Synchronization and Dephasing of Many-Body States in Optical Lattices

M. B. Hastings\textsuperscript{1,2} and L. S. Levitov\textsuperscript{3,2}

\textsuperscript{1}Center for Nonlinear Studies and Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, 87545
\textsuperscript{2}Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106
\textsuperscript{3}Department of Physics, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA, 02139

We introduce an approach to describe quantum-coherent evolution of a system of cold atoms in an optical lattice triggered by a change in superlattice potential. Using a time-dependent mean field description, we map the problem to a strong coupling limit of previously studied time-dependent BCS model. We compare the mean field dynamics to a simulation using light-cone methods and find reasonable agreement for numerically accessible times. The mean field model is integrable, and gives rise to a rich behavior, in particular to beats and recurrences in the order parameter, as well as singularities in the momentum distribution, directly measurable in cold atom experiment.

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The approach to thermal equilibrium has been a central problem in statistical mechanics since Boltzmann's H-theorem. Recent advances in ultracold atoms make it possible to probe this approach in quantum-coherent many-body systems, due to the ability to change interactions in optical lattices\textsuperscript{1,2} on a fast timescale.

These new experimental opportunities stimulated theoretical work on quantum dynamics in many-body systems. Improvements in simulation algorithms, such as time-dependent density-matrix renormalization group\textsuperscript{3,4} and light-cone methods\textsuperscript{5}, make it possible to study these systems numerically for short times. However, the increase in entanglement entropy limits the simulation time\textsuperscript{6}, calling for the development of new approaches.

One simple-to-realize way to start a system out of equilibrium is to begin with an additional period-two modulation in a translationally invariant system. One case of this is an XXZ spin chain started from a Neel state at large Ising coupling\textsuperscript{6}. Another case proposed recently is a Bose gas in an optical lattice, with a period-two superlattice initially superimposed\textsuperscript{7}, causing the system to begin in a state with alternating filled and empty sites. The superlattice is then removed, and the system evolves under Bose-Hubbard dynamics.

In this article we study interacting spinless fermions in a one-dimensional lattice, described by the Hamiltonian

\[ H = \Delta \sum_{i=1}^{N} \left( \hat{a}_{i}^{\dagger} \hat{a}_{i+1} + h.c. \right) + \sum_{i=1}^{N} \lambda \hat{n}_{i} \hat{n}_{i+1}, \quad (1) \]

where $\Delta$ is the hopping amplitude, $\hat{n}_{i} = \hat{a}_{i}^{\dagger} \hat{a}_{i} - \frac{1}{2}$. The initial state, taken to be alternating filled and empty sites, $\hat{n}_{i} = \pm \frac{1}{2}$, is created by an additional period-two potential that is removed at $t = 0$, after which the system evolves under $H$. The Hamiltonian (1) describes the regime in which multiple occupancy of lattice sites is inhibited by repulsive interaction and/or the Pauli principle.

To understand the evolution governed by (1) we employ a mean-field description of the problem (1) which uses the staggered density

\[ \rho_{\tau}(t) = \frac{1}{N} \sum_{i=1...N} (-1)^{i} \langle \hat{n}_{i} \rangle \quad (2) \]

as an order parameter. We show that the resulting mean-field dynamics is mathematically equivalent to time-dependent BCS dynamics\textsuperscript{3,5,10,11}, with, however, very different initial conditions. Comparison to the numerical results\textsuperscript{5} for the Jordan-Wigner-equivalent XXZ spin chain is used to test validity of the mean-field approach.

We find that instead of simple relaxation to a steady state, the order parameter time evolution exhibits revivals. These revivals are understood as resulting from a buildup of singularities in the fermion momentum distribution, illustrated in Fig. 1. The formation of a steady

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{figure1.png}
\caption{Buildup of singular momentum distribution of pseudospin $S_{k}$, a semicircle (11) with the edge at $k_{c} = \arcsin \lambda$. A series of traces computed for $\lambda = 0.5$ are shown at times $t = 0, 25, 50, ..., 175$, eventually converging to Eq. (11). Inset: the corresponding limiting fermion momentum distribution $\langle n(k) \rangle = \langle a_{k}^{\dagger} a_{k} \rangle$ (14).}
\end{figure}
state with a singular momentum distribution can be directly tested in a free flight imaging experiment [13].

