = f_{\sigma}^{\dagger} f_{\sigma} \quad (\sigma = \uparrow, \downarrow) \quad (2b)$$

to be satisfied on each site, thereby enslaving the bosonic fields.

The Hamiltonian in the so enlarged Fock space is

$$\mathcal{H}_{\text{KR}} = \sum_{\sigma} \sum_{i=1}^2 \left( \varepsilon f_{\sigma,i}^{\dagger} f_{\sigma,i} - t f_{\sigma,i}^{\dagger} z_{\sigma,i}^{\dagger} z_{\sigma,i-1} f_{\sigma,i-1} \right) + U \sum_{i=1}^2 d_i^{\dagger} d_i + V \prod_{i=1}^2 \left( 2 - 2e_i^{\dagger} e_i - \sum_{\sigma} p_{\sigma,i}^{\dagger} p_{\sigma,i} \right) \quad (3)$$

where

$$z_{\sigma,i} = e_i^{\dagger} L_{\sigma,i} R_{\sigma,i} p_{\sigma,i} + p_{-\sigma,i}^{\dagger} L_{\sigma,i} R_{\sigma,i} d_i \quad (4)$$

is the occupancy change operator. The latter is renormalized by inverse square root factors

$$L_{\sigma,i} = \left( 1 - p_{\sigma,i}^{\dagger} p_{\sigma,i} - d_i^{\dagger} d_i \right)^{-\frac{1}{2}} \quad (5a)$$

$$R_{\sigma,i} = \left( 1 - e_i^{\dagger} e_i - p_{-\sigma,i}^{\dagger} p_{-\sigma,i} \right)^{-\frac{1}{2}} \quad (5b)$$

These so-called 'Kotliar roots' modify the saddle-point approximation so that it yields the Gutzwiller approximation result [54]. Furthermore, they act exactly as the identity operator within the physical subspace, as we show below. Yet, as emphasized by Schönhammer [92], their exact computation within the functional integral formalism poses a formidable challenge, as there was not any rigorous procedure to substitute these functions of boson operators in the Lagrangian by field expressions, after the Hamiltonian is written in the normal order form [93]. This step is usually neglected since, by doing so, the Gutzwiller approximation is recovered as a saddle-point, which is variationally controlled in the large-dimensionality limit [94–96]. The purpose of the present paper is then to remedy this loophole, and to show that the radial gauge KR representation, with a proper regularization scheme, allows to overcome these mathematical hurdles when exactly evaluating the Kotliar roots within the functional integrals.

In this formalism the physical constraints (2) are enforced by the three Lagrange multipliers  $\lambda_i$ , resp.  $\lambda_{\sigma,i}$ , associated to each site. At this stage it should be noted that the functional integral over the fermionic and bosonic fields cannot be performed right away. Indeed, in order to ensure convergence,  $\lambda_i$  has to be continued into the complex plane as

$$\tilde{\lambda}_i = \lambda_i - i\lambda_0 \quad (6)$$

with  $\lambda_0 > 0$  (or  $\lambda_0 + U > 0$  if  $U < 0$ ) so that the integration contour is shifted into the lower half-plane [64, 97, 98].

The expression of the Lagrangian in the Cartesian representation of the slave boson fields reads

$$\mathcal{L}^{(c)}(\tau) = \mathcal{L}_f^{(c)}(\tau) + \mathcal{L}_b^{(c)}(\tau). \quad (7)$$

It entails the dynamics of the auxiliary fermionic and bosonic fields, together with the constraints (2) specific to the KR setup. The fermionic contribution is quadratic in the fermion fields with

$$\mathcal{L}_f^{(c)}(\tau) = \sum_{\sigma} \sum_{i=1}^2 \left( f_{\sigma,i}^*(\tau) (\partial_{\tau} + \varepsilon + i\lambda_{\sigma,i}) f_{\sigma,i}(\tau) - t f_{\sigma,i}^*(\tau) z_{\sigma,i}^*(\tau) z_{\sigma,i-1}(\tau) f_{\sigma,i-1}(\tau) \right). \quad (8)$$

The remaining part

$$\begin{aligned} \mathcal{L}_b^{(c)}(\tau) = & \sum_{i=1}^2 \left( -i\tilde{\lambda}_i + e_i^*(\tau) (\partial_\tau + i\tilde{\lambda}_i) e_i(\tau) \right. \\ & + d_i^*(\tau) (\partial_\tau + U + i\tilde{\lambda}_i - i\lambda_{\uparrow,i} - i\lambda_{\downarrow,i}) d_i(\tau) \\ & + \sum_{\sigma} p_{\sigma,i}^*(\tau) (\partial_\tau + i\tilde{\lambda}_i - i\lambda_{\sigma,i}) p_{\sigma,i}(\tau) \Big) \\ & + V \prod_{i=1}^2 \left( 2 - 2e_i^*(\tau) e_i(\tau) - \sum_{\sigma} p_{\sigma,i}^*(\tau) p_{\sigma,i}(\tau) \right) \end{aligned} \quad (9)$$

is only composed with boson fields, up to the constant terms. And we get the partition function in the Cartesian gauge as

$$\begin{aligned} \mathcal{Z} = & \int_{-\pi/\beta}^{\pi/\beta} \prod_{i=1}^2 \left( \frac{\beta d\lambda_i}{2\pi} \prod_{\sigma} \frac{\beta d\lambda_{\sigma,i}}{2\pi} \right) \int \prod_{\sigma} D[f_{\sigma}, f_{\sigma}^*] \\ & \times \int D[e, e^*] D[d, d^*] \prod_{\sigma} D[p_{\sigma}, p_{\sigma}^*] e^{-\int_0^{\beta} d\tau \mathcal{L}^{(c)}(\tau)}. \end{aligned} \quad (10)$$

In this representation, the physical electron creation and annihilation operators are mapped onto auxiliary operators as

$$c_{\sigma,i} \mapsto z_{\sigma,i} f_{\sigma,i} \quad \text{and} \quad c_{\sigma,i}^{\dagger} \mapsto f_{\sigma,i}^{\dagger} z_{\sigma,i}^{\dagger}. \quad (11)$$

They properly anticommute provided the constraints (2) are satisfied. This representation of the physical electron operators is invariant under the gauge transformations

$$\begin{cases} f_{\sigma,i} \mapsto e^{-i\chi_{\sigma,i}} f_{\sigma,i} \\ e_i \mapsto e^{i\theta_i} e_i \\ p_{\sigma,i} \mapsto e^{i(\chi_{\sigma,i} + \theta_i)} p_{\sigma,i} \\ d_i \mapsto e^{i(\chi_{\uparrow,i} + \chi_{\downarrow,i} + \theta_i)} d_i. \end{cases} \quad (12)$$

The local gauge symmetry group is therefore  $U(1) \times U(1) \times U(1)$  on each site. The Lagrangian, Eq. (7), also possesses

this symmetry. Expressing the bosonic fields in amplitude and phase variables as

$$e_i(\tau) = \sqrt{R_{e,i}(\tau)} e^{i\theta_i(\tau)} \quad (13a)$$

$$p_{\sigma,i}(\tau) = \sqrt{R_{\sigma,i}(\tau)} e^{i(\chi_{\sigma,i}(\tau) + \theta_i(\tau))} \quad (13b)$$

allows to gauge away the phases of three of the four slave boson fields provided one introduces the three time-dependent Lagrange multipliers

$$\alpha_i(\tau) = \lambda_i + \partial_\tau \theta_i(\tau) \quad (14a)$$

$$\beta_{\sigma,i}(\tau) = \lambda_{\sigma,i} - \partial_\tau \chi_{\sigma,i}(\tau). \quad (14b)$$

Here the radial slave boson fields are implemented in the continuum limit following, e. g., Ref. [61–63]. Similar gauge symmetry groups have been identified in the spin rotation invariant representation [57] and in the case of the two-band model [99].

### 3 Functional integrals in the radial gauge

For the exact evaluation of the functional integrals, the representation in the radial gauge has to be set up on a discretized time mesh from the beginning. Moreover, the constraints now have to be satisfied at every time step. Extending the procedure introduced in Ref. [64] for Barnes' slave boson to the KR representation one may compute the thermal average  $\langle \mathbb{Q} \rangle$  of a quantity  $\mathbb{Q}$  as

$$\begin{aligned} \mathcal{Z} \langle \mathbb{Q} \rangle = & \lim_{\nu \rightarrow 0} \lim_{N \rightarrow \infty} \lim_{\eta \rightarrow 0^+} \left\{ \prod_{n=1}^N \prod_{i=1}^2 \left( \int_{-\eta}^{\eta} dR_{e,i,n} dR_{\uparrow,i,n} dR_{\downarrow,i,n} \int_{-\infty}^{\infty} \frac{\delta d\alpha_{i,n}}{2\pi} \frac{\delta d\beta_{\uparrow,i,n}}{2\pi} \frac{\delta d\beta_{\downarrow,i,n}}{2\pi} \int \frac{dd_{i,n} dd_{i,n}^*}{2\pi i} \int \prod_{\sigma} df_{\sigma,i,n} df_{\sigma,i,n}^* \right) \right. \\ & \left. \times Q e^{-S} \right\} \end{aligned} \quad (15)$$

where  $Q$  is its discrete-time representation, and the action reads

$$\begin{aligned} S = & \sum_{n=1}^N \left\{ \sum_{i=1}^2 \left[ \sum_{\sigma} f_{\sigma,i,n}^* \left( f_{\sigma,i,n} - e^{-\delta(\epsilon + i\beta_{\sigma,i,n})} f_{\sigma,i,n-1} + \delta t z_{\sigma,i,n}^* z_{\sigma,i-1,n-1} f_{\sigma,i-1,n-1} \right) - i\delta \tilde{\alpha}_{i,n} + i\delta \sum_{\sigma} (\tilde{\alpha}_{i,n} - \beta_{\sigma,i,n}) R_{\sigma,i,n} \right. \right. \\ & \left. \left. + i\delta \tilde{\alpha}_{i,n} R_{e,i,n} + d_{i,n}^* \left( d_{i,n} - e^{-\delta(U + i\tilde{\alpha}_{i,n} - i\beta_{\uparrow,i,n} - i\beta_{\downarrow,i,n})} d_{i,n-1} \right) \right] + \delta V \prod_{i=1}^2 \left( 2 - 2R_{e,i,n} - \sum_{\sigma} R_{\sigma,i,n} \right) \right\}. \end{aligned} \quad (16)$$

Here the integer  $N$  is the number of imaginary-time slices with duration

$$\delta = \frac{\beta}{N} \quad (17)$$

while  $\nu$  and  $\eta$  are regulators, the purposes of which will be explained below. The integral expression of the partition function  $\mathcal{Z}$  is obtained with  $\mathbb{Q} = Q = 1$ . Note that we have introduced the shorthand notation

$$\tilde{\alpha} \equiv \alpha - i\lambda_0. \quad (18)$$

As previously discussed, the functional integral has to be evaluated with  $\alpha$  replaced by  $(\alpha - i\lambda_0)$  with  $\lambda_0 > 0$ , in order to ensure convergence.

