Dynamics of two-site Fermi-Hubbard and Bose-Hubbard systems

K. Ziegler*

Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

(Received 27 September 2009; revised manuscript received 4 February 2010; published 10 March 2010)

This paper analyzes dynamical properties of small Fermi-Hubbard and Bose-Hubbard systems, focusing on the structure of the underlying Hilbert space. We evaluate time-dependent quantities such as the return probability to the initial state and the spin imbalance of spin-1/2 fermions. For the symmetric two-site Fermi-Hubbard model we find that the spin imbalance and the return probability are controlled by two and three frequencies, respectively. The spin imbalance and the return probability are identical for the asymmetric Falicov-Kimball limit and controlled by only one frequency. In general, the transition probabilities between the initial state and the energy eigenstates depend strongly on the particle-particle interaction. This is discussed for "self-trapping" of spinless bosons in a double-well potential. We observe that the available Hilbert space is reduced significantly by strong interaction.

DOI: 10.1103/PhysRevA.81.034701 PACS number(s): 34.50.−s, 31.15.ac, 03.67.Lx

The dynamics of many-body quantum states has been studied with a high accuracy in ultracold gases, either for bosons [1–5] or for fermions [6,7]. The main advantage of employing an ultracold gas is that there are many parameters in the experiment that can be adjusted to control the initial state as well as the dynamics of the system. This means, in particular, that an ultracold gas can be prepared in almost any state $|\Psi_0\rangle$, not just in the ground state. After its preparation at time $t = 0$, the state evolves in time $t > 0$ for a system with Hamiltonian H, which describes the kinematics and the interaction of the atomic particles, according to

$$|\Psi_t\rangle = e^{-iHt}|\Psi_0\rangle. \tag{1}$$

In the following we consider the simplest possible case, namely, a model with two sites. As the first example we study two fermions with spin-1/2, and the second example is a system of N spinless bosons in a double well. Despite their simplicity, these examples reveal dynamical properties that may also have implications for more complex systems. For instance, an interesting question is whether or not all states of the underlying Hilbert space can be reached from a given initial state, which time scales appear, and how this can be controlled by adjusting the parameters of the system such as the tunneling rate and the interaction strength.

The dynamics of atomic systems with a finite number of atoms has been an active field of research for several decades, with a focus on oscillating behavior between different atomic states [8,9]. More recently, ultracold gases in an optical lattice have been a successful platform for such investigations [1,4, 10]. In particular, small systems of spin-1/2 fermions have also attracted considerable attention from the quantum computation community [8,11]. A typical initial state is a (paramagnetic) Mott state, where the orientation of the individual spins can be used for information storage. Since for N particles this state has an exponential degeneracy 2^N, the time evolution in terms of, for instance, a Hubbard Hamiltonian can lead to a complex dynamics. Of particular interest is how the spin population of a given site changes with time.

Experiments with a Bose gas in an optical double well have revealed that the population dynamics is controlled by direct tunneling of atoms and by a second-order (superexchange) process, characterized by two frequencies [1,10]. The appearance of the characteristic frequencies in finite bosonic systems was calculated in strong-coupling perturbation theory [12,13] and in time-dependent Hartree approximation [14,15]. In a more recent paper by Trotzky *et al.* [4] the spin imbalance of two spin-1/2 atoms in a double well was studied. Such a system can be described by a two-site Bose-Hubbard (BH) model, which is often called the two-mode approximation [14]. With increasing values of J/U, where J is the tunneling rate and U is the local interaction strength, the oscillating spin imbalance was increasingly influenced by a second frequency. This implies that both,the tunneling rate of the atoms and the interaction strength determine the dynamics of the many-body system. In this paper we study this effect in terms of a Fermi-Hubbard (FH) model. The focus is on the return probability of the many-body state. This is an important quantity for recovering information that was stored in the initial state.

There are several options for an analytic calculation of physical quantities in a finite many-body system. Perturbative methods are very successful and reliable approaches to physical problems and can be considered exact if their regimes of validity are respected. On the contrary, in most cases they fail near a singularity, where their validity is violated. Nevertheless, they can still be used in these cases as approximation methods by using an asymptotic partial summation of the perturbation series. Hartree-Fock approximations belong to this type of approximation and have been used in the case of finite many-body systems [14,15]. Other self-consistent approaches to many-body systems have been very successful, such as the dynamical mean-field theory [16]. A disadvantage of all these approaches is that the (nonlinear) self-consistent equations are very complex, such that their treatment usually requires intensive numerical work.