The mean-field approximation can be constructed by replacing $\hat{n}_i\hat{n}_{i+1} \approx -2\rho_\tau(t)\sum_i (-1)^i\hat{n}_i$ in the fermionic Hamiltonian [11], which gives

$$H_{\text{mf}} = \frac{1}{2} \sum_i \left( a_i^\dagger a_i + \text{h.c.} \right) - 2\lambda\rho_\tau(t)\sum_i (-1)^i\hat{n}_i$$

(without loss of generality we set the hopping amplitude to $\Delta = \frac{1}{2}$). In the evolution governed by $H_{\text{mf}}$ the quantity $\rho_\tau(t)$ is determined self-consistently via Eq. (2).

To establish equivalence of the problem [3] to the BCS dynamics [8, 9, 10, 11] we consider a translation invariant system on a ring, with momentum states $|k\rangle$, $-\pi < k < \pi$. Initially, the system is half-filled and each pair of momentum states, $|k\rangle$ and $|k + \pi\rangle$, contains exactly one particle. Momentum-nonconserving terms in the Hamiltonian [3] couple momenta $k$ and $k + \pi$. Thus, at all times we can write the many-body wavefunction in a BCS-like form

$$\Psi(t) = \prod_{-\pi/2 \leq k < \pi/2} \left( u_k(t)a_i^\dagger(k + \pi) + v_k(t)a_i^\dagger(k) \right)|0\rangle,$$

where $|0\rangle$ is the vacuum state. The initial conditions are $u_k(0) = v_k(0) = \sqrt{2}$. The evolution equations are

$$\partial_t u_k(t) = i\cos(k)u_k(t) + 2\lambda\rho_\tau(t)v_k(t),$$
$$\partial_t v_k(t) = -i\cos(k)v_k(t) + 2\lambda\rho_\tau(t)u_k(t),$$

with the self-consistency condition [2] taking the form

$$\rho_\tau(t) = \frac{1}{N/2} \sum_{-\pi/2 \leq k < \pi/2} \text{Re}(u_k(t)v_k(t)).$$

Note that there are $N/2$ different values of $k$ in the sum in Eq. (6), so that $-1/2 \leq \rho_\tau(t) \leq 1/2$.

Given a pair, $u_k$, $v_k$, we define pseudo-spins [12] by $S_k^x = \frac{1}{2}(|u_k|^2 - |v_k|^2)$, $S_k^z = iS_k^y = \eta_k u_k v_k$. In terms of these classical variables the Hamiltonian reads

$$H_S = -\sum_{-\pi/2 \leq k < \pi/2} 2\cos(k)S_k^z + \frac{2\lambda}{N/2} \sum_{k,k'} S_k^x S_{k'}^x,$$

which, together with the usual Poisson brackets, $\{S_n, S_k\} = i\epsilon_{abc}S_a$, reproduces the dynamics [3].

The canonical BCS Hamiltonian [12] differs from [7] in one important respect: the BCS problem has an additional coupling $S_k^x S_{k+\pi}^x$. We circumvent this problem in two steps. First, we extend the Hamiltonian [7] to a twice larger momentum range $-\pi < k < \pi$, doubling the number of $k$-states. Simultaneously we replace the coupling $2\lambda/(N/2)$ by $2\lambda/N$. Consider any pair of momenta, $k$ and $k + \pi$; these two pseudospins feel opposite $z$ fields and the same $x$ field, so they evolve as

$$S_{k+\pi}^x(t) = S_k^x(t), \quad S_{k+\pi}^z(t) = -S_k^z(t),$$

where individual spin polarizations for $-\pi/2 < k < \pi/2$ evolve in the same way as in the original problem [7].