The functional integral Eq. (15) may be equivalently recast in the more suggestive formulation

$$\mathcal{Z}(\mathbb{Q}) = \lim_{\nu \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P}(\langle Q \rangle_{f_i, f_i, d}). \quad (19)$$

Here the operator  $\mathcal{P}$ , which will be detailed below, 'projects onto the physical subspace' the correlation  $\langle Q \rangle_{f_i, f_i, d}$  that is obtained as the thermal average of  $Q$  over the different configurations of the pseudofermion and  $d$ -boson fields within the enlarged Fock space: It discards all the contributions that do not comply with the constraints (2), while properly weighting the remaining ones.

The partition function may thus be computed as

$$\mathcal{Z} = \lim_{\nu \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P}(Z_{df}) \quad (20)$$

where the joint partition function  $Z_{df}$  of the  $d$  boson and the auxiliary fermions is evaluated as the functional integral

$$Z_{df} = \langle 1 \rangle_{f_i, f_i, d} \quad (21)$$

with

$$\langle \dots \rangle_{f_\sigma} \equiv \int \prod_{n=1}^N \prod_{i=1}^2 df_{\sigma, i, n} df_{\sigma, i, n}^* \dots e^{-S_\sigma}, \quad (22a)$$

$$\langle \dots \rangle_d \equiv \int \prod_{n=1}^N \prod_{i=1}^2 \frac{dd_{i, n} dd_{i, n}^*}{2\pi i} \dots e^{-S_d}, \quad (22b)$$

where  $S_\sigma$  and  $S_d$  are the terms in the action (16) that are quadratic in the variables  $f_{\sigma, i, n}$  and  $d_{i, n}$ , respectively.

The fermionic action  $S_f = S_\uparrow + S_\downarrow$  is the sum of the quadratic forms represented by the  $2N \times 2N$  matrix

$$[S_\sigma] = \begin{bmatrix} \mathbb{1}_2 & & & -[M_{\sigma, 1}] \\ [M_{\sigma, 2}] & \mathbb{1}_2 & & \\ & \ddots & \ddots & \\ & & [M_{\sigma, N}] & \mathbb{1}_2 \end{bmatrix} \quad (23)$$

within the basis  $\{f_{\sigma, 1, 1}, f_{\sigma, 2, 1}, \dots, f_{\sigma, 1, N}, f_{\sigma, 2, N}\}$  for each spin projection. Here  $\mathbb{1}_2$  is the  $2 \times 2$  identity matrix, and the block

$$[M_{\sigma, n}] = \begin{bmatrix} -L_{\sigma, 1, n} & T_{\sigma, 1, n} \\ T_{\sigma, 2, n} & -L_{\sigma, 2, n} \end{bmatrix} \quad (24)$$

involves

$$L_{\sigma, i, n} = e^{-\delta(\varepsilon + i\beta_{\sigma, i, n})} \quad (25a)$$

$$T_{\sigma, i, n} = \delta t z_{\sigma, i, n}^* z_{\sigma, i-1, n-1}. \quad (25b)$$

The representations in the radial gauge of the operators  $z_{\sigma, i}$  and  $z_{\sigma, i}^\dagger$  are, respectively,

$$z_{\sigma, i, n} = \frac{\sqrt{R_{e, i, n+1} R_{\sigma, i, n}} + \sqrt{R_{-\sigma, i, n+1}} d_{i, n}}{\sqrt{R_{e, i, n+1} + R_{-\sigma, i, n+1} - i\nu} \sqrt{1 - R_{e, i, n} - R_{-\sigma, i, n} + i\nu}} \\ z_{\sigma, i, n}^* = \frac{\sqrt{R_{\sigma, i, n+1} R_{e, i, n}} + d_{i, n}^* \sqrt{R_{-\sigma, i, n}}}{\sqrt{1 - R_{e, i, n+1} - R_{-\sigma, i, n+1} - i\nu} \sqrt{R_{e, i, n} + R_{-\sigma, i, n} + i\nu}} \quad (26)$$

where the radial variable  $R_{e, i, n}$  ( $R_{\sigma, i, n}$ ) corresponds to the squared amplitude of the complex  $e_{i, n}$  ( $p_{\sigma, i, n}$ ) bosonic field. First, note that  $z_{\sigma, i, n}^*$  is not the complex conjugate of  $z_{\sigma, i, n}$  as the time steps of radial variables are not the same. Second, the above expressions of the  $z$  factors differ from the usual ones. Indeed, we made use of the physical constraints (2) to replace the number of  $d$  bosons in the denominators by its counterpart in terms of radial slave-boson variables, which eases the evaluation of the functional integrals. The regulator  $\nu$  is taken to zero after performing the continuous-time limit  $N \rightarrow \infty$ . It is introduced in the discrete-time representation in order to take care of the vanishingly small contribution of spurious processes which appear when computing the partition function, as it ensures that the  $z$  factors are not singular in the physical subspace.

The part of the action  $S_d = S_{d_1} + S_{d_2}$  that is quadratic in the  $d$  boson field, is the sum of the contributions from each site

$$S_{d_i} = \sum_{m=1}^N \sum_{n=1}^N d_{i, m}^* [S_{d_i}]_{m, n} d_{i, n} \\ = \sum_{n=1}^N d_{i, n}^* (d_{i, n} - d_{i, n-1} e^{\delta(-U - i\tilde{\alpha}_{i, n} + i\beta_{\uparrow, i, n} + i\beta_{\downarrow, i, n})}) \quad (27)$$

where  $d_{i, 0} \equiv d_{i, N}$  in the second line to satisfy periodic boundary conditions in the imaginary time. When expanding the exponential in Eq. (27) to lowest order in  $\delta$ , the familiar form following from the Trotter-Suzuki decomposition is recovered. Yet, the latter may only be applied for bounded values of the Lagrange multipliers while



Eq. (27) is well behaved when integrating the multipliers along the real axis.

The remaining terms of the action are gathered in the integral operator

$$\mathcal{P} \equiv \prod_{n=1}^N \mathcal{P}_n \quad (28)$$

where

$$\mathcal{P}_n \equiv \int_{R_n} e^{-\delta V_n} \int_{\alpha \beta_n} e^{i \delta \sum_{i=1}^2 \left( \tilde{\alpha}_{i,n} (1 - R_{e,i,n} - \sum_{\sigma} R_{\sigma,i,n}) + \sum_{\sigma} \beta_{\sigma,i,n} R_{\sigma,i,n} \right)} \quad (29)$$

is defined with the non-local Coulomb potential

$$V_n = V \prod_{i=1}^2 (2 - 2R_{e,i,n} - R_{\uparrow,i,n} - R_{\downarrow,i,n}) \quad (30)$$

and the shorthand notations

$$\int_{R_n} \equiv \lim_{\eta \rightarrow 0^+} \int_{-\eta}^{\infty} \prod_{i=1}^2 \{ dR_{e,i,n} dR_{\uparrow,i,n} dR_{\downarrow,i,n} \}, \quad (31a)$$

$$\int_{\alpha \beta_n} \equiv \int_{-\infty}^{\infty} \prod_{i=1}^2 \left\{ \frac{\delta d\alpha_{i,n}}{2\pi} \frac{\delta d\beta_{\uparrow,i,n}}{2\pi} \frac{\delta d\beta_{\downarrow,i,n}}{2\pi} \right\}. \quad (31b)$$

Note that it takes an infinitesimal regulator  $-\eta$  for the integration bounds to have well defined delta functions enforcing the constraints.

The integration over the fields will be carried out in the following order. First, integrating the fields  $f_{\sigma}$  and  $d$  yields the joint partition function  $Z_{df}$  as a sum over all the discrete-time evolutions that are governed by the KR Hamiltonian (3). Note that at this stage, the dynamics is not restricted to the subspace of physical states. Then, we perform the integration over the Lagrange multipliers and the radial fields through the operator  $\mathcal{P}$ , Eq. (28). This removes the contributions of the unphysical trajectories in the evaluation of the partition function  $\mathcal{Z}$ , and it multiplies the physical ones by their respective weight factor associated with the non-local Coulomb interaction energy. The latter integrations are straightforward for static settings where no hopping can occur. The computation is more involved in the presence of hopping processes because the boson number distribution is modified on all relevant pairs of sites. The calculations prove that  $\mathcal{P}$  does filter out all irrelevant evolutions as intended, so that the remaining contributions yield the expected expression of the partition function in the continuous-time limit.

Other thermal averages may be integrated in the same fashion. The most similar computation certainly is evaluating a pure correlation of radial boson fields since for any function  $\mathcal{F}$  of only radial variables,

$$\langle \mathcal{F}(R_a, R_b, \dots) \rangle_{f_{\uparrow}, f_{\downarrow}, d} = \mathcal{F}(R_a, R_b, \dots) Z_{df}. \quad (32)$$

A whole range of static thermal averages and correlation functions may be expressed in terms of them. Let us focus here on the  $R_e$  field as an example, with the evaluation of the hole density  $\langle R_{e,1} \rangle$  on site 1 given by

$$\mathcal{Z} \langle R_{e,1} \rangle = \lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P} (R_{e,1,1} Z_{df}), \quad (33)$$

and of the auto-correlation function  $\langle R_{e,2}(\tau) R_{e,1}(0) \rangle$  given by

$$\mathcal{Z} \langle R_{e,2}(\tau) R_{e,1}(0) \rangle = \lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P} (R_{e,2,m} R_{e,1,1} Z_{df}) \quad (34)$$

where  $\lim_{N \rightarrow \infty} \left( \frac{m\beta}{N} \right) = \tau$ .

As an illustration for the evaluation of the temperature Green's function, the paper will describe the integration of only one electron propagator, which will then simply be noted  $\mathcal{G}$  for compactness. However, the presentation of the procedure is quite general, and all the key steps in the derivation of the Green's function are expounded. Below, we consider the auto-correlation associated with the creation of an electron with spin up on site 1 at imaginary time 0, followed by its annihilation on the same site at the imaginary-time variable  $\tau$ . It may be calculated as

$$\mathcal{Z} \mathcal{G} = - \lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P} \left( \left\langle z_{\uparrow,1,m} f_{\uparrow,1,m} f_{\uparrow,1,1}^* z_{\uparrow,1,1}^{\star} \right\rangle_{f_{\uparrow}, f_{\downarrow}, d} \right). \quad (35)$$

Thus, the computation of the partition function, expectation values and dynamical correlation functions bear strong similarities when they are expressed as functional integrals.