An alternative to the perturbative approach and to self-consistent approximations is the recursive projection method (RPM) [17,18]. It is a systematic exploration of the Hilbert space, using a recursive calculation of the resolvent $(z - H)^{-1}$. The RPM enables us to extract systematically the poles of the

*klaus.ziegler@physik.uni-augsburg.de

resolvent in a subspace of the underlying physical Hilbert space. This method, combined with a truncation of recursion, is related to the Lanczos procedure [19]. The RPM has been explained elsewhere in the literature [17,18]; here we give only a brief summary and apply it to the Hubbard models.

Recursive projection method: The structure of our physical system is completely determined by a Hamiltonian H that acts on Hilbert space $\mathcal{H}$. Then the central idea of the RPM is that the dynamics starts from an initial state which lives in a subspace $\mathcal{H}_0 \subset \mathcal{H}$. It should consist of a basis that is dynamically separable, meaning that the Hamiltonian does not allow movement directly from one basis state to another. Once this subspace has been chosen specifically, the rest of the RPM is entirely determined by the Hamiltonian H, and the dynamics, given by the time-evolution operator, determines which part of $\mathcal{H}$ is reached by the physical system. This depends on the transition probabilities between the initial states and the eigenstates of H. A problem is to control the trajectories of the system through $\mathcal{H}$. This can be solved by considering the resolvent $(z-H)^{-1}$ rather than the time evolution operator. These quantities are related as

$$e^{-iHt} = \int_\Gamma (z-H)^{-1} e^{-izt} \frac{dz}{2\pi i}, \tag{2}$$

where the closed contour Γ encloses all (real) eigenvalues of H. Now we project with projector P_0 onto the Hilbert space $\mathcal{H}_0$. The corresponding projected resolvent is $G_0(z) = P_0(z-H)^{-1}P_0$. Then the RPM includes two steps.

1. Hilbert space $\mathcal{H}_{2j+2}$ $(j=0,1,\ldots)$ is created by acting with the operator $(\mathbf{1}-P_0-P_2-\cdots-P_{2j})HP_{2j}$ on $\mathcal{H}$. In other words, a basis set from all the states created by $(\mathbf{1}-P_0-P_2-\cdots-P_{2j})HP_{2j}$ is a basis of $\mathcal{H}_{2j+2}$.
2. The resolvent G_{2j} on $\mathcal{H}_{2j}$ is evaluated through the recurrence relation

$$G_{2j} = \left(z - H'_{2j}\right)^{-1}_{2j}, \tag{3}$$

with the effective Hamiltonian H'_{2j} on $\mathcal{H}_{2j}$:

$$H'_{2j} = P_{2j}HP_{2j} + P_{2j}HG_{2j+2}HP_{2j}. \tag{4}$$

The recursion terminates in a finite-dimensional Hilbert space with the effective Hamiltonian $H'_{2n} = P_{2n}HP_{2n}$. This is the only effective Hamiltonian that is explicitly given, provided we know the projection P_n. To use this as the initial effective Hamiltonian, we introduce $k = n-j$ as the running index in the recurrence relation. Then we have

$$G_{2(n-k)} = \left(z - H'_{2(n-k)}\right)^{-1}_{2(n-k)}, \tag{5}$$

and with $g_k \equiv G_{2(n-k)}$, $h_k \equiv H'_{2(n-k)}$, we obtain the recurrence relation

$$g_k = (z-h_k)^{-1}_{2(n-k)}, \tag{6}$$

where

$$h_k = P_{2(n-k)}HP_{2(n-k)} + P_{2(n-k)}Hg_{k-1}HP_{2(n-k)}, \tag{7}$$

with $h_0 = P_{2n}HP_{2n}$.

Model: The FH model describes locally interacting fermions with spin $\sigma = \uparrow, \downarrow$; the BH model, locally interacting spinless bosons. For fermions this reads

$$H_F = -\sum_{\sigma=\uparrow,\downarrow} J_\sigma (c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}), \tag{8}$$

with fermionic creation operators $c^\dagger_{\mathbf{j}\sigma}$, annihilation operators $c_{\mathbf{j}\sigma}$, and density operators $n_{\mathbf{j}\sigma} = c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{j}\sigma}$. For bosons with bosonic creation operators $b^\dagger_{\mathbf{j}}$, annihilation operators $b_{\mathbf{j}}$, and density operators $n_{\mathbf{j}} = b^\dagger_{\mathbf{j}}b_{\mathbf{j}}$, the Hamiltonian reads

$$H_B = -J(b^\dagger_{1\sigma}b_{2\sigma} + b^\dagger_{2\sigma}b_{1\sigma}) + U\left(n_1^2 + n_2^2\right). \tag{9}$$

This Hamiltonian is also known as the two-mode approximation of a continuous Bose gas in a double-well potential [14].