After the states are doubled, the net $y$ polarization $\sum_k S_k^y$ is taken over the extended range $-\pi < k < \pi$ vanishes at all times, while the net $x$ polarization $\sum_k S_k^x$ does not change, and so we can then add the interaction $S_k^x S_{k+\pi}^x$ to the original Hamiltonian [7] without changing the dynamics. Thus, we arrive at the BCS Hamiltonian:

$$H_{\text{BCS}} = -\sum_{-\pi \leq k < \pi} 2\cos(k)S_k^z + \frac{2\lambda}{N} \sum_{k,k'} S_k^x S_{k'}^x + S_k^y S_{k+\pi}^y.$$
mean-field dynamics shows a revival: the amplitude of oscillations begins to increase again. This revival is not far outside the times reached with the light-cone methods, and may be accessible with more numerical effort.

As we will see below, for \( \lambda > 1 \) the mean-field dynamics predicts a non-vanishing asymptotic value \( \rho_{\pi}(t \to \infty) \), while simulation of the XXZ chain indicates that \( \rho_{\pi}(t) \) rapidly decays to zero. Nevertheless, as illustrated in Fig. 2(b), even at short times, with both \( M(t) \) and \( \rho_{\pi}(t) \) decaying faster than for \( \lambda = 0.5 \).

Turning to discuss different regimes, we note that because both the Hamiltonian \( \mathcal{H} \) and the initial values \( u_x(0) \) and \( v_x(0) \) are real, the mean-field dynamics of \( \rho_{\pi}(t) \) is time reversal invariant. Further, the initial state is invariant under the orthogonal operator \( \mathcal{O} = \prod_k S_k^z \), which anti-commutes with the first term in \( \mathcal{H}_{mf} \) and commutes with the second. Combining these two statements, we see that the dynamics depends only on the magnitude of \( \lambda \) and not on its sign (all this is also true for the XXZ chain started in the Neel state, where we set \( \mathcal{O} = \prod_{k \text{ odd}} S_k^z \).

In the absence of interaction, \( \lambda = 0 \), the decay of \( \rho_{\pi}(t) \) follows \( \cos(2t + \delta)/t^{1/2} \) with \( \delta = \pi/2 \). At \( 0 < |\lambda| < 1 \), the system is in a "dephasing" regime, and \( \rho_{\pi} \) is well-described at long times by a sum of two frequencies beating together with a power-law envelope decaying as \( t^{-3/2} \):

\[
\rho_{\pi}(t) \sim \left( a_1 \cos(\omega_1 t + \delta_1) + a_2 \cos(\omega_2 t + \delta_2) \right)/t^{3/2}.
\] (10)

We will see that this unexpected behavior, leading to revivals in \( \rho_{\pi}(t) \), signals formation of a singularity in \( k \) space of the asymptotic polarization \( S_k^z \). Below, we use integrals of motion of the BCS dynamics to show, in agreement with numerics, that \( \omega_1 = 2 \), \( \omega_2 = 2\sqrt{1 - \lambda^2} \).

One can expect that strong interaction will stabilize the state with density modulation \( \rho_{\pi}(t) \). In agreement with this intuition, we find that for \( |\lambda| > 1 \) the system is in the "polarized" regime, with non-vanishing \( \rho_{\pi}(t \to \infty) = (1/2)\sqrt{T - 1/\lambda^2} \). We obtain this asymptotic value analytically, and confirm it numerically. The approach to the asymptotic value is described by \( \rho_{\pi}(t) - \sqrt{1 - 1/\lambda^2} \sim \cos(\omega t + \delta)/t^{1/2} \) at the phase transition at \( \lambda = 1 \), we observe numerically that \( \rho_{\pi}(t) \sim \cos(2t + \delta)/t^{3/2} \).

The behavior in the dephasing regime can be qualitatively understood as follows. In the non-interacting case, all of the pseudo-spins remain in the \( x-y \) plane, with \( S_k^z(t) = 0 \). Initially, they all point in the \( x \)-direction, and dephase over time, leading to the \( 1/\sqrt{T} \) decay in \( \rho_{\pi} \). When interaction is turned on, the spins begin to move out of the \( x-y \) plane and polarize in the \( z \)-direction. The appearance of a net \( z \)-polarization is required by conservation of energy: as the ferromagnetic \( S^zS^\ast \) term in the energy \( \mathcal{H} \) is becoming less negative because of dephasing, the \( S^z \) contribution must become more negative.