## 4 Integration over $f_{\sigma}$ fields : $N$ -time products

For the partition function, or a pure correlation of radial boson fields, integrating the fermion fields yields

$$Z_f = \langle 1 \rangle_{f_{\uparrow}, f_{\downarrow}} = \det[S_{\uparrow}] \times \det[S_{\downarrow}]. \quad (36)$$

Each determinant may be written as the trace of a time-ordered matrix product :

$$\det[S_{\sigma}] = \text{Tr}[U_{\sigma, N;1}]. \quad (37)$$

The product represents the imaginary-time evolution operator for  $f_{\sigma}$  pseudofermions between the time steps 1 and  $N$ , and it is defined, for  $n_f \geq n_i$ , as

$$\begin{aligned} [U_{\sigma, n_f; n_i}] &= \mathcal{T} \left\{ \prod_{n=n_i}^{n_f} [K_{\sigma, n}] \right\} \\ &= [K_{\sigma, n_f}] [K_{\sigma, n_f-1}] \cdots [K_{\sigma, n_i}] \end{aligned} \quad (38)$$

with

$$[K_{\sigma,n}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & L_{\sigma,1,n} & T_{\sigma,1,n} & 0 \\ 0 & T_{\sigma,2,n} & L_{\sigma,2,n} & 0 \\ 0 & 0 & 0 & L_{\sigma,1,n}L_{\sigma,2,n} \end{bmatrix}. \quad (39)$$

Please note that Eqs. (37)–(38) are equivalent to Eq. (30) in Ref. [65]. The three blocks in  $[K_{\sigma,n}]$  describe the dynamics of the states involving respectively zero, one, and two auxiliary fermions of spin projection  $\sigma$ . The entry  $L_{\sigma,i,n}$  is associated with a fermion  $f_{\sigma}$  staying still on site  $i$  at time step  $n$ , while  $T_{\sigma,i,n}$  corresponds to its hopping from site  $i-1$  onto site  $i$ .

The tensor product

$$[K_n] = [K_{\uparrow,n}] \otimes [K_{\downarrow,n}] \quad (40)$$

thus describes the dynamics of the total system of pseudofermions. And its partition function may be expanded as a sum over all multi-fermion state evolutions along a closed trajectory :

$$\begin{aligned} Z_f &= \text{Tr}[U_{\uparrow,N:1}] \times \text{Tr}[U_{\downarrow,N:1}] = \text{Tr}([U_{\uparrow,N:1}] \otimes [U_{\downarrow,N:1}]) \\ &= \text{Tr}\left(\mathcal{T} \left\{ \prod_{n=1}^N [K_n] \right\}\right). \end{aligned} \quad (41)$$

The different terms in the trace will be called  $N$ -time products. They are products of matrix elements representing the position of each pseudofermion at every time step. Note that, according to the structure of the matrices  $[K_{\sigma,n}]$ , an element  $L_{\sigma,i,n}$  or  $T_{\sigma,i,n}$  can only be followed by either  $L_{\sigma,i,n+1}$  or  $T_{\sigma,i+1,n+1}$ . Explicitly, the contributions to  $Z_f$  from the sectors with zero to four fermions are

$$\begin{cases} 0: 1 \\ 1: \text{Tr}\left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\uparrow} + \text{Tr}\left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\downarrow} \\ 2: [LL]_{\uparrow} + [LL]_{\downarrow} + \text{Tr}\left(\left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\uparrow} \otimes \left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\downarrow}\right) \\ 3: [LL]_{\uparrow} \text{Tr}\left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\downarrow} + [LL]_{\downarrow} \text{Tr}\left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\uparrow} \\ 4: [LL]_{\uparrow} [LL]_{\downarrow} \end{cases} \quad (42)$$

where the time-ordered matrix product

$$\left[\begin{smallmatrix} L & T \\ T & L \end{smallmatrix}\right]_{\sigma} \equiv \mathcal{T} \left\{ \prod_{n=1}^N \left[\begin{smallmatrix} L_{\sigma,1,n} & T_{\sigma,1,n} \\ T_{\sigma,2,n} & L_{\sigma,2,n} \end{smallmatrix}\right] \right\} \quad (43)$$

yields all the discrete-time evolutions of a single fermion with spin projection  $\sigma$ , while

$$[LL]_{\sigma} \equiv \prod_{n=1}^N L_{\sigma,1,n} L_{\sigma,2,n} \quad (44)$$

is the sole possibility for a pair of them.

As shown in Appendix A, the unnormalized correlation  $\langle z_{\uparrow,1,m} f_{\uparrow,1,m} f_{\uparrow,1,1}^* z_{\uparrow,1,1}^* \rangle_{f_{\uparrow}}$  may be computed as the trace of the matrix

$$[G_{\uparrow}] = z_{\uparrow,1,m} z_{\uparrow,1,1}^* [U_{\uparrow,N:m+1}] [F_1] [U_{\uparrow,m:2}] [F_1]^{\dagger} [K_{\uparrow,1}] \quad (45)$$

where

$$[F_1]^{\dagger} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad [F_1] = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (46)$$

enact the creation and annihilation, respectively, of a particle on site 1, within the basis  $\{|0\rangle, f_{\uparrow,1}^{\dagger}|0\rangle, f_{\uparrow,2}^{\dagger}|0\rangle, f_{\uparrow,1}^{\dagger}f_{\uparrow,2}^{\dagger}|0\rangle\}$ . Hence, the full integration over pseudofermion fields yields

$$G_f = \langle z_{\uparrow,1,m} f_{\uparrow,1,m} f_{\uparrow,1,1}^* z_{\uparrow,1,1}^* \rangle_{f_{\uparrow}, f_{\downarrow}} = \text{Tr}([G_{\uparrow}] \otimes [U_{\downarrow,N:1}]). \quad (47)$$

Similarly to  $Z_f$ , each  $N$ -time product here is a product of entries  $L_{\sigma,i,n}$  or  $T_{\sigma,i,n}$  describing the pseudofermion positions during an evolution. However, the number of matrix elements is not the same for every time step since an extra  $f_{\uparrow}$  particle is present between  $n=2$  and  $n=m$ . Furthermore, the product also includes the supplemental factor  $z_{\uparrow,1,1}^*$  associated with the addition of the latter, and the factor  $z_{\uparrow,1,m}$  for its removal. Besides, it always contains  $L_{\uparrow,1,m}$  or  $T_{\uparrow,1,m}$ , which reflects the fact that the particle is on site 1 when it is removed from the cluster. And conversely, there is not any entry  $L_{\uparrow,1,1}$  nor  $T_{\uparrow,1,1}$  because site 1 has to be free of  $f_{\uparrow}$  pseudofermion at the beginning.

Below, we coin an  $N$ -time product as regular if any factor  $z_{\sigma,i,n}$  within it is accompanied by the matrix element  $L_{\sigma,i,n}$ , and any  $z_{\sigma,i,n}^*$  is followed by  $L_{\sigma,i,n+1}$ . Since the hopping term  $T_{\sigma,i,n}$  contains  $z_{\sigma,i,n}^* z_{\sigma,i-1,n-1}$ , it has then to be immediately preceded by  $L_{\sigma,i-1,n-1}$  and succeeded by  $L_{\sigma,i,n+1}$ . In other words, a regular product does not possess any clustered factors  $T_{\sigma,i+1,n+1} T_{\sigma,i,n}$ , and it corresponds to an evolution during which there is not any successive hoppings of the same pseudofermion (note that the products with  $T_{\sigma,i,N}$  and  $T_{\sigma,i+1,1}$  on both extremities are irregular for the trace is invariant under a circular shift). The motive for the above definition is to ensure the inverse square roots in  $z$  factors are eventually valued to unity within physical  $N$ -time products. In this prospect,  $R_{e,i,n}$  and  $R_{-\sigma,i,n}$  have thus to vanish in  $z_{\sigma,i,n}$  when enforcing the constraints Eqs. 2. One can easily check that this requirement is fulfilled when an  $f_{\sigma}$  particle is on the site  $i$

at the time step  $n$ , which is equivalent to state the  $N$ -time product contains the factor  $L_{\sigma,i,n}$ . Besides,  $R_{e,1,n+1} = 1$  or  $R_{-\sigma,i,n+1} = 1$  must be satisfied as well. However, this is always the case because  $z_{\sigma,i,n}$  is associated with the removal of an  $f_{\sigma}$  pseudofermion from site  $i$ , so there is not any at the next time step. As for the factor  $z_{\sigma,i,n}^*$ , one needs that  $R_{e,i,n+1} = R_{-\sigma,i,n+1} = 0$  in physical evolutions, while  $R_{e,i,n} = 1$  or  $R_{-\sigma,i,n} = 1$ . The former property is enforced if and only if  $L_{\sigma,i,n+1}$  is present, while the latter is always satisfied since there cannot be more than one  $f_{\sigma}$  pseudofermion on each site, so  $z_{\sigma,i,n}^*$  and  $L_{\sigma,i,n}$  never appear together in the same  $N$ -time product.

## 5 Integration over the complex bosonic $d$ field

Akin to the fermionic ones the  $d$ -boson field couples the time steps through its dynamics. It furthermore enters  $Z_f$  and  $G_f$  through the factors  $z_{\sigma,i,n}$  and  $z_{\sigma,i,n}^*$  which are parts of the hopping terms. Hence, integrating their  $N$ -time products requires to evaluate weighted integrals of products with an equal number of factors  $d_i$  and  $d_i^*$  (the correlations of the other kinds of product vanish). Since  $d_1$  and  $d_2$  are not coupled, one only needs the partition function of the 'non-interacting'  $d_i$  boson

$$Z_{d_i} = \langle 1 \rangle_{d_i} \quad (48)$$

and its unnormalized  $k$ -particle correlations

$$G_{d_i}(m_1, \dots, m_k | n_1, \dots, n_k) = \langle d_{i,m_1} \cdots d_{i,m_k} d_{i,n_k}^* \cdots d_{i,n_1}^* \rangle_{d_i} \quad (49)$$

where

$$\langle \dots \rangle_{d_i} \equiv \int \prod_{n=1}^N \frac{dd_{i,n} dd_{i,n}^*}{2\pi i} \dots e^{-S_{d_i}}. \quad (50)$$

The first of the three physical constraints (2) imposes that the  $d$  boson is a hard core particle : On each site there is at most one  $d$  boson at a time. Therefore, most of the correlations will be canceled by the integral operator  $\mathcal{P}$  at the end of the evaluation, and the only relevant products are the ones where the creation and annihilation fields strictly alternate when time ordered.