There are two interesting quantities directly related to $|\Psi_t\rangle$. One is the return probability to the initial state $P_t = |\langle\Psi_0|\Psi_t\rangle|^2$; the other is the spin imbalance between the two sites in a double well [4],

$$N_{12}(t) = \tfrac{1}{2}\langle\Psi_t|n_{\uparrow 1} - n_{\downarrow 1} + n_{\downarrow 2} - n_{\uparrow 2}|\Psi_t\rangle. \tag{10}$$

The latter describes the exchange dynamics of the two spins $\uparrow$ and $\downarrow$, located at the two sites. N_{12} vanishes if the sites are not singly occupied.

The return probability to the initial state is obtained from the inverse Laplace transform of the resolvent through the relation

$$\langle\Psi_0|\Psi_t\rangle = \int_\Gamma e^{-izt}\langle\Psi_0|(z-H)^{-1}|\Psi_0\rangle\frac{dz}{2\pi i}. \tag{11}$$

The many-body spectral density can be calculated from this expression for $z = E + i\epsilon$ as

$$-\mathrm{Im}\langle\Psi_0|(E+i\epsilon-H)^{-1}|\Psi_0\rangle, \tag{12}$$

which is a rational function with poles $z = E_j$ $(j=0,1,\ldots)$. By plotting this expression as a function of E, we can identify graphically the poles E_j $(j=0,1,\ldots)$ of G_0 and the overlap of $|E_j\rangle$ with the initial state. The energy levels E_j are the locations of the Lorentzian peaks, and $|\langle E_j|\Psi_0\rangle|^2/\epsilon$ correspond to the height of the Lorentzian peaks. The knowledge of E_j and $|\langle E_j|\Psi_0\rangle|^2$ enables us to determine the expression for the dynamical overlap function.

Dynamics of two fermions in a double well: Considering only two fermions with opposite spin, the Hamiltonian acts on a four-dimensional Hilbert space and can be diagonalized directly with eigenvalues 0, U, and $U/2 \pm \sqrt{(U^2/4)+4J^2}$ for the symmetric case $J_\downarrow = J_\uparrow \equiv J$. Also, the RPM with one fermion per well is simple because it terminates already for $n=1$, after creating a single pair of an empty and a doubly occupied well. The effective Hamiltonians then read

$$H'_2 = U, \quad H'_0 = \frac{1}{z-U}P_0H^2P_0. \tag{13}$$

H'_0 can also be expressed as a Heisenberg spin Hamiltonian [18]:

$$H'_0 = \sum_{<\mathbf{j},\mathbf{j}'>}\left[a_{\uparrow\downarrow}\left(S^x_{\mathbf{j}}S^x_{\mathbf{j}'} + S^y_{\mathbf{j}}S^y_{\mathbf{j}'}\right) + a_{\uparrow\uparrow}\left(S^z_{\mathbf{j}}S^z_{\mathbf{j}'} - 1/4\right)\right], \tag{14}$$

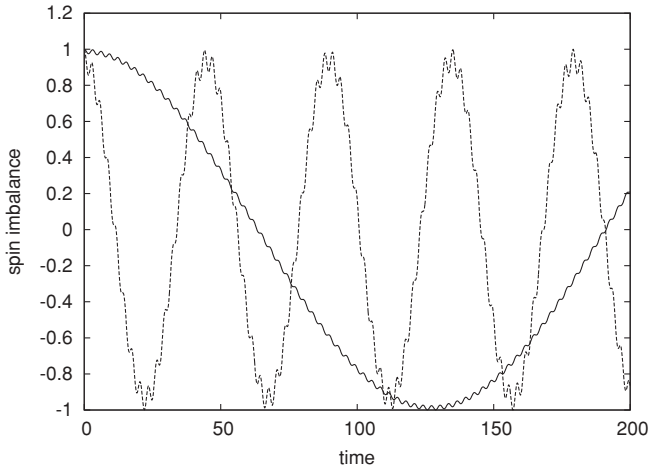

FIG. 1. The spin imbalance for the initial state $|\Psi_0\rangle = |\uparrow,\downarrow\rangle$ is plotted for $U = 2$ with $J/U = 0.05$ (solid curve) and $J/U = 0.3$ (dashed curve). Two frequencies contribute to each curve, corresponding to the lowest and highest energy levels of the system.

