Few-Particle Green's Functions for Strongly Correlated Systems on Infinite Lattices

Mona Berciu

Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada, V6T 1Z1

(Received 3 March 2011; published 7 December 2011)

We show how few-particle Green's functions can be calculated efficiently for models with nearest-neighbor hopping, for infinite lattices in any dimension. As an example, for one-dimensional spinless fermions with both nearest-neighbor and second-nearest-neighbor interactions, we investigate the ground states for up to 5 fermions. This allows us not only to find the stability region of various bound complexes, but also to infer the phase diagram at small but finite concentrations.

DOI: 10.1103/PhysRevLett.107.246403 PACS numbers: 71.10.Li, 31.15.ac, 71.35.Pq

Recently, there has been considerable interest in few-particle solutions of interacting Hamiltonians. For example, in Ref. [1] it was shown that knowledge of the two- and three-body solutions allows for quantitatively accurate predictions of finite-temperature thermodynamic quantities for many-body systems. As another example, in the context of atomic and molecular physics, the predicted universal three-body Efimov structures [2] have now been seen experimentally [3], giving new impetus to their study and work on various generalizations [4].

While the above work is for free space where particles have parabolic dispersions, there is equally strong interest in the lattice version of such few-body problems. For example, while stable excitons—bound pairs composed of an electron and a hole—appear in many materials, it is less clear when a so-called charged exciton or trion, consisting of two holes and one electron or vice versa, is stable. That this can happen has been recently demonstrated in GaAs quantum wells [5] and in carbon nanotubes [6]. (Note that trion theory is still mostly based on continuous models and variational solutions, e.g., see Ref. [7].) Studying bigger bound complexes, for example, biexciton pairs, is the next logical step.

Few-particle bound states are relevant not only for the materials where they appear, but also in the interpretation of certain spectroscopic data. For instance, the role played by bound two-particle states, leading to atomiclike multiplet structures in the Auger spectra of narrow band insulating oxides, is well established [8]. At low dopings, more complicated complexes may form and leave their fingerprints in various spectroscopic features. It is therefore useful to be able to study relatively easily few-particle solutions on an infinite lattice.

In this Letter we show that few-particle Green's functions can be calculated efficiently for strongly correlated lattice Hamiltonians in the thermodynamic limit, at least so long as the hopping involves only nearest-neighbor (NN) sites. For simplicity and to illustrate the technique and its usefulness, we focus here on a one-dimensional (1D) model of spinless fermions with nearest-neighbor and next-nearest-neighbor (NNN) interactions. However, the method generalizes straightforwardly to higher dimensions, longer (but finite) range interactions, mixtures of fermions (including spinful fermions) and/or bosons, etc. Such problems are of direct interest either in solid state physics or for cold atoms in optical lattices.

For two-fermion Green's functions ($N_f = 2$), our method is equivalent to that of Ref. [8] but is recast in a simpler form which allows, in 1D, for an analytical solution for any finite-range interaction. More importantly, it has a simple generalization for $N_f > 2$. We study cases with up to $N_f = 5$ and show that these suffice not only to sort out the stability of few-particle bound states, but also to infer the low density phase diagram.

Consider, then, spinless fermions on a 1D chain with $N \to \infty$ sites, described by the Hamiltonian

$$\mathcal{H} = -t\sum_i (c_i^\dagger c_{i+i} + \text{H.c.}) + U_1 \sum_i n_i n_{i+1} + U_2 \sum_i n_i n_{i+2},$$

where c_i removes a spinless fermion from site i located at $R_i = ia$ and $n_i = c_i^\dagger c_i$. Note that this 1D Hamiltonian is not integrable in the sense of having a Bethe ansatz solution. Because our solution is not linked in any way to such integrability, it can be generalized to higher dimensions, as already mentioned. To illustrate the main idea behind our solution, we discuss in some detail the solution for $N_f = 2$ fermions, after which we generalize to $N_f > 2$. Other possible generalizations, mentioned above, are discussed in the Supplemental Material [9].

Because the Hamiltonian is invariant to translations, the total momentum of the pair is a good quantum number. As a result, we work with the $N_f = 2$ states,

$$|k, n\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ik(R_i + na/2)} c_i^\dagger c_{i+n}^\dagger |0\rangle,$$

which describe fermions at a relative distance $n \geq 1$.