The thermal averages are cast here in a form which is suitable for the computation with the operator  $\mathcal{P}$ . One obtains

$$Z_{d_i} = \det[S_{d_i}]^{-1} = (1 - \xi_i)^{-1} = \sum_{D_i=0}^{\infty} \xi_i^{D_i} \quad (51)$$

with

$$\xi_i = e^{-\beta U} \prod_{n=1}^N e^{i\delta(-\tilde{\alpha}_{i,n} + \beta_{\uparrow,i,n} + \beta_{\downarrow,i,n})}. \quad (52)$$

According to Wick's theorem [93], multi-particle correlations can be expressed in terms of single-particle ones, which are given by the elements of the inverse matrix  $[S_{d_i}^{-1}]$ . Explicitly,

$$G_{d_i}(m_1, \dots, n_k) = \sum_{s \in \mathfrak{S}_k} G_{d_i}^{(s)}(m_1, \dots, n_k) \quad (53)$$

where the sum runs over all complete contractions (multiplied by  $Z_{d_i}$ )

$$G_{d_i}^{(s)}(m_1, \dots, n_k) = Z_{d_i} [S_{d_i}^{-1}]_{m_{s(k)}, n_k} \cdots [S_{d_i}^{-1}]_{m_{s(1)}, n_1} \quad (54)$$

and

$$[S_{d_i}^{-1}]_{m,n} = \begin{cases} Z_{d_i} \prod_{q \in \llbracket n+1, m \rrbracket} e^{\delta(-U - i\tilde{\alpha}_{i,q} + i\beta_{\uparrow,i,q} + i\beta_{\downarrow,i,q})} & \text{if } m > n, \\ Z_{d_i} & \text{if } m = n, \\ Z_{d_i} \prod_{q \notin \llbracket m+1, n \rrbracket} e^{\delta(-U - i\tilde{\alpha}_{i,q} + i\beta_{\uparrow,i,q} + i\beta_{\downarrow,i,q})} & \text{if } m < n \end{cases} \quad (55)$$

with  $q \notin \llbracket m+1, n \rrbracket$  standing for  $q \in \llbracket 1, N \rrbracket \setminus \llbracket m+1, n \rrbracket$ . Using the equality

$$\begin{aligned} Z_{d_i}^{k+1} &= (1 - \xi_i)^{-(k+1)} = \frac{1}{k!} \frac{d^k}{d\xi_i^k} \left( \frac{1}{1 - \xi_i} \right) \\ &= \frac{1}{k!} \frac{d^k}{d\xi_i^k} \left( \sum_{D_i=0}^{\infty} \xi_i^{D_i} \right) = \sum_{D_i=0}^{\infty} \binom{D_i + k}{k} \xi_i^{D_i}, \end{aligned} \quad (56)$$

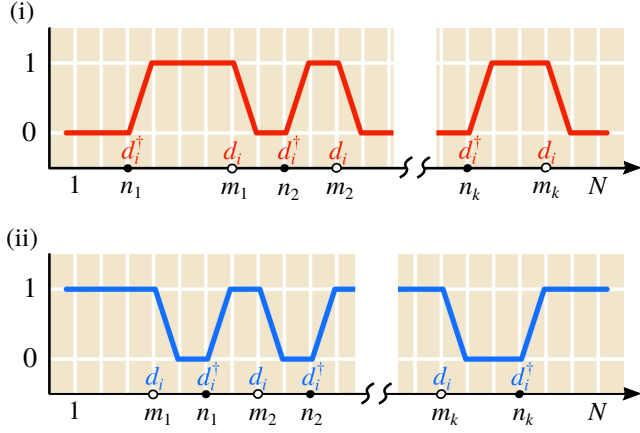
a complete contraction can then be cast into the generic form

$$\begin{aligned} G_{d_i}^{(s)}(m_1, \dots, n_k) &= \sum_{D_i=0}^{\infty} \binom{D_i + k}{k} \prod_{n=1}^N e^{\delta(D_i + D_n^{(s)})(-U - i\tilde{\alpha}_{i,n} + i\beta_{\uparrow,i,n} + i\beta_{\downarrow,i,n})} \end{aligned} \quad (57)$$

where  $D_n^{(s)}$  is written instead of the more rigorous notation  $D_n^{(s)}(m_1, \dots, n_k)$  in order to shorten expressions. By taking  $k = 0$  and  $D_n^{(s)} = 0$ , the expansion (51) of  $Z_{d_i}$  is recovered. Hence, any thermal average over the  $d_i$  field can be cast as a sum of terms of the form (57), and the latter will be used when discussing general properties of  $d$ -boson correlations.

As evidenced by the Coulomb amplitude  $U$ , the sum  $D_i + D_n^{(s)}$  corresponds to the number of  $d$  bosons on site  $i$  at time step  $n$  during the system evolution associated





**Figure 1** (Color online) Discrete-time variation of the double occupancy  $D_n^{(s)}$  in a complete contraction complying with the physical constraints (i) for the time step order  $n_1 < \dots < m_k$ , and (ii) for  $m_1 < \dots < n_k$ .

with that particular complete contraction. Note that  $D_i$  can take any integer value since the double occupancy is not restricted in the enlarged Fock space. However, the Lagrange multipliers promote the sum as the number of  $d$  bosons in the physical constraints (2). The latter equalities impose that  $D_i + D_n^{(s)} \leq 1$  so that the series in the generic form (57) actually stops at  $D_i = 0$  when the operator  $\mathcal{P}$  is applied on a  $k$ -particle correlation, and it is eventually discarded if  $D_n^{(s)} > 1$  at any time step.

Considering Eq. (55), one thus deduces that in a constraint-compliant complete contraction, there cannot be more than one single-particle correlation of the kind  $\langle d_{i,n}^* d_{i,m} \rangle$  with  $m < n$ . In this case,  $m$  is the smallest among the  $2k$  time steps and  $n$  the largest one. The other contractions are necessarily of the type  $\langle d_{i,m} d_{i,n}^* \rangle$  with  $m \geq n$ , and their time ranges do not overlap. Hence the hard-core nature of the boson imposes that creations and annihilations of  $d$  bosons must chronologically alternate in a non-vanishing correlation. If there is a time step  $n$  in the sequence at which both  $d_i$  and  $d_i^*$  are evaluated, the two corresponding complex variables must be gathered in the same contraction. Indeed, such instance can occur when calculating the thermal average of a product containing a pair  $T_{\sigma',i-1,n+1} T_{\sigma,i,n}$ . Following the dynamics of pseudofermions embodied by the matrices  $[K_{\sigma,n}]$  (Eq. (39)), no factor  $L_{\sigma,i,n}$  is then present at time step  $n$ : The  $f_\sigma$  particle does not stand on site  $i$  at the very instant of its hopping, so the site cannot be doubly occupied. Therefore,  $D_n^{(s)}$  must vanish in order to comply with physical constraints, which is possible only if the vari-

able  $d_{i,n}$  is contracted in a equal-time expectation value. As a result, in the Wick expansion of a non-vanishing  $k$ -particle correlation, only one complete contraction is relevant since the operator  $\mathcal{P}$  cancels all the other ones. This one is  $\prod_{j=1}^k [S_{d_i}^{-1}]_{m_j, n_j}$  for  $m_k \geq n_k \geq \dots \geq m_1 \geq n_1$ , and  $[S_{d_i}^{-1}]_{m_1, n_k} \prod_{j=1}^{k-1} [S_{d_i}^{-1}]_{m_{j+1}, n_j}$  for  $n_k \geq m_k \geq \dots \geq n_1 \geq m_1$  (see Fig. 1).

The remaining details of the  $d$ -field integration will be discussed in the next sections in conjunction with the filtering by  $\mathcal{P}$  of the joint correlations

$$Z_{df} = \langle Z_f \rangle_d \quad \text{and} \quad G_{df} = \langle G_f \rangle_d. \quad (58)$$

In short, the contributions to  $Z_{df}$  from the subspaces with zero to four fermions are

$$\begin{cases} 0: Z_{d_1} Z_{d_2} \\ 1: \langle \text{Tr} \left[ \begin{smallmatrix} L & T \\ T & L \end{smallmatrix} \right]_{\uparrow} \rangle_d + \langle \text{Tr} \left[ \begin{smallmatrix} L & T \\ T & L \end{smallmatrix} \right]_{\downarrow} \rangle_d \\ 2: ([LL]_{\uparrow} + [LL]_{\downarrow}) Z_{d_1} Z_{d_2} + \langle \text{Tr} \left( \left[ \begin{smallmatrix} L & T \\ T & L \end{smallmatrix} \right]_{\uparrow} \otimes \left[ \begin{smallmatrix} L & T \\ T & L \end{smallmatrix} \right]_{\downarrow} \right) \rangle_d \\ 3: [LL]_{\uparrow} \langle \text{Tr} \left[ \begin{smallmatrix} L & T \\ T & L \end{smallmatrix} \right]_{\downarrow} \rangle_d + [LL]_{\downarrow} \langle \text{Tr} \left[ \begin{smallmatrix} L & T \\ T & L \end{smallmatrix} \right]_{\uparrow} \rangle_d \\ 4: [LL]_{\uparrow} [LL]_{\downarrow} Z_{d_1} Z_{d_2} \end{cases} \quad (59)$$

The terms that contain the product  $Z_{d_1} Z_{d_2}$  result from static configurations. The other contributions, as well as the computation of  $G_{df}$ , involve higher-order correlations of the  $d$  field which are associated with fermion hoppings.

## 6 Integrations over radial slave-boson fields and constraints

The joint partition function  $Z_{df}$  and the joint Green's function  $G_{df}$  have been rewritten as sums over the different  $d$ -averaged  $N$ -time products describing all the discrete-time evolutions of  $f_\sigma$  pseudofermions and  $d$  bosons within the enlarged Fock space. Static contributions are just products of factors  $L_\sigma$  multiplied by  $Z_{d_1} Z_{d_2}$ , while dynamical  $N$ -time products contain higher-order correlations of  $d$  bosons, which are generated when accounting for fermion motion. Since any hopping process may be associated with four different sequences of boson number changes (see Eq. (26)), a  $d$ -averaged  $N$ -time product in  $Z_{df}$  with  $K$  hopping factors  $T_\sigma$  is a linear combination of  $4^K$  correlations  $G_{d_1} G_{d_2}$  ( $4^{K+1}$  in the case of  $G_{df}$ ). However, among the latter, only one corresponds to the physical variations of site occupancy that follow from the evolution of the pseudofermion distribution, and as shown below, the operator  $\mathcal{P}$  discards all the other ones.