with z-dependent spin-spin coupling coefficients,

$$a_{\uparrow\uparrow} = 2\frac{J_\uparrow^2 + J_\downarrow^2}{U - z}, \quad a_{\uparrow\downarrow} = 4\frac{J_\uparrow J_\downarrow}{U - z}, \tag{15}$$

and with the spin-1/2 operators $S^x = (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow)/2$, $S^y = -i(c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow)/2$, and $S^z = (n_\uparrow - n_\downarrow)/2$. The singly occupied eigenstates of H_0' are linear combinations of $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$. If λ is an eigenvalue of $(z-U)H_0'$ with $\lambda = -(J_\uparrow \pm J_\downarrow)^2$, for the poles of the projected resolvent G_0, we get

$$z = \frac{U}{2}\left[1 \pm \sqrt{1 - (4\lambda/U^2)}\right] \sim \begin{cases} U - \lambda/U \\ \lambda/U \end{cases} \tag{16}$$

from the RPM. The asymptotic expressions hold for $\lambda/U \sim 0$. For a strong interaction parameter U, only one pole is accessible by perturbation theory, such that the appearance of two poles can be understood as a simple nonperturbative effect: the Brillouin-Wigner perturbation theory in powers of λ/U [21] gives only the low-energy pole for $G_0(z)$, namely, $z = \lambda/U$ [12], and neglects the high-energy pole $z \sim U - (\lambda/U)$. Experimentally, however, both energies have been observed in a double-well potential [4].

The spin imbalance of Eq. (10) can be rewritten in terms of the spin operator S^z as $\langle\Psi_t|S_1^z - S_2^z|\Psi_t\rangle$, since $S^z = (n_\uparrow - n_\downarrow)/2$. To understand the dynamics of the two-site FH model, we study the spin imbalance and the return probability for two specific cases: the symmetric FH model, with $J_\downarrow = J_\uparrow = 1/2$, and the Falicov-Kimball limit, $J_\uparrow = 0$, $J_\downarrow > 0$ [20]. The eigenvalues $z_{3/4} = U/2 \pm \sqrt{(U^2/4) + 1}$ of the symmetric FH model appear as frequencies in

$$\langle\Psi_0|\Psi_t\rangle = C_0 + C_1 e^{-iz_3 t} + C_2 e^{-iz_4 t}$$

and in the spin imbalance (cf. Fig. 1)

$$\langle\Psi_t|S_1^z - S_2^z|\Psi_t\rangle = C_1\cos(z_4 t) + C_2\cos(z_3 t),$$

with coefficients $C_0 = 1/2$ and

$$C_{1/2} = \frac{1}{(\sqrt{U^2+4} \pm U)\sqrt{U^2+4}}.$$

Then the time-dependent behavior of the return probability is characterized by three different frequencies: z_3, z_4, and $z_3 - z_4$.

Falicov-Kimball limit: In this case the eigenvalues are doubly degenerate for all values of $J_\downarrow$: $z_{3/4} = U/2 \pm \sqrt{(U^2/4) + J_\downarrow^2}$. This simplifies the dynamics. In particular, the spin imbalance becomes identical to the return probability, $\langle\Psi_t|S_1^z - S_2^z|\Psi_t\rangle = P_t$, and the transition matrix element reads

$$\langle\Psi_0|\Psi_t\rangle = C_1 e^{-iz_3 t} + C_2 e^{-iz_4 t},$$

with $C_1 = (z_3 - U)/(z_3 - z_4)$ and $C_2 = -(z_4 - U)/(z_3 - z_4)$. The oscillating behavior is characterized by a single frequency:

$$P_t = C_1^2 + C_2^2 + 2C_1 C_2 \cos(\sqrt{U^2 + 4J_\downarrow^2}\, t).$$

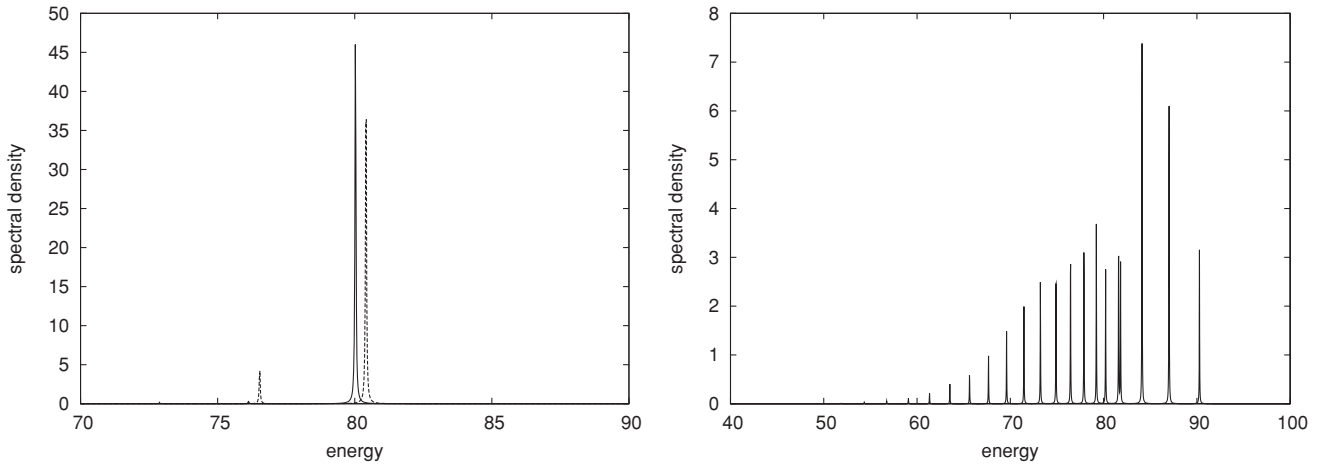

FIG. 2. Spectral density of the BH model of $N = 40$ bosons, $U = 0.05$, and $\epsilon = 0.02$. For $J = 0.05$ (solid curve) and $J = 0.2$ (dashed curve), there is only one dominant energy level, of 41 energy levels (left). The initial state is the state where all atoms are in one well. This is a signature of "self-trapping." The spectral density of the BH model of $N = 40$ bosons, $U = 0.05$, $\epsilon = 0.02$, and $J = 1$ (right). This clearly indicates that, with increasing tunneling rate J, more and more states can be reached dynamically with reasonable probability.

Dynamics of N *bosons in a double well:* A system of N spinless bosons, distributed over two wells, lives in an $(N+1)$-dimensional Hilbert space. Using the basis $|n_1, n_2\rangle$, a special case for the initial state is $n_1 = N$, $n_2 = 0$: $|\Psi_0\rangle = |N, 0\rangle$. Then all projected spaces $\mathcal{H}_{2j}$ are one dimensional and spanned by $|N-j, j\rangle$. The RPM leads to the recurrence relation

$$g_k = \frac{1}{z - U[k^2 + (N-k)^2] - J^2(N-k+1)kg_{k-1}}, \quad (17)$$

with initial value $g_0 = 1/(z - UN^2)$. Then the projected resolvent for the initial state $|\Psi_0\rangle = |N, 0\rangle$ reads

$$\langle N, 0|G_0|N, 0\rangle = \langle N, 0|(z-H)^{-1}|N, 0\rangle = g_N.$$

The evaluation of g_N from Eq. (17) is a simple task and leads to a rational function, consisting of a polynomial of order $N+1$ in the denominator.

According to the Hartee approximation of the double-well potential [14], the spectral properties change qualitatively when the number of bosons exceeds a critical value $N_c \approx J/U$, where the regime with $N > N_c$ is characterized by "self-trapping," in which the symmetry of the two wells is spontaneously broken. For $N < N_c$, on the contrary, the regime is characterized by an oscillating behavior with frequencies related to the tunneling rate. When the number of particles N approaches the critical value N_c, the frequency of the oscillations goes down to zero, indicating a real critical behavior. However, this is an artifact of the classical nonlinear equation obtained by the Hartree approximation. For a quantum system on a finite-dimensional Hilbert space, we expect no genuine critical behavior. Nevertheless, a crossover between two regimes is possible, where in one regime the time scale for escaping from the initial states can be very large and the escape is very unlikely. Such a behavior can be studied by the many-body spectral function.