We define the two-particle Green's functions,

$$G(m, n; k, \omega) = \langle k, m | \hat{G}(\omega) | k, n \rangle,$$

where $\hat{G}(\omega) = [\omega + i\eta - \mathcal{H}]^{-1}$ with $\eta \to 0_+$ and we set $\hbar = 1$. From the Lehmann representation,

$$G(m, n; k, \omega) = \sum_{\alpha} \frac{\langle k, m|k, \alpha\rangle\langle k, \alpha|k, n\rangle}{\omega - E_{2,\alpha}(k) + i\eta},$$

where $\{|k, \alpha\rangle\}$ are the two-particle eigenstates with total momentum k, $\mathcal{H}|k, \alpha\rangle = E_{2,\alpha}(k)|k, \alpha\rangle$. Thus, this propagator allows us to find the $N_f = 2$ spectrum and also to get information about its eigenfunctions. Its Fourier transform $G(m, n; k, t) \propto \langle k, m| \exp(-i\mathcal{H}t)|k, n\rangle$ is the amplitude of probability that if initially the two particles (with total momentum k) are at a relative distance na, they will be at a relative distance ma after time t.

Matrix elements of the identity $1 = \hat{G}(\omega)(\omega + i\eta - \mathcal{H})$ lead to $\delta_{n,m} = (\omega + i\eta)G(m, n; k, \omega) - \langle k, m|\hat{G}(\omega)\mathcal{H}|k, n\rangle$. Since $\mathcal{H}|k, n\rangle = U(n)|k, n\rangle - f(k)[|k, n-1\rangle + |k, n+1\rangle]$, where $U(n) = U_1\delta_{n,1} + U_2\delta_{n,2}$ and $f(k) = 2t\cos\frac{ka}{2}$, we get a simple recurrence relation:

$$\delta_{n,m} = [\omega + i\eta - U(n)]G(m, n; k, \omega) + f(k) \times [G(m, n-1; k, \omega) + G(m, n+1; k, \omega)]. \quad (1)$$

This is trivial to solve for an infinite chain if one realizes that, for any m of interest, $G(m, n; k, \omega) \to 0$ as $n \to \infty$. This is obvious if ω is outside the free two-particle continuum where eigenstates, if any, are bound and therefore wave functions decay exponentially with n. It is also true inside the free two-particle continuum. Even though here the wave functions are plane waves, η defines an effective lifetime $\tau \sim 1/\eta$. As such, $G(m, n; k, t) \to 0$ if na is large compared to the typical distance that particles travel within τ. Thus, the recurrence relation can be solved starting from $G(m, M_c + 1; k, \omega) = 0$ for a sufficiently large cutoff M_c. Of course, the $N_f = 2$ case can be solved analytically exactly (see below). However, the idea can be used for $N_f > 2$ cases, where a numerical solution is needed. Noting that the few-particle Green's functions become arbitrarily small as a "relative distance" M (to be defined below) increases, the recurrence relations can be solved propagating the solution from a cutoff M_c towards small M. M_c is then increased until convergence is reached. The effects of η and M_c on the numerical solution are discussed in the Supplemental Material [9].

First, though, we complete the $N_f = 2$ discussion, which has an analytical solution (for details see [9]; we also show there how to deal with a finite-size system in this case). At the Brillouin zone (BZ) edge, since $f(k = \pi/a) = 0$ we find

$$G\left(1, n; \frac{\pi}{a}, \omega\right) = \frac{\delta_{n,1}}{\omega + i\eta - U_1},$$

as expected since $|\frac{\pi}{a}, 1\rangle$ is an eigenstate of $\mathcal{H}$ with energy U_1. For any $ka \neq \pi$, we find

$$G(1, 1; k, \omega) = \left[\omega + i\eta - U_1 - \frac{[f(k)]^2}{\omega + i\eta - U_2 + z(k, \omega)f(k)}\right]^{-1},$$

and for any $n \geq 2$,

$$G(1, n; k, \omega) = -\frac{[z(k, \omega)]^{n-1} f(k) G(1, 1; k, \omega)}{\omega + i\eta - U_2 + z(k, \omega)f(k)}.$$

Values for $m > 1$ can be obtained similarly. Here, $z(k, \omega)$ is the root of the characteristic equation of this recurrence relation, $(\omega + i\eta) + f(k)(z + \frac{1}{z}) = 0$, for which $|z(k, \omega)| < 1$ [9]. This shows that indeed $G(1, n; k, \omega) \to 0$ as $n \to \infty$. It is also easy to check that inside the free two-particle continuum, $|\omega| < 2f(k)$, we have $1 - |z(k, \omega)| \sim \eta$, so here G decays exponentially only because $\eta > 0$.