In order to clarify how physical constraints are eventually enforced within the computation,  $d_i$ -boson correlations are expanded according to Wick's theorem as sums of expressions of the form (57). Lagrange multipliers then enter the complete contractions  $G_{d_i}^{(s)}$  (and  $Z_{d_i}$ ), as well as the integral operator  $\mathcal{P}$  and the matrix elements  $L_\sigma$ . As a result, they are gathered in the arguments of imaginary exponentials, which are the Fourier transforms of Dirac delta functions (noted  $\hat{\delta}$  below) implementing Eqs. (2) on every site and at every time step [90]. For each term  $G_{d_1}^{(s_1)} G_{d_2}^{(s_2)}$  of an  $N$ -time product, integrating out Lagrange multipliers yields the product of simple integrals

$$\int_{-\infty}^{\infty} \frac{\delta \alpha_{i,n}}{2\pi} e^{i\delta \alpha_{i,n} (1 - R_{e,i,n} - R_{\uparrow,i,n} - R_{\downarrow,i,n} - D_i - D_n^{(s_i)})} = \hat{\delta} (1 - R_{e,i,n} - R_{\uparrow,i,n} - R_{\downarrow,i,n} - D_i - D_n^{(s_i)}) \quad (60)$$

and

$$\int_{-\infty}^{\infty} \frac{\delta \beta_{\sigma,i,n}}{2\pi} e^{i\delta \beta_{\sigma,i,n} (D_i + D_n^{(s_i)} + R_{-\sigma,i,n} - F_{\sigma,i}(n))} = \hat{\delta} (D_i + D_n^{(s_i)} + R_{\sigma,i,n} - F_{\sigma,i}(n)) \quad (61)$$

where the number of  $f_\sigma$  fermions  $F_{\sigma,i}(n) = 1$  if the  $N$ -time product contains  $L_{\sigma,i,n}$ , and  $F_{\sigma,i}(n) = 0$  otherwise. Because radial boson fields are restricted to positive values, the delta functions unequivocally bind boson numbers to pseudofermion numbers. One thus deduces that when both  $L_{\uparrow,i,n}$  and  $L_{\downarrow,i,n}$  are present, the only finite boson value that is allowed on site  $i$  at time step  $n$  is the double occupancy  $D_i + D_n^{(s_i)} = 1$ . If there is one single factor  $L_{\sigma,i,n}$ , then  $R_{\sigma,i,n} = 1$ . And without any factor  $L_{\sigma,i,n}$ , the constraints imply that only the empty-site amplitude  $R_{e,i,n} = 1$  is of relevance.

As a consequence, the full integration of each  $N$ -time product sets the value of double occupancy at every time step, which will thereafter be noted  $D_i(n)$ . More specifically, for a static  $N$ -time product, the expansion (51) of the partition function  $Z_{d_i}$  is actually stripped down to one single term. The latter corresponds to the number  $D_i = 0$  for systems with zero or with two pseudofermions of equal spin orientations, and  $D_i = 1$  in the four-pseudofermion case. In the dynamical sector, the static evolution of a cluster with one single pseudofermion yields  $D_i = 0$ , while  $D_i = 1$  on the doubly occupied site and 0 on the other one when the system contains three pseudofermions or two with opposite spin projections. Moreover, for an  $N$ -time product that contains hopping factors, one can conclude that the operator  $\mathcal{P}$  discards all unphysical correlations  $G_{d_1} G_{d_2}$ . Indeed, the delta functions ensure that there is only one boson species at a time on each site. So at least one of the two radial-field values,  $R_{e,i-1,n}$  or  $R_{-\sigma,i-1,n}$ ,

entering the numerator of each factor  $z_{\sigma,i-1,n-1}$  eventually vanishes. Since the same holds true for  $z_{\sigma,i,n}^*$  as well, with  $R_{e,i,n}$  or  $R_{-\sigma,i,n}$ , every factor  $T_{\sigma,i,n}$  is then actually reduced to one of the four combinations of boson number changes. As a result, the final integration over radial fields does not keep more than one of the correlations. Furthermore, as discussed in the previous section, the operator  $\mathcal{P}$  refines the Wick expansion of the remaining one down to its sole complete contraction  $G_{d_1}^{(s_1)} G_{d_2}^{(s_2)}$  that respects the hard-core property of  $d$  bosons, with  $D_i = 0$  and  $D_{d_i}^{(s_i)} = D_i(n)$  in the expansion (57).

At last, since the contribution to the action from the  $V$ -potential depends only on radial boson fields, see Eq. (29), the delta functions ensure that each  $N$ -time product is correctly weighted with the physical value of the non-local Coulomb interaction energy at every time step.

As shown in Appendix B, the contributions to the thermal averages from irregular  $N$ -time products vanish in the limit  $N \rightarrow \infty$ . Hence only the results from the full integration of regular ones are of interest, and are summarized here.

We introduce the compact notation

$$(AB \cdots \otimes XY \cdots)_n \equiv A_{\uparrow,n} B_{\uparrow,n} \cdots X_{\downarrow,n} Y_{\downarrow,n} \cdots \quad (62)$$

for the product of all the matrix elements that occur at time step  $n$  in an  $N$ -time product. The effect of the integration over the  $d$  field, followed by the application of the integral operator  $\mathcal{P}$ , is to replace them according to the following mapping – for the configurations with zero to four pseudofermions :

$$\begin{aligned} 0 : (1 \otimes 1)_n &\mapsto 1 \\ 1 : (L_i \otimes 1)_n &\mapsto e^{-\delta \varepsilon} & (T_i \otimes 1)_n &\mapsto \delta t_v \\ 2 : (L_1 L_2 \otimes 1)_n &\mapsto e^{-\delta(2\varepsilon+V)} \\ (L_i \otimes L_i)_n &\mapsto e^{-\delta(2\varepsilon+U)} & (L_i \otimes L_{i-1})_n &\mapsto e^{-\delta(2\varepsilon+V)} \\ (T_i \otimes L_i)_n &\mapsto \delta t_v e^{-\delta \varepsilon} & (T_i \otimes L_{i-1})_n &\mapsto \delta t_v e^{-\delta \varepsilon} \\ (T_i \otimes T_i)_n &\mapsto 0 & (T_i \otimes T_{i-1})_n &\mapsto (\delta t_v)^2 \\ 3 : (L_i \otimes L_1 L_2)_n &\mapsto e^{-\delta(3\varepsilon+U+2V)} \\ (T_i \otimes L_1 L_2)_n &\mapsto \delta t_v e^{-\delta(2\varepsilon+V)} \\ 4 : (L_1 L_2 \otimes L_1 L_2)_n &\mapsto e^{-\delta(4\varepsilon+2U+4V)} \end{aligned} \quad (63)$$

with

$$t_v = \frac{t}{1 + v^2}. \quad (64)$$

Because of spin symmetry, the combinations obtained from inverting spin orientations result into the same values, so they have been omitted. These rules apply likewise

when computing the partition function  $\mathcal{Z}$  and the Green's function  $\mathcal{G}$ . However for the latter, there are also the extra  $z$  factors which are mapped as

$$z_{\uparrow,1,m} z_{\uparrow,1,1}^* \mapsto (1 + v^2)^{-1}. \quad (65)$$

For the calculation of a correlation  $\langle \mathcal{F}(R_a, R_b, \dots) \rangle$ , where the function is a product of only radial variables, the procedure is only slightly different from the above mapping. Indeed, each  $N$ -time product is now multiplied by the physical value of  $\mathcal{F}$  that follows from the evolution of pseudofermions. Since the final value is either 0 or 1, this has the effect to discard some of the  $N$ -time products. This may be implemented by nullifying the results of certain combinations from the above list, for the very time steps at which the radial fields are evaluated. For instance, when computing the hole density with the factor  $R_{e,1,1}$ , only the mapping for  $n = 1$  is modified. The affected combinations correspond to configurations with  $R_{e,1,1} = 0$ , i.e. with an occupied site 1, which now yield a vanishing factor: They are  $(L_1 \otimes 1)_1$ ,  $(L_1 L_2 \otimes 1)_1$ ,  $(L_1 \otimes L_1)_1$ ,  $(L_i \otimes L_{i-1})_1$ ,  $(T_i \otimes L_1)_1$ , all the products for three and four pseudofermions, and the corresponding ones obtained by flipping spin orientations. And for the computation of the correlation  $\langle R_{e,2,m} R_{e,1,1} \rangle$ , the list of nullified combinations is extended with the ones associated with an occupied site 2 at  $n = m$ : They are  $(L_2 \otimes 1)_m$ , and so on.

## 7 Recovering the results derived from the Hamiltonian formulation

At the beginning of the integral evaluation, time steps were intertwined, as illustrated by the expression of the hopping element  $T_{\sigma,i,n}$ , see Eqs. (25b) and (26). However, this is no longer the case once the computation with the operator  $\mathcal{P}$  is completed. Actually, the factors within the end value of every regular  $N$ -time product do not even depend on the time step, apart marginally at  $n = 1$  and  $n = m$  for the correlations in which these time steps play a particular role. The projection onto the physical subspace of a thermal average may thus be recast into a more compact form. And as shown below, in the continuous-time limit, the latter results in the same expression as the one directly derived from the Hamiltonian in the original physical Fock space. This demonstrates the validity of the integration procedure within the radial gauge formulation.

### 7.1 Partition function

Starting from the pseudo-fermion partition function  $Z_f$  given by Eq. (41), we have derived the corresponding joint correlation  $Z_{df}$  and its  $\mathcal{P}$ -projection. It contains both regular and irregular contributions. However, the latter do not contribute to the partition function in the continuous-time limit (see Appendix B), and by neglecting them, a simpler expression for the projection of the joint partition function is obtained as

$$\begin{aligned} \mathcal{P}(Z_{df}) &= \mathcal{P}(\langle \text{Tr}([U_{1,N:1}] \otimes [U_{1,N:1}]) \rangle_d) \\ &= \text{Tr}([\kappa]^N) + o(1). \end{aligned} \quad (66)$$

Here  $[\kappa]$  is the time-independent  $16 \times 16$  matrix that results from applying the mapping Eq. (63) on the infinitesimal-evolution matrix  $[K_{1,n}] \otimes [K_{1,n}]$  of the pseudofermion system. It reads to the first order in  $N^{-1}$ ,

$$[\kappa] = \mathbb{1}_{16} - \frac{\beta}{N} [H_v] + o\left(\frac{\mathbb{1}_{16}}{N}\right). \quad (67)$$