However, the asymptotic distribution of \( S^z \) is not the thermal distribution. Instead, it shows a square-root singularity at \( k = k_c \equiv \arcsin \lambda \) (see Fig. 1). We find, analytically and numerically (see Fig 10), that \( S_k^z(t \to \infty) = 0 \) for \( |k| > k_c \), whereas

\[
S_k^z(t \to \infty) = \frac{1}{2} \sqrt{\cos^2 k - 1 + \lambda^2}, \quad |k| \leq k_c.
\] (11)

The van Hove singularity at the band edge and the singularity at \( k_c \) give rise to the frequencies \( \omega_1, \omega_2 \) in (10).

An analytic insight into the behavior in the dephasing regime can be gained as follows. The BCS dynamics has infinitely many commuting integrals of motion that can be written as an energy dependent Lax vector \( \mathcal{L} \):

\[
\mathcal{L}(\xi) = \mathbf{z} + 2\lambda \sum_{\xi' \neq \xi} \frac{S_{\xi'}}{\xi - \xi'},
\]

where in our case \( \xi = \cos k \) and \( \sum_{\xi' \neq \xi} S_{\xi'} = \int \cdots \Delta_k \frac{dk}{2\pi} \).

The asymptotic polarization can be found by comparing the values \( \mathcal{L}(\xi) \) in the initial and asymptotic states \( \mathcal{L}(\xi) \). The initial state, polarized in the \( x \) direction, gives

\[
\mathcal{L}^2(\xi) = L_1^2 + L_3^2 = 1 + \lambda^2/(\xi^2 - 1).
\] (12)

In the asymptotic state, because the \( x \) and \( y \) components are dephased, we can approximate:

\[
\mathcal{L}^2(\xi) \approx L_3^2 = \left( 1 + 2\lambda \int_{-\pi}^{\pi} \frac{S_k^z dk}{(\xi - \cos k)2\pi} \right)^2.
\] (13)

Comparing (12) and (13) we obtain an integral equation

\[
2\lambda \int_{-\pi}^{\pi} \frac{S_k^z dk}{(\xi - \cos k)2\pi} = \sqrt{\frac{\xi^2 - 1 + \lambda^2}{\xi^2 - 1}} - 1
\] (14)

where \( \xi \) is treated as a complex variable, \( \text{Im} \xi > 0 \). Changing variable to \( x = \cos k \), we rewrite (14) as

\[
\frac{1}{2\pi} \int_{-1}^{1} \frac{f(x) dx}{\xi - x} = \sqrt{\frac{\xi^2 - 1 + \lambda^2}{\xi^2 - 1}} - 1
\] (15)

where \( f(x) = 4\lambda S^2(x)/\sqrt{1 - x^2} \) is the unknown function. This equation can be solved using Cauchy’s formula, by writing \( f(x) = f_+(x) + f_-(x) \), the functions \( f_{\pm}(x) \) being analytic in the upper/lower complex half-plane, respectively. The result is \( f(x) = 2 \text{Im} \sqrt{\frac{x^2 - 1 + \lambda^2}{1 - x^2}} \), which yields the semicircle dependence (11).

The \( t^{-3/2} \) power law envelope in (10) is more difficult to understand. Consider the band edge singularity at \( k = 0 \). At \( \lambda = 0 \), this gives rise to a \( 1/\sqrt{T} \) contribution to \( \rho_{\pi} \) due to a coherent contribution of the modes with \( k \leq 1/\sqrt{T} \). For \( \lambda > 0 \), the \( x-y \) component of the spins near \( k = 0 \) is proportional to \( k \), which suggests in a scaling picture that \( S^x(0) \) should decay with an envelope of \( 1/\sqrt{T} \), which we do observe numerically. Thus, if the order parameter were due to a coherent contribution of spins with \( k \leq 1/\sqrt{T} \), we would expect a \( 1/t \) decay in \( \rho_{\pi} \).
FIG. 3: The quantity $S_{\text{cum}}^x(k) = \frac{1}{N} \sum_{0 < k' < k} S_{k'}^x$, for $\lambda = 0$ (black) and $\lambda = 0.5$ (red). Snapshots at $t = 400$ are shown, with $y$-axis multiplied by an arbitrary scaling factor in both cases.

rather than $1/t^{3/2}$ as observed. To understand this better, we analyze the cumulative order parameter $S_{\text{cum}}^x(k)$, plotting it as Fig. 3 for a particular snapshot in time. It can be seen that the contribution of the low-lying modes is largely canceled out by higher modes in the interacting case, while the contribution of the higher modes averages out in the non-interacting case.