To study the two-particle spectrum, we plot the two-particle spectral weight, $A_2(k, \omega) = -\frac{1}{\pi}\,\mathrm{Im}G(1, 1; k, \omega)$, in Fig. 1 for $U_2 = 0$ and three values of U_1. By definition, $A_2(k, \omega)$ is finite at energies in the two-particle spectrum, and its value is related to the probability to find the fermions as NN in that eigenstate. If $U_1 = 0$, $A_2(k, \omega)$ is finite in the free two-particle continuum, ranging from $-4t$ to $4t$ if $k = 0$, while at $k = \pi/a$ only $\omega = 0$ is an eigenstate; hence, the δ function (Lorentzian) seen here. As an attractive U_1 is turned on, the $k = \pi/a$ peak tracks U_1, and a bound state is pulled below the continuum at nearby k values. For $U_1 > -2t$, this bound state exists only near the BZ edge, while near the Γ point the weak attraction shifts spectral weight to the bottom of the two-particle continuum but is not enough to push a discrete state below it. For $U_1 < -2t$, the bound state becomes the low-energy state at all k. This shows that, for certain ranges of parameters, bound pairs are only stable in some regions of the BZ, which moreover are not necessarily near $k = 0$. It would be interesting to investigate their effects on various response functions.

However, hereafter we focus on the $k = 0$ ground state (GS). Figure 2(a) shows whether in the GS the pair is bound or not, for $U_1 < 0$ and $U_2 > 0$. (Note that such

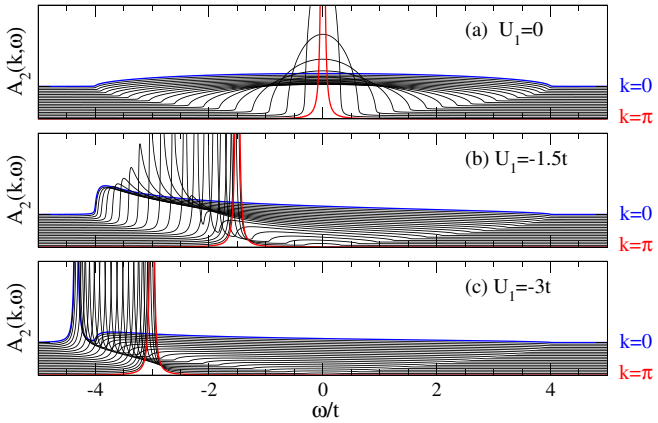

FIG. 1 (color online). $A_2(k, \omega)$ for $U_2 = 0$ and (a) $U_1 = 0$, (b) $U_1 = -1.5t$, and (c) $U_1 = -3t$. As the NN attraction is turned on, a bound state splits from the free two-particle continuum shown in (a). It exists at all momenta if $U_1 < -2t$, but only for large momenta if $U_1 > -2t$. Here $\eta = 0.01$.

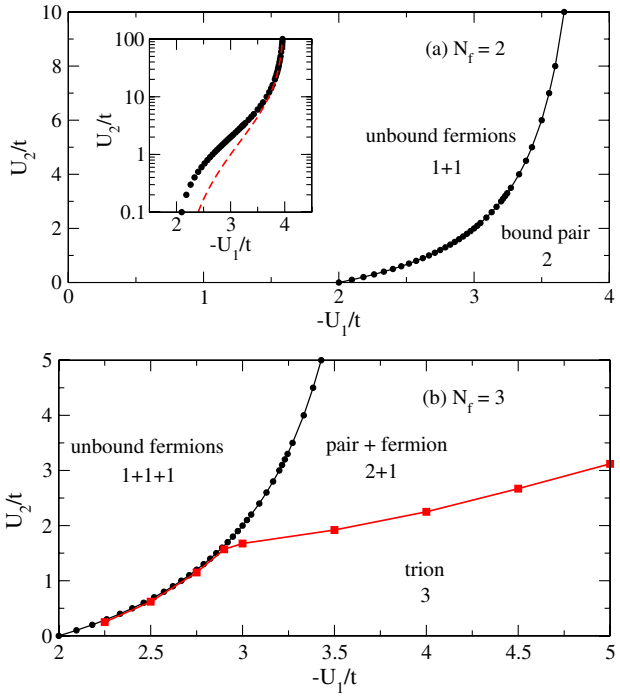

FIG. 2 (color online). Stability diagram for (a) $N_f = 2$ and (b) $N_f = 3$ fermion systems, indicating the nature of the GS. The inset in (a) shows that bound pairs are always stable if $U_1 < -4t$. The dashed line is a perturbational prediction.