The mapping Eq. (63) allows us to work out the matrix elements of  $[H_v]$ . They turn out to be identical to the ones of the matrix  $[H]$  that represents the original Hamiltonian, Eq. (1), at the exception of the hopping amplitude which, here, reads  $t_v$  as given in Eq. (64), instead of  $t$ . At this point, the regulator  $v$  has played its role: It has allowed to handle the irregular contributions by rendering them finite, but it has no further impact on the final result when the limit  $v \rightarrow 0$  is taken. One can note that within a representation that does not include the Kotliar square roots, the exact same calculation would have resulted in the same expressions with  $t$  instead of  $t_v$ . Explicitly,

$$[H_v] = \begin{bmatrix} [H_v^{(\uparrow:0)}] & & & \\ & [H_v^{(\uparrow:1a)}] & [H_v^{(\uparrow:1b)}] & \\ & [H_v^{(\uparrow:1c)}] & [H_v^{(\uparrow:1d)}] & \\ & & & [H_v^{(\uparrow:2)}] \end{bmatrix} \quad (68)$$

where

$$[H_v^{(\uparrow:0)}] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon & -t_v & 0 \\ 0 & -t_v & \varepsilon & 0 \\ 0 & 0 & 0 & 2\varepsilon + V \end{bmatrix} \quad (69)$$

describes the dynamics of the states without any spin-up electron – the reader is reminded that  $\varepsilon$  stands for the difference in energy between the orbital level and the

chemical potential,

$$[H_v^{(\uparrow;1a)}] = \begin{bmatrix} \varepsilon & 0 & 0 & 0 \\ 0 & 2\varepsilon + U & -t_v & 0 \\ 0 & -t_v & 2\varepsilon + V & 0 \\ 0 & 0 & 0 & 3\varepsilon + U + 2V \end{bmatrix},$$

$$[H_v^{(\uparrow;1b)}] = [H_v^{(\uparrow;1c)}] = -t_v \mathbb{1}_4,$$

$$[H_v^{(\uparrow;1d)}] = \begin{bmatrix} \varepsilon & 0 & 0 & 0 \\ 0 & 2\varepsilon + V & -t_v & 0 \\ 0 & -t_v & 2\varepsilon + U & 0 \\ 0 & 0 & 0 & 3\varepsilon + U + 2V \end{bmatrix}, \quad (70)$$

represent the Hamiltonian of the states with one spin-up electron, and

$$[H_v^{(\uparrow;2)}] = \begin{bmatrix} 2\varepsilon + V & 0 & 0 & 0 \\ 0 & 3\varepsilon + U + 2V & -t_v & 0 \\ 0 & -t_v & 3\varepsilon + U + 2V & 0 \\ 0 & 0 & 0 & 4\varepsilon + 2U + 4V \end{bmatrix} \quad (71)$$

corresponds to the states with two spin-up electrons.

And using the expansion Eq. (67) of the matrix  $[\kappa]$ , the partition function is finally obtained as

$$\begin{aligned} \mathcal{Z} &= \lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P}(Z_{df}) = \lim_{v \rightarrow 0} \text{Tr} \left( \lim_{N \rightarrow \infty} [\kappa]^N \right) \\ &= \lim_{v \rightarrow 0} \text{Tr} \left( e^{-\beta(H_v)} \right) = \text{Tr} \left( e^{-\beta(H)} \right) \end{aligned} \quad (72)$$

with  $[H_{v=0}] = [H]$ .

## 7.2 Green's function

As with the evaluation of the partition function, the irregular contributions to the Green's function vanish in the continuous-time limit. Hence they can be neglected, and using the mapping Eq. (63), the projection of the joint Green's function  $G_{df}$  can be cast as

$$\begin{aligned} \mathcal{P}(G_{df}) &= \mathcal{P}(\langle \text{Tr}([G_\uparrow] \otimes [U_{\downarrow,N;1}]) \rangle_d) \\ &= \frac{1}{1+v^2} \text{Tr} \left( [\kappa]^{N-m} [F_{\uparrow,1}] [\kappa]^{m-1} [F_{\uparrow,1}]^\dagger [\kappa] \right) + o(1) \end{aligned} \quad (73)$$

where the matrices

$$[F_{\uparrow,1}]^\dagger = [F_1]^\dagger \otimes \mathbb{1}_4, \quad [F_{\uparrow,1}] = [F_1] \otimes \mathbb{1}_4 \quad (74)$$

represent the creation and the annihilation operators of a spin-up electron on site 1, respectively. Accordingly, we

finally obtain

$$\begin{aligned} \mathcal{ZG} &= -\lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P}(G_{df}) \\ &= -\text{Tr} \left( e^{-(\beta-\tau)[H]} [F_{\uparrow,1}] e^{-\tau[H]} [F_{\uparrow,1}]^\dagger \right), \end{aligned} \quad (75)$$

which is the expected result.

## 7.3 Thermal averages of radial slave boson fields : the example of the radial field $R_e$

The probability of site 1 to be empty at time step 1 follows from

$$\begin{aligned} \mathcal{P}(R_{e,1,1} Z_{df}) &= \mathcal{P}(R_{e,1,1} \langle \text{Tr}([U_{\uparrow,N;1}] \otimes [U_{\downarrow,N;1}]) \rangle_d) \\ &= \text{Tr} \left( [\kappa]^{N-1} [\kappa_{e_1}] \right) + o(1). \end{aligned} \quad (76)$$

Here  $[\kappa_{e_1}]$  is the matrix obtained from  $[\kappa]$  by nullifying the entries that correspond to the infinitesimal evolutions during which the site 1 is occupied. In the continuous-time limit, it takes the simpler form

$$[n_{e_1}]_{i,j} = \delta_{i,1} \delta_{j,1} + \delta_{i,3} \delta_{j,3} + \delta_{i,9} \delta_{j,9} + \delta_{i,11} \delta_{j,11} \quad (77)$$

which represents the hole-number operator on site 1. And the hole density on site 1 is then given by

$$\begin{aligned} \mathcal{Z} \langle R_{e,1} \rangle &= \lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P}(R_{e,1,1} Z_{df}) \\ &= \text{Tr} \left( e^{-\beta[H]} [n_{e_1}] \right) \end{aligned} \quad (78)$$

which vanishes when the system is fully filled, only. Hence, unlike complex bosonic fields, the exact averaged value of a radial slave boson field is generically finite, without being in conflict with Elitzur's theorem.

Introducing the matrix  $[\kappa_{e_2}]$  that is obtained from  $[\kappa]$  by nullifying the matrix elements associated with an occupied site 2, the regular part of the projection on the physical subspace

$$\begin{aligned} \mathcal{P}(R_{e,2,m} R_{e,1,1} Z_{df}) &= \mathcal{P}(R_{e,2,m} R_{e,1,1} \langle \text{Tr}([U_{\uparrow,N;1}] \otimes [U_{\downarrow,N;1}]) \rangle_d) \\ &= \text{Tr} \left( [\kappa]^{N-m} [\kappa_{e_2}] [\kappa]^{m-1} [\kappa_{e_1}] \right) + o(1). \end{aligned} \quad (79)$$

Since the continuous-time limit of  $[\kappa_{e_2}]$  is the matrix

$$[n_{e_2}]_{i,j} = \delta_{i,1} \delta_{j,1} + \delta_{i,2} \delta_{j,2} + \delta_{i,5} \delta_{j,5} + \delta_{i,6} \delta_{j,6} \quad (80)$$

of the hole-number operator on site 2,

$$\begin{aligned} \mathcal{Z} \langle R_{e,2}(\tau) R_{e,1}(0) \rangle &= \lim_{v \rightarrow 0} \lim_{N \rightarrow \infty} \mathcal{P}(R_{e,2,m} R_{e,1,1} Z_{df}) \\ &= \text{Tr} \left( e^{-(\beta-\tau)[H]} [n_{e_2}] e^{-\tau[H]} [n_{e_1}] \right), \end{aligned} \quad (81)$$

which is the expected result.

Our calculations performed in the radial gauge demonstrate that the Kotliar roots may be translated from their operator forms, Eq. (5), to the corresponding regularized expressions in terms of radial slave boson fields, Eq. (26). The radial representation allows to overcome the hurdle of the normal ordering procedure for the square roots. Thus, we have not only obtained the exact partition function, but also the correct Green's function as well as the proper correlation functions.

## 8 Summary and conclusion

Summarizing, we have tested the Kotliar and Ruckenstein slave-boson representation by thoroughly calculating exactly the functional integral formulation of thermodynamical and dynamical properties of the finite- $U$  extended Hubbard model on a two-site cluster. Our study is focused on the radial gauge, which is here shown to be free of redundant degrees of freedom. Our calculations demonstrate that the formulation (Eq. (15)), that has been set up from the outset, is faithful. In particular, it remedies the apparent shortcoming of the KR representation related to the normal ordering procedure. Indeed, accounting for it when the Kotliar roots are included in the calculation is a formidable task. Yet, our work shows that it is unnecessary as, starting from the original formulation [54], it is possible to rewrite the arguments of the roots in terms of radial slave bosons, only, without any loss of generality. This applies to the evaluation of the partition function, averaged values and correlation functions of radial slave-boson fields, and the electronic Green's function, to quote a few (see Sec. 7). We further obtained that the Kotliar roots need to be properly regularized within the discrete-time computation of the functional integrals (see Eq. (26)) to cope with otherwise singular values associated to multiple hopping processes occurring at consecutive time steps. We then showed that they are not numerous enough to yield a finite contribution to the expectation values in the continuous-time limit. Hence, this representation is well defined. Accordingly, the criticisms raised by Schönhammer [92] are answered, and, recalling that radial slave bosons do not undergo Bose condensation, the numerous works based on the saddle-point approximation are put on a firmer ground. Let us also emphasize that using radial slave bosons largely simplifies the handling of non-local interactions as they naturally arise as terms quadratic in the radial fields, akin to the Hubbard interaction. Furthermore, we do not expect further hurdles to appear when tackling larger clusters. One may

also perform the same calculations without introducing the Kotliar roots. In that case, no unexpected difficulty arises while the irregular contributions are not singular any longer, though the complex and dynamical  $d$  boson field keeps the calculation of the partition function far more complicated than in the  $U = \infty$  case. In that limit, all bosons are radial fields, which have no dynamics on their own. Regarding the extended Hubbard model, the present representation paves the way to better controlled calculations of charge fluctuations in the thermodynamic limit.

## A Pseudofermion Green's function

Standard results for Gaussian integrals over Grassmann variables [93] yield the correlation

$$\langle f_{\uparrow,1,m} f_{\uparrow,1,1}^* \rangle_{f_{\uparrow}} = [S_{\uparrow}^{-1}]_{2m-1,1} \det[S_{\uparrow}] \quad (82)$$

which is also equal to the minor  $\mathcal{M}_{1,2m-1}$  of  $[S_1]$  obtained by removing the first row and the  $(2m-1)$ -th column. In order to show the latter can be computed as  $\text{Tr}[G_1]/(z_{1,1,m}z_{1,1,1}^*)$  as well, it is first expressed with the help of the middle blocks  $[K_{1,n}^{(1)}]$  of the dynamics matrices  $[K_{1,n}]$ , see Eq. (39), instead of the blocks  $[M_{1,n}]$ . In the following, the spin subscript  $\uparrow$  will be omitted for compactness. Multiplying by  $-1$  its  $N$  rows and its  $N$  columns that contain the entries  $L_{2,n}$ , the minor can be evaluated as the determinant

$$\left| \begin{array}{cccccccc} & & & & & & & \overbrace{K_1^{(1)}} \\ 0 & 1 & & & & & & \\ \left[ -K_2^{(1)} \right] & \mathbb{1}_2 & & & & & & \\ & \ddots & \ddots & & & & & \\ & & \ddots & \ddots & & & & \\ & & & \mathbb{1}_2 & & & & \\ & & & \left[ -K_m^{(1)} \right] & & & & \\ & & & & 0 & & & \\ & & & & 1 & & & \\ & & & -K_{m+1}^{(1)} & & \mathbb{1}_2 & & \\ & & & & & \left[ -K_{m+2}^{(1)} \right] & \ddots & \\ & & & & & & \ddots & \\ & & & & & & & \ddots \\ & & & & & & & \left[ -K_N^{(1)} \right] \mathbb{1}_2 \end{array} \right| \quad (83)$$

where we have introduced the notations  $\overline{M}$ ,  $\underline{M}$ ,  $[M$ , and  $M]$  for the top row, the bottom row, the left column, and the right column of a  $2 \times 2$  matrix  $[M]$ , respectively.