There are two types of characteristic quantities: the energy levels E_k and the transition probabilities $|\langle\Psi_0|E_k\rangle|^2$ between the initial state and the eigenstates of the Hamiltonian. Both quantities appear explicitly in the many-body spectral density of Eq. (12). For the initial state $|N, 0\rangle$ the many-body spectral density is plotted for several parameter values in Fig. 2. This clearly indicates that the distribution of transition probabilities is narrow for strong interactions and becomes broader with increasing U. For sufficiently large U all transition probabilities $|\langle\Psi_0|E_k\rangle|^2$ are extremely small except for one (cf. upper panel in Fig. 2). This implies that the system cannot escape from its initial state. This strong-interaction behavior can be linked to the semiclassical self-trapping of the Hartree approximation.

Conclusions: The dynamics of finite FH and BH models is characterized by a discrete set of energy levels and nonzero overlaps of the eigenfunctions with the initial state. By employing the RPM, we have calculated these quantities to determine the spin imbalance, return probability, and many-body spectral function for the FH and BH models in a double well.

The author is grateful to Professor A. F. R. de Toldeo Piza for bringing Ref. [17] to his attention. This work was supported by the Aspen Center for Physics.

[1] S. Fölling *et al.*, Nature **448**, 1029 (2007).
[2] I. B. Spielman, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. **98**, 080404 (2007).
[3] T. Salger, C. Geckeler, S. Kling, and M. Weitz, Phys. Rev. Lett. **99**, 190405 (2007).
[4] S. Trotzky *et al.*, Science **319**, 295 (2008).
[5] P. Würtz, T. Langen, T. Gericke, A. Koglbauer, and H. Ott, Phys. Rev. Lett. **103**, 080404 (2009).
[6] Y. Shin, M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Phys. Rev. Lett. **97**, 030401 (2006); G. B. Partridge *et al.*, *ibid.* **97**, 190407 (2006); N. Strohmaier *et al.*, *ibid.* **99**, 220601 (2007).
[7] M. Inguscio, W. Ketterle, and C. Salomon, eds., *Ultra-cold Fermi Gases* (IOS Press, Amsterdam, 2007).
[8] M. Lewenstein *et al.*, Adv. Phys. **56**, 243 (2007).
[9] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg, *Atom-Photon Interactions* (John Wiley, New York, 1992).
[10] J. Estéve, C. Gross, A. Weller, S. Giovanazzi, and M. K. Oberthaler, Nature **455**, 1216 (2008).
[11] J. I. Cirac, in *Ultra-cold Fermi Gases*, edited by M. Inguscio, W. Ketterle and C. Salomon (IOS Press, Amsterdam, 2007).
[12] L.-M. Duan, E. Demler, and M. D. Lukin, Phys. Rev. Lett. **91**, 090402 (2003).
[13] A. M. Rey, V. Gritsev, I. Bloch, E. Demler, and M. D. Lukin, Phys. Rev. Lett. **99**, 140601 (2007).
[14] G. J. Milburn, J. Corney, E. M. Wright, and D. F. Walls, Phys. Rev. A **55**, 4318 (1997).
[15] S. Zöllner, H.-D. Meyer, and P. Schmelcher, Phys. Rev. A **78**, 013621 (2008).
[16] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989); A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996); A. Georges, in *Ultra-cold Fermi Gases*, edited by M. Inguscio, W. Ketterle, and C. Salomon (IOS Press, Amsterdam, 2007).
[17] H. Feshbach, A. K. Kerman, and R. H. Lemmer, Ann. Phys. (NY) **41**, 230 (1967).
[18] K. Ziegler, Phys. Rev. A **68**, 053602 (2003); Phys. Rev. B **72**, 075120 (2005); Phys. Rev. A **77**, 013623 (2008).
[19] A. S. Householder, *Theory of Matrices in Numerical Analysis* (Dover, New York, 1974).
[20] L. M. Falicov and J. C. Kimball, Phys. Rev. Lett. **22**, 997 (1969); J. K. Freericks, Phys. Rev. B **48**, 3881 (1993); P. Farkasovsky, Z. Phys. B **102**, 91 (1996); Eur. Phys. Lett. **84**, 37010 (2008); J. K. Freericks and V. Zlatić, Rev. Mod. Phys. **75**, 1333 (2003).
[21] E. Fradkin, *Field Theories of Condensed Matter Systems* (Addison Wesley, Reading, MA, 1991).