interactions, attractive at short range and repulsive at longer range, appear in systems with highly polarizable ions [10].) For $U_1 < -4t$ a bound pair is always stable; even if it had infinite mass, a NN pair of energy U_1 is below the minimum energy of two free fermions, of $-4t$. Of course, the kinetic energy of the pair further enhances its stability region. The dashed line in the inset shows a perturbational estimate for $t \ll |U_1 - U_2|$ [9].

This $N_f = 2$ stability diagram, however, has no predictive power for what happens if more fermions are in the system. For example, if $N_f = 3$, we expect regions where the GS consists of 3 fermions, of a bound pair plus a fermion, or of a bound "trion." To identify these regions we study $N_f = 3$ Green's functions, by direct generalization of the $N_f = 2$ approach. Briefly, for any $n_1 \geq 1$, $n_2 \geq 1$, we define three-particle states,

$$|k, n_1, n_2\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} c^\dagger_{i-n_1} c^\dagger_i c^\dagger_{i+n_2} |0\rangle,$$

and three-particle Green's functions,

$$G(m_1, m_2; n_1, n_2; k, \omega) = \langle k, m_1, m_2 | \hat{G}(\omega) | k, n_1, n_2 \rangle.$$

Recurrence relations for these propagators are generated just as for the $N_f = 2$ case. If we define a "relative distance" $M = n_1 + n_2$, hopping of the outside fermions will link Green's functions with a given M to those with $M \pm 1$. If the central fermion hops, one of the n_1, n_2 values increases by one and the other decreases by one; therefore, M remains the same. Thus, the equation of motion links Green's functions with consecutive $M - 1, M, M + 1$ values, leading to recurrence relations that can be solved in terms of continued fractions of matrices, if we use the insight that propagators vanish as $M \to \infty$. Generalization to larger N_f values is now straightforward [9].

In higher dimension, we need to combine the "relative distance" with the "Manhattan distance" [11]. For example, in 2D for $N_f = 3$, we associate the plane wave with the coordinates i_x and i_y of the "central" particle for that axis. The other particles' coordinates are $i_x - n_{1,x}, i_x + n_{2,x}$, respectively, $i_y - n_{1,y}, i_y + n_{2,y}$, where $n_{i,\alpha} \geq 0$, $i = 1, 2$, $\alpha = x, y$. If we choose $M = \sum_{i,\alpha} n_{i,\alpha}$ then NN hopping links together only Green's functions with $M - 1, M, M + 1$. Thus, m particles in 2D are computationally similar to $2m - 1$ particles in 1D. In both cases, $2(m - 1)$ positive integers specify the relative positions, and M is their sum. The key observation is that the equations of motion still group into recurrence relations linking only quantities with $M - 1, M, M + 1$, allowing for an efficient solution (for more details, see [9]).

To study the spectrum of the $N_f = 3$, 1D system, we plot $A_3(k, \omega) = -\frac{1}{\pi} \mathrm{Im} G(1, 1; 1, 1; k, \omega)$. This must have finite spectral weight for $\omega \geq E_{2,\mathrm{GS}} - 2t$, corresponding to a continuum of states describing a fermion far away from a pair. (If $E_{2,\mathrm{GS}} = -4t$, this continuum starts at $-6t$ and describes 3 free fermions.) If the continuum is the lowest spectral feature, then the GS is either a pair + fermion or three fermions, mirroring the $N_f = 2$ situation. However, if a discrete state appears below this continuum, then the GS is a stable bound trion [9]. The stability diagram is plotted in Fig. 2(b) and shows a region where trions are stable, at large attractive U_1 and weak repulsive U_2. This is expected since binding a 3rd fermion to a stable pair lowers its energy by roughly $U_1 + U_2$, while a free fermion can lower the total energy by at most $-2t$.