The minor is then calculated by repeating the expansions according to the last two columns. The first iteration



yields

$$\mathcal{M}_{1,2m-1} = \mathcal{D}_{0,N>} - T_{2,1}\mathcal{D}_{1,N>} - L_{2,1}\mathcal{D}_{2,N>} \quad (84)$$

where the determinant  $\mathcal{D}_{0,N>}$  is

$$\begin{vmatrix} 0 & 1 & & & & \\ [-K_2^{(1)}] & \mathbb{1}_2 & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \mathbb{1}_2 & & \\ & & & [-K_m^{(1)}] & 0 & \\ & & & & 1 & \\ & & & & -K_{m+1}^{(1)} & \mathbb{1}_2 \\ & & & & & [K_{m+2}^{(1)}] & \ddots \\ & & & & & \ddots & \ddots \\ & & & & & & [-K_{N-1}^{(1)}] & \mathbb{1}_2 \end{vmatrix} \quad (85)$$

and, for  $n > m + 1$ , we define  $\mathcal{D}_{1,n>}$  as

$$\begin{vmatrix} [-K_2^{(1)}] & \mathbb{1}_2 & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \mathbb{1}_2 & & \\ & & & [-K_m^{(1)}] & 0 & \\ & & & & 1 & \\ & & & & -K_{m+1}^{(1)} & \mathbb{1}_2 \\ & & & & & [K_{m+2}^{(1)}] & \ddots \\ & & & & & \ddots & \ddots \\ & & & & & & [-K_{n-1}^{(1)}] & \mathbb{1}_2 \\ & & & & & & & [-K_n^{(1)}] \end{vmatrix} \quad (86)$$

while  $\mathcal{D}_{2,n>}$  has the same structure as  $\mathcal{D}_{1,n>}$ , except for its last row where  $[-K_n^{(1)}]$  is replaced by  $[-K_n^{(1)}]$ .

The first term  $\mathcal{D}_{0,N>}$  can be straight away simplified, thanks to the blocks  $\mathbb{1}_2$  on the right part of its diagonal. It is equal to the determinant  $\mathcal{D}_{1,m<}$ , which is defined as

$$\mathcal{D}_{1,n<} = \begin{vmatrix} 0 & 1 & & & \\ [-K_2^{(1)}] & \mathbb{1}_2 & & & \\ & \ddots & \ddots & & \\ & & & \mathbb{1}_2 & \\ & & & & [-K_{n-1}^{(1)}] & \mathbb{1}_2 \\ & & & & & [-K_n^{(1)}] \end{vmatrix} \quad (87)$$

for  $2 \leq n < m + 1$ . The latter follows the recursion relation

$$\begin{bmatrix} \mathcal{D}_{1,n<} \\ \mathcal{D}_{2,n<} \end{bmatrix} = \begin{bmatrix} L_{1,n} & T_{1,n} \\ T_{2,n} & L_{2,n} \end{bmatrix} \begin{bmatrix} \mathcal{D}_{1,n-1<} \\ \mathcal{D}_{2,n-1<} \end{bmatrix} = [K_n^{(1)}] \begin{bmatrix} \mathcal{D}_{1,n-1<} \\ \mathcal{D}_{2,n-1<} \end{bmatrix}$$

with  $\mathcal{D}_{2,n<}$  being identical to  $\mathcal{D}_{1,n<}$ , except for its last row where  $[-K_n^{(1)}]$  is replaced by  $[-K_n^{(1)}]$ . Since

$$\mathcal{D}_{1,2<} = \begin{vmatrix} 0 & 1 \\ [-K_2^{(1)}] \end{vmatrix} = L_{1,2} \quad \text{and} \quad \mathcal{D}_{2,2<} = \begin{vmatrix} 0 & 1 \\ -K_2^{(1)} \end{vmatrix} = T_{2,2}, \quad (89)$$

one then obtains

$$\mathcal{D}_{0,N>} = \begin{bmatrix} 1 & 0 \end{bmatrix} [K_m^{(1)}] [K_{m-1}^{(1)}] \dots [K_2^{(1)}] \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \quad (90)$$

The block-diagonal structure of the dynamics matrix  $[K_n]$  allows to readily verify that the previous expression can also be written as

$$\mathcal{D}_{0,N>} = [E_0][G][E_0]^\dagger / (z_{1,m} z_{1,1}^*) \quad (91)$$

where  $[E_0] = [1 \ 0 \ 0 \ 0]$  is the row vector of the zero-pseudofermion state.

Expanding the determinants  $\mathcal{D}_{1,n>}$  and  $\mathcal{D}_{2,n>}$  according to their last two columns yield the same recursion relation as the previously obtained one :

$$\begin{bmatrix} \mathcal{D}_{1,n>} \\ \mathcal{D}_{2,n>} \end{bmatrix} = [K_n^{(1)}] \begin{bmatrix} \mathcal{D}_{1,n-1>} \\ \mathcal{D}_{2,n-1>} \end{bmatrix}. \quad (92)$$

Hence

$$\begin{bmatrix} \mathcal{D}_{1,N>} \\ \mathcal{D}_{2,N>} \end{bmatrix} = [K_N^{(1)}] [K_{N-1}^{(1)}] \dots [K_{m+2}^{(1)}] \begin{bmatrix} -T_{1,m+1} \\ -L_{2,m+1} \end{bmatrix} \mathcal{D}_{3,m<} \quad (93)$$

with

$$\mathcal{D}_{3,m<} = \begin{vmatrix} [-K_2^{(1)}] & \mathbb{1}_2 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & \mathbb{1}_2 & \\ & & & & [-K_m^{(1)}] \end{vmatrix} = \prod_{n=2}^m L_{1,n} L_{2,n} \quad (94)$$

Here, we have omitted the terms  $T_{1,n} T_{2,n} = o(\frac{1}{N})$  that are in the factors  $\det(-[K_n^{(1)}])$  : Their total contribution vanishes in the continuous-time limit. It is then easy to check that

$$-T_{2,1}\mathcal{D}_{1,N>} = [E_1][G][E_1]^\dagger / (z_{1,m} z_{1,1}^*), \quad (95)$$

$$-L_{2,1}\mathcal{D}_{2,N>} = [E_2][G][E_2]^\dagger / (z_{1,m} z_{1,1}^*), \quad (96)$$

where  $[E_1] = [0 \ 1 \ 0 \ 0]$  and  $[E_2] = [0 \ 0 \ 1 \ 0]$  are the row vectors of the states with one pseudofermion on site 1 and on site 2, respectively.

And since

$$[E_3][G][E_3]^\dagger = 0 \quad (97)$$

with the row vector  $[E_3] = [0 \ 0 \ 0 \ 1]$  of the state with one pseudofermion on both sites, one can conclude that

$$\mathcal{M}_{1,2m-1} = \text{Tr}[G]/(z_{1,m}z_{1,1}^*). \quad (98)$$

## B Limit of irregular contributions

It is shown that the contribution from irregular products to the matrix representation of the evolution operator vanishes in the continuous-time limit. This can be understood by reasoning with a fixed number  $k$  of hopping factors while increasing  $N$  to infinity. One then finds that the number of irregular products with  $k$  hoppings does not grow fast enough to compensate the decreasing factor  $\delta^k = (\beta/N)^k$ , so that their sum tends to zero. However, since there is an infinite number of  $k$  values, adding all the vanishingly small contributions has to be performed with care.

First, let us prove the assertion when the infinitesimal evolution operator is represented by a  $p \times p$  matrix of the form

$$[\mathcal{K}] = [\mathcal{L}] + \frac{1}{N}[\mathcal{T}]. \quad (99)$$

Here  $[\mathcal{L}]$  is a diagonal matrix with its norm  $\|[\mathcal{L}]\| \leq 1$ , where the infinity norm of a matrix is defined as

$$\|[\mathcal{M}]\| = \max_{i,j} |[\mathcal{M}]_{i,j}|. \quad (100)$$

The hopping entries are  $O(1/N)$  and they are gathered, among others, in  $[\mathcal{T}]/N$ . The matrix  $[\mathcal{T}]$  is bounded with  $\|[\mathcal{T}]\| \leq r/p$ , where  $r$  is a positive constant. This is the case for the evolution matrix  $[\kappa]$  given by Eq. (67). And it is also true for the matrix

$$[\mathcal{K}_v] = \mathbb{1}_{16} + \frac{1}{N}[\mathcal{T}_v] \quad \text{with} \quad [\mathcal{T}_v]_{i,j} = \left| \frac{2\beta t}{v} \right|, \quad (101)$$

which will be used below to bound the irregular contributions to the thermal averages discussed in the manuscript.

The matrix of the evolution operator over a time range  $\tau \in ]0, \beta]$  is obtained as the limit of  $[\mathcal{K}]^m$  with the exponent  $m$  set as the integer part of  $\tau N/\beta$ . Expanding the power  $[\mathcal{K}]^m$  using expression (99) yields a sum of  $2^m$  different  $m$ -time products of matrices. Extending the definition introduced for a product of matrix elements, a matrix product is coined irregular when there are at least two adjacent factors  $[\mathcal{T}]$  (or at both ends of the product), and

regular otherwise. Noting the contributions to the expansion from regular and irregular terms as  $\text{Reg}([\mathcal{K}]^m)$  and  $\text{Irr}([\mathcal{K}]^m)$ , respectively, one has the obvious equality

$$\text{Irr}([\mathcal{K}]^m) = [\mathcal{K}]^m - \text{Reg}([\mathcal{K}]^m). \quad (102)$$

The definition ensures the irregular matrix products contain all the irregular  $m$ -time products of matrix entries. Actually, they also contain a part of the regular ones (e.g. regular products with alternating hoppings of different pseudofermions). However, the contribution from the latter to the evolution matrix can be neglected since, as it is shown below,  $\|\text{Irr}([\mathcal{K}]^m)\|$  vanishes when  $N \rightarrow \infty$ .