To identify the boundary of the dephasing regime, we recall that in the BCS problem the large-$t$ asymptotic is governed by the complex roots of the spectral equation $L^2(\xi) = 0$. In our case, for the initial state polarized in the $x$-direction, the spectral equation can be factorized as $L^2 = (L_3 + iL_1)(L_3 - iL_1) = 0$, giving

$$1 \pm i2\lambda \int_{-\pi}^{\pi} \frac{dk}{4\pi(\xi - \cos k)} = 1 \pm \sqrt{1 - \xi^2} = 0 \quad (16)$$

This equation has complex imaginary roots $\xi = \pm i\sqrt{1 - \lambda^{-2}}$ if $\lambda > 1$, and has no complex solutions for $\lambda < 1$. Thus, for $\lambda > 1$, we have a non-zero asymptotic value of $\rho_x = \frac{1}{2}\sqrt{1 - \lambda^{-2}}$, which we confirmed by numerical simulations.

We have tried non-integrable deformations of the model, by making the $S_x S^x$ coupling between modes weakly dependent on $k$. Even a very small change removes the singularity at $k_c$, though a smooth kink remains, causing the contribution to $\rho_x(t)$ at frequency $\omega_x = 2\cos k_c$ to decay exponentially in time, rather than as a power law. At early times, beats are still observable.

Now we briefly discuss application of our results to bosons in an optical lattice, described by [15]

$$H_{\text{BH}} = \Delta \sum_i \left( b_i^\dagger b_{i+1} + \text{h.c.} \right) + U \sum_i (b_i^\dagger b_i + 1/2)^2 \quad (17)$$

As above, the initial state of alternating filled and empty sites is imposed by an additional period-two potential.

Because the mean-field dynamics with the staggered density order parameter $\rho_\pi(t) = \frac{1}{N} \sum_i (-1)^i (b_i^\dagger b_i - 1/2)$ does not depend on statistics, the bosonic and fermionic Hamiltonians yield the same mean-field evolution. In fact, in the bosonic case, for any initial conditions where we alternate a site with $n$ particles with an empty site, we obtain the same mean-field equations up to rescaling $U$ by dividing it by $n$. We expect the mean-field to become more accurate for larger $n$.

As a result, the mean-field theory for the bosonic system predicts the asymptotic momentum distribution $n(k) = \langle b_k^\dagger b_k \rangle$ which is similar to fermionic $n(k)$ (see Fig. [1]). This momentum distribution can be measured in a cold atom experiment using time-of-flight.

Unlike the fermion problem, the Bose-Hubbard model is not integrable, and therefore at long times the momentum distribution of the particles should thermalize. Still, at short times the kink in the distribution may be observable. If present, it will manifest itself also in revivals of the staggered density amplitude $\rho_\pi(t)$.

As the interaction $U$ increases, it is no longer valid to use mean-field theory. However, because at $U = \infty$ the bosonic problem reduces to non-interacting fermions, for large $U$ we can use second order perturbation theory to map the problem onto a system of hard-core bosons with weak attractive interactions $\frac{4\Delta^2}{U} \sum_i b_i^\dagger b_{i+1}^\dagger b_{i+1} b_i + \frac{2\Delta^2}{U} \sum_i b_i^\dagger b_{i+1}^\dagger b_{i-1} b_i + \text{h.c.}$ For large $U$, both terms are now weak and can be treated by mean-field theory. The treatment of the first term is as before, whereas the second term leads to a momentum dependent coupling in the Bose mean-field which breaks integrability.

In contrast to that, the fermion problem is integrable, and thus its dynamics is not be ergodic. Thus our main results, the revivals in the order parameter and the formation of a singular momentum distribution, may persist in the fermion case even at the times longer than those described by our mean-field approach.

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