The fact that stable trions are found for $N_f = 3$ does not, however, guarantee that they appear at finite concentrations. Just as the pair + fermion is unstable to trion formation, trions may be unstable to bigger bound complexes, if more particles are present. Indeed, a study of cases with $N_f = 4$ and 5 fermions proves that trions are actually unstable. This is shown in Fig. 3(a) where we plot the energy of the $N_f = 5$ GS versus U_2 (line marked "5") at $U_1 = -3.5t$. The other lines show energies where a continuum could appear, e.g., $E_{2+2+1} = 2E_{2,\mathrm{GS}} - 2t$ is the lowest energy of two pairs plus a fermion, $E_{2+3} = E_{2,\mathrm{GS}} + E_{3,\mathrm{GS}}$ is the lowest energy for a pair plus a trion, etc. The arrows indicate various dissociations. Arrow 1 shows when a pair becomes more stable than 2 fermions ($E_{2+1+1+1} < E_{1+1+1+1+1}$), while arrow 2 shows when a trion becomes more stable than a pair + fermion ($E_{3+1+1} < E_{2+1+1+1}$); see Figs. 2(a) and 2(b). A trion + fermion is unstable to

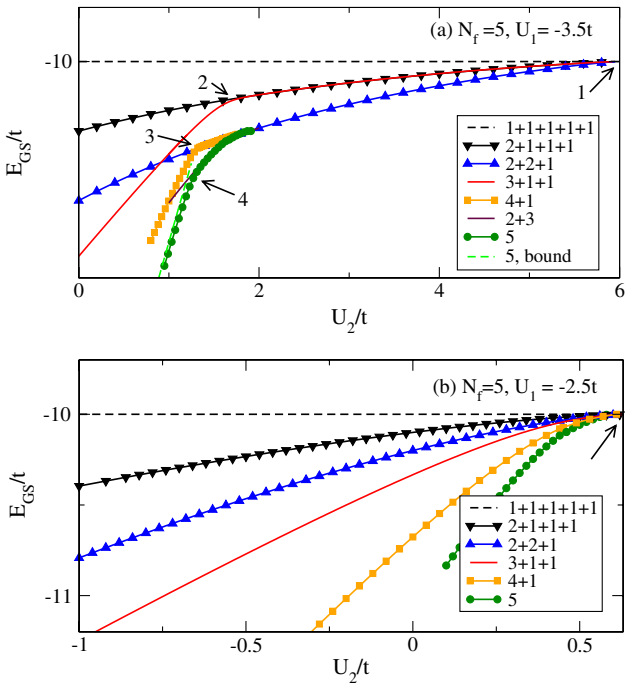

FIG. 3 (color online). $N_f = 5$ GS energy (green circles, label 5) versus U_2 for (a) $U_1 = -3.5t$ and (b) $U_1 = -2.5t$. Other lines show the lowest energies of various complexes and arrows indicate dissociations (see text for details).

either two pairs (at larger U_2) or a 4-fermion bound complex (smaller U_2). The boundary between the two is marked by arrow 3 ($E_{4+1} = E_{2+2+1}$). But 4-fermion bound states are not stable either, since $E_{4+1} < \min(E_{2+3}, E_5)$ (arrow 4 marks where the 5-fermion bound complex breaks into a pair + trion). Below it, E_5 is indeed in good agreement with the perturbational estimate for the energy of a 5-bound complex $E_{5,B} = 4U_1 + 3U_2 + 2t^2/(U_1 + t^2/U_1 - 2t^2/(U_1 + U_2))$, shown by the dashed line indexed "5, bound."

What happens as N_f increases becomes clear if we realize that arrows 3 and 4 point to essentially the same U_2 value. If more fermions are added, below this U_2 we expect a bigger and bigger bound complex—in other words, phase separation occurs and the system splits into a fermion rich and a fermion poor region. Above this, a gas of pairs is stable (plus one trion, if N_f is odd). That this inference is correct is verified by the following argument. This critical value should be given by the condition that adding two more particles to a fermion rich region (which changes energy by about $2U_1 + 2U_2$, because of extra interactions) should be energetically favorable to having a bound pair far away. From $2U_2 + 2U_1 < E_{2,\mathrm{GS}}$ we find $U_2 = 1.29t$ if $U_1 = -3.5t$, in good agreement with the value $U_2 = 1.3t$ pointed to by arrows 3 and 4.