The total number of products with  $k$  factors  $[\mathcal{T}]$  is

$$a_{m,k} = \begin{cases} \binom{m}{k} & \text{if } 0 \leq k \leq m \\ 0 & \text{if } k > m, \end{cases} \quad (103)$$

and the number of regular ones is

$$b_{m,k} = \begin{cases} 1 & \text{if } k = 0 \\ \binom{m-k}{k} + \binom{m-k-1}{k-1} & \text{if } 1 \leq k \leq \frac{m}{2} \\ 0 & \text{if } k > \frac{m}{2}. \end{cases} \quad (104)$$

Indeed, for  $1 \leq k \leq \frac{m}{2}$ , there are  $\binom{m-k}{k}$  ones with  $[\mathcal{L}]$  at the right end, and  $\binom{m-k-1}{k-1}$  ones with  $[\mathcal{T}]$  at the right end: The ones with a factor  $[\mathcal{L}]$  on the right may be seen as sequences of  $m-k$  positions to be filled with  $k$  products  $[\mathcal{T}][\mathcal{L}]$  and  $m-2k$  factors  $[\mathcal{L}]$ , while the ones with a factor  $[\mathcal{T}]$  on the right may be seen as sequences composed of  $k-1$  products  $[\mathcal{T}][\mathcal{L}]$  and  $m-2k$  factors  $[\mathcal{L}]$ , sandwiched between  $[\mathcal{L}]$  and  $[\mathcal{T}]$ .

In order to prove that  $\text{Irr}([\mathcal{K}]^m)$  vanishes in the continuous-time limit, let us show that for any real number  $\epsilon > 0$ , there is a rank  $N_\epsilon$  above which  $\|\text{Irr}([\mathcal{K}]^m)\| \leq \epsilon$ .

First, since the norm of a product of two  $p \times p$  matrices verifies the inequality  $\|[A][B]\| \leq p\|[A]\|\|[B]\|$  in the general case, and  $\|[A][B]\| \leq \|[A]\|\|[B]\|$  when one of the matrices is diagonal, the norm of a product with  $k$  factors  $[\mathcal{T}]/N$  and  $m-k$  factors  $[\mathcal{L}]$  is smaller than  $(r/N)^k$ . Hence,

$$\|\text{Irr}([\mathcal{K}]^m)\| \leq \sum_{k=2}^m (a_{m,k} - b_{m,k}) \left(\frac{r}{N}\right)^k. \quad (105)$$

Then, for any integer  $n \geq 2$ ,

$$\begin{aligned} \|\text{Irr}([\mathcal{K}]^m)\| &\leq \sum_{k=2}^n (a_{m,k} - b_{m,k}) \left(\frac{r}{N}\right)^k + \sum_{k=n+1}^{\infty} a_{m,k} \left(\frac{r}{N}\right)^k \\ &\leq \sum_{k=2}^n (a_{m,k} - b_{m,k}) \left(\frac{r}{N}\right)^k + \sum_{k=n+1}^{\infty} \frac{r^k}{k!}. \end{aligned} \quad (106)$$

The infinite sum in the last line is the tail of the power series of  $e^r$ . Thus there exists an integer  $n_e$  such that if  $n \geq n_e$ , then the tail is smaller than  $\frac{\epsilon}{2}$ , and

$$\|\text{Irr}([\mathcal{K}]^m)\| \leq \sum_{k=2}^{n_e} (a_{m,k} - b_{m,k}) \left(\frac{r}{N}\right)^k + \frac{\epsilon}{2}. \quad (107)$$

Now, all the integers  $k$  on the right-hand side of the inequality are lower than the fixed value  $n_e$ , and the sum can be made as small as wished by increasing  $N$  (and so  $m$ , as well). Indeed, with  $m \geq 2n_e$ , all  $k$  values are smaller than  $m/2$ , and

$$0 \leq (a_{m,k} - b_{m,k}) \left(\frac{r}{N}\right)^k \leq \left( \binom{m}{k} - \binom{m-k}{k} \right) \left(\frac{r}{N}\right)^k \leq \frac{m^k - (m-k)^k}{N^k} \times \frac{r^k}{k!} \quad (108)$$

where  $n^k \equiv \frac{n!}{(n-k)!}$ . For a fixed integer  $k$ ,  $\frac{m^k}{N^k}$  and  $\frac{(m-k)^k}{N^k}$  converge to the same limit  $\tau^k$  when  $N \rightarrow \infty$ , so their difference vanishes. As a consequence, there exists an integer  $N_e > 2n_e \beta / \tau$  such that if  $N \geq N_e$ , then for all  $k \in \llbracket 2, n_e \rrbracket$ ,

$$0 \leq (a_{m,k} - b_{m,k}) \left(\frac{r}{N}\right)^k \leq \frac{\epsilon}{2} e^{-r} \times \frac{r^k}{k!}, \quad (109)$$

so that

$$\|\text{Irr}([\mathcal{K}]^m)\| \leq \frac{\epsilon}{2} e^{-r} \left( \sum_{k=2}^{n_e} \frac{r^k}{k!} \right) + \frac{\epsilon}{2} \leq \epsilon. \quad (110)$$

Hence, one can conclude that

$$\lim_{N \rightarrow \infty} \|\text{Irr}([\mathcal{K}]^m)\| = 0. \quad (111)$$

Now, Eq. (66) can be justified. First, in an irregular  $N$ -time product, there are consecutive time-steps at which a pseudofermion hops back and forth. For this kind of process, when the physical constraints are satisfied, the evaluation by  $\mathcal{P}$  of a  $z$  factor, Eq. (26), yields a term with module  $(|v|\sqrt{1+v^2})^{-1/2}$  or 0. In contrast, it yields  $(1+v^2)^{-1/2}$  when the hopping process is regular. So a hopping term  $T_{\sigma,i,n}$  results in a factor which may always be bounded by  $\beta t / (|v|N)$  when  $|v| < 1$ . As a result, the total irregular contribution to  $\mathcal{P}(Z_{df})$  is smaller in module than the trace of  $\text{Irr}([\mathcal{K}_v]^N)$ , with the matrix  $[\mathcal{K}_v]$  given by Eq. (101). Since the irregular parts of  $[\mathcal{K}_v]^N$  and of  $[\kappa]^N$  vanish in the continuous-time limit, their traces and the irregular contribution to  $\mathcal{P}(Z_{df})$  vanish as well, which proves Eq. (66).

Similarly, the total irregular contribution to  $\mathcal{P}(G_{df})$  may be dominated in module by the trace of the irregular part of the matrix product

$$[\mathcal{G}_v] = \frac{1}{|v|} [\mathcal{K}_v]^{N-m} [F_{\uparrow,1}] [\mathcal{K}_v]^{m-1} [F_{\uparrow,1}]^\dagger [\mathcal{K}_v] \quad (112)$$

which is

$$\begin{aligned} \text{Irr}[\mathcal{G}_v] &= \frac{1}{|v|} \left( \text{Irr}([\mathcal{K}_v]^{N-m}) [F_{\uparrow,1}] [\mathcal{K}_v]^{m-1} [F_{\uparrow,1}]^\dagger [\mathcal{K}_v] \right. \\ &\quad + [\mathcal{K}_v]^{N-m} [F_{\uparrow,1}] \text{Irr}([\mathcal{K}_v]^{m-1}) [F_{\uparrow,1}]^\dagger [\mathcal{K}_v] \\ &\quad + \text{Irr}([\mathcal{K}_v]^{N-m}) [F_{\uparrow,1}] \text{Irr}([\mathcal{K}_v]^{m-1}) [F_{\uparrow,1}]^\dagger [\mathcal{K}_v] \\ &\quad \left. + O\left(\frac{1}{N}\right) \right). \end{aligned} \quad (113)$$

Indeed, expanding the product  $[\mathcal{G}_v]$  by using Eq. (101) (without commuting the matrices nor simplifying the products of identity matrices), one finds that the majority of irregular  $(N+2)$ -time matrix products are the ones that contain at least a pair of adjacent factors  $[\mathcal{T}_v]$  either on the left or on the right of the factor  $[F_{\uparrow,1}]$ , or on both sides. The remaining irregular ones belong to the set of products with a factor  $[\mathcal{T}_v]$  adjacent to  $[F_{\uparrow,1}]$  or  $[F_{\uparrow,1}]^\dagger$ , or a pair of  $[\mathcal{T}_v]$  on both ends of the product. It is straightforward to show that their sum is  $O(N^{-1})$ . For the latter types, the sums of the irregular  $(N+2)$ -time products are :

- $\frac{1}{|v|N} [\mathcal{K}_v]^{N-m-1} [\mathcal{T}_v] [F_{\uparrow,1}] [\mathcal{K}_v]^{m-1} [F_{\uparrow,1}]^\dagger [\mathcal{K}_v]$ ,
- $\frac{1}{|v|N} [\mathcal{K}_v]^{N-m} [F_{\uparrow,1}] [\mathcal{T}_v] [\mathcal{K}_v]^{m-2} [F_{\uparrow,1}]^\dagger [\mathcal{K}_v]$ ,
- $\frac{1}{|v|N} [\mathcal{K}_v]^{N-m} [F_{\uparrow,1}] [\mathcal{K}_v]^{m-2} [\mathcal{T}_v] [F_{\uparrow,1}]^\dagger [\mathcal{K}_v]$ ,
- $\frac{1}{|v|N} [\mathcal{K}_v]^{N-m} [F_{\uparrow,1}] [\mathcal{K}_v]^{m-1} [F_{\uparrow,1}]^\dagger [\mathcal{T}_v]$ ,
- $\frac{1}{|v|N^2} [\mathcal{T}_v] [\mathcal{K}_v]^{N-m-1} [F_{\uparrow,1}] [\mathcal{K}_v]^{m-1} [F_{\uparrow,1}]^\dagger [\mathcal{T}_v]$ .

Since the matrix powers  $[\mathcal{K}_v]^{N-m}$  and  $[\mathcal{K}_v]^{m-1}$  converge while their irregular parts vanish, one can deduce that the matrix  $\text{Irr}[\mathcal{G}_v]$  vanishes in the continuous-time limit. And, using similar arguments, the same conclusion may be drawn for the irregular part of the matrix product

$$[\mathbf{G}] = \frac{1}{1+v^2} [\kappa]^{N-m} [F_{\uparrow,1}] [\kappa]^{m-2} [F_{\uparrow,1}]^\dagger [\kappa], \quad (114)$$

which completes the proof of Eq. (73). The demonstrations of Eq. (76) and Eq. (79) follow the same line of reasoning without further difficulties.

**Key words.** Hubbard Model, slave boson, radial gauge, normal order procedure, functional integration

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