Thus, based on these few-particles results, we can infer the phase diagram of this model at small concentrations, shown in Fig. 4. The dashed line shows the estimate discussed above, accurate for large U_1, U_2 (at smaller U_1, t comes into play since the extra fermions need not be fully localized at the edge of the fermion rich region). If $U_1 > -2.6t$, the transition is from phase separation to unbound fermions as U_2 increases. This is shown, for $U_1 = -2.5t$, in Fig. 3(b): here each bigger complex is more stable than any smaller ones, if $U_2 < 0.63t$ (arrow).

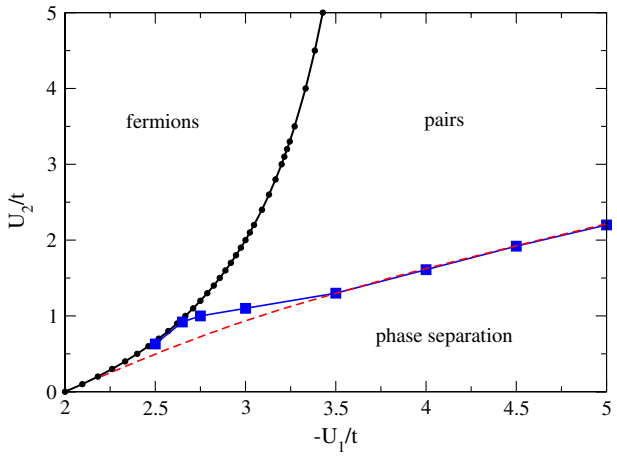

FIG. 4 (color online). Phase diagram at small concentrations. The GS consists of either unbound fermions or pairs, or it phase separates into fermion rich and fermion poor regions. The dashed line is an estimate for phase separation (see text).

While we are not aware of numerical studies of this model, the good agreement with various asymptotic estimates as well as with known results for spin-$\frac{1}{2}$ Hamiltonians [9] supports the accuracy of our results. This work shows that even such a simple model has a rich behavior that can be uncovered with this method.

To summarize, we have shown how to calculate few-particle Green's functions on an infinite 1D chain. The information obtained from them sheds light on the stability of few-particle bound states. It also illustrates the dangers of an insufficient analysis—if we stopped at $N_f = 3$, we would conclude that trions are stable in a large region of the parameter space, in this model. Analysis for larger N_f shows that addition of more particles leads to instability of trions, and furthermore allows us to find the phase diagram for small concentrations.

Although these results are for a 1D model, as discussed above this method generalizes to higher dimensions if the hopping is nearest-neighbor only. This opens the way to study the stability of trions and biexcitons in realistic lattice models. Such work is currently under way.

I thank I. Affleck, G. Sawatzky, P. Stamp, F. Zhou, and S. Yarlagadda for useful discussions. This work was supported by NSERC and CIfAR.

[1] X.-J. Liu, H. Hu, and P. D. Drummond, Phys. Rev. Lett. **102**, 160401 (2009); Phys. Rev. A **82**, 023619 (2010); Phys. Rev. B **82**, 054524 (2010).

[2] V. Efimov, Phys. Lett. B **33**, 563 (1970); Sov. J. Nucl. Phys. **12**, 589 (1971); JETP Lett. **16**, 34 (1972).
[3] For example, see S. E. Pollack, D. Dries, and R. G. Hulet, Science **326**, 1683 (2009).
[4] For example, see D. J. MacNeill and F. Zhou, Phys. Rev. Lett. **106**, 145301 (2011).
[5] F. J. Teran *et al.*, Phys. Rev. B **71**, 161309(R) (2005).
[6] R. Matsunaga, K. Matsuda, and Y. Kanemitsu, Phys. Rev. Lett. **106**, 037404 (2011).
[7] T. F. Ronnow, T. G. Pedersen, and H. D. Cornean, Phys. Rev. B **81**, 205446 (2010).
[8] G. A. Sawatzky, Phys. Rev. Lett. **39**, 504 (1977).
[9] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.107.246403 for further details and generalizations.
[10] M. Berciu, I. Elfimov, and G. A. Sawatzky, Phys. Rev. B **79**, 214507 (2009).
[11] M. Berciu and A. Cook, Europhys. Lett. **92**, 40 003 (2010).