TIGHT BINDING MODELS IN COLD ATOMS PHYSICS*

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Cold atomic gases placed in optical lattice potentials offer a unique tool to study simple tight binding models. Both the standard cases known from the condensed matter theory as well as novel situations may be addressed. Cold atoms setting allows for a precise control of parameters of the systems discussed, stimulating new questions and problems. The attempts to treat disorder in a controlled fashion are addressed in detail.

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1. Introduction

Ultra-cold atoms in optical lattices are a unique tool for studying models and situations that are typically met in condensed matter theory. A laser light, detuned from the atomic transition, affects external atomic degrees of freedom. For sufficient detuning, the upper states can be eliminated adiabatically from the description, the atom (in the ground state) moves in a potential proportional to laser intensity and inversely proportional to the detuning [1]. A standing wave laser field produces a stationary one-dimensional (1D) periodic potential with the lattice constant being a half of the light's wavelength. A cubic three-dimensional (3D) lattice is realised with 3 pairs of mutually orthogonal beams, *etc.*

As shown in a seminal now work [2] sufficiently cold atomic sample placed in such a lattice is very well described by the so called Bose–Hubbard tight binding model. Bose–Hubbard since atomic bosonic samples have been efficiently cooled first. Present techniques allow to cool efficiently fermionic samples as well as mixtures of fermions and bosons, enabling studies of the correspond systems in optical lattices as well.

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Bose–Hubbard system is interesting since it exhibits the so called quantum phase transition [3]. It is the first experimental attempt at the observation of this transition in cold atomic setting [4] that triggered a huge interest in similar systems. By now several different applications have been envisaged ranging from high T_c superconductivity [5], disordered systems [6, 7], various spin models [8] or novel quantum magnets [9] to quantum computing settings [10]. An excellent review on the subject [11] appeared recently. Therefore, I shall concentrate here mostly on one particular situation namely on the most basic Bose–Hubbard model (BHM) paying a particular attention to effects due to the presence of the disorder.

This contribution is arranged as follows. I shall briefly review how the Bose–Hubbard model appears naturally in cold atoms studies showing how easily one can tune basic model parameters. This flexibility allows for studies of quantum phase transitions. In the next section I consider the effect of disorder and the possibility of the existence of the novel phase — the Bose glass — discussing both the theoretical models and the first experimental attempts in that direction. Later I shall describe recent attempts to observe Anderson localisation in shallow optical potentials as well as I shall mention briefly possible generalisations towards mixtures of bosons and fermions.

2. Bose–Hubbard model

Consider a very cold sample of bosons placed in the periodic potential $V_{\rm latt}$ as well as in an additional potential $V_{\rm ext}$. The latter may be due to an optical (or magnetic) trap holding the condensate, additional optical fields, disorder *etc.* If lattice is one or two dimensional only, we assume that in the perpendicular directions the atoms are tightly confined, *i.e.*, there exist a tight (harmonic) trap assuring that the perpendicular motion is restricted to the corresponding ground state.

The Hamiltonian of the system may be expressed in the following second-quantised form

$$\begin{aligned} H &= \int d^3x\, \hat{\Psi}^\dagger(\boldsymbol{x}) \left(\frac{\boldsymbol{p}^2}{2M} + V_{\rm latt}(\boldsymbol{x}) + V_{\rm ext}(\boldsymbol{x}) \right) \hat{\Psi}(\boldsymbol{x}) \\ &\quad + \frac{1}{2} \int d^3x d^3x' \hat{\Psi}^\dagger(\boldsymbol{x}) \hat{\Psi}^\dagger(\boldsymbol{x}') V_{\rm int}(\boldsymbol{x}, \boldsymbol{x}') \hat{\Psi}(\boldsymbol{x}') \hat{\Psi}(\boldsymbol{x}) \,, \end{aligned} \tag{1}$$

where $\hat{\Psi}(\boldsymbol{x})$ is the boson field operator. The boson–boson interaction is taken as a contact potential $V_{\rm int}(\boldsymbol{x}, \boldsymbol{x}') = g\delta(\boldsymbol{x} - \boldsymbol{x}')$ For s-wave scattering $g = 4\pi a_s/M$ with a_s being the s-wave scattering length.

The Hamiltonian (1) is a starting point to two possible extreme cases. For very weak lattices, making a standard "semi-classical" approximation by substituting a classical wave function $\Psi(\boldsymbol{x})$ for $\hat{\Psi}(\boldsymbol{x})$ we arrive at the Gross–Pitaevskii description of the condensate in $V_{\rm latt}(\boldsymbol{x}) + V_{\rm ext}(\boldsymbol{x})$ potential. Such

a situation has been discussed in numerous cases (for a review see [12]), our interest will be mainly to review the situation in the presence of the disorder.

For the other limit, with deep lattice potential, the basis describing localisation in different lattice sites would be physically relevant. For particles occupying the lowest band of the periodic potential only, the so called Wannier functions $W(\boldsymbol{x}-\boldsymbol{x}_j)$ localised at sites $\boldsymbol{x}_j$ are the best choice. The Wannier functions are linear combinations of Bloch functions of the lowest band with different quasi momenta $\boldsymbol{q}$, $\phi_{\boldsymbol{q}}(\boldsymbol{x})$

$$W(\boldsymbol{x}-\boldsymbol{x}_j)=\Theta^{-3/2}\sum_{\boldsymbol{q}} e^{-i\boldsymbol{q}\cdot\boldsymbol{x}_j}\,\phi_{\boldsymbol{q}}(\boldsymbol{x})\,. \tag{2}$$

Expressing $\hat{\Psi}(\boldsymbol{x})=\sum_{j=1} W(\boldsymbol{x}-\boldsymbol{x}_j)\hat{a}_j$ where $\hat{a}_j$ is an annihilation operator for boson at j site allows to express the Hamiltonian (1) in the form

$$H=-\sum_{i,j} J_{ij}\hat{a}_i^{\dagger}\hat{a}_j+\frac{1}{2}\sum_{i,j,k,l} U_{ijkl}\hat{a}_i^{\dagger}\hat{a}_j^{\dagger}\hat{a}_k\hat{a}_l\,, \tag{3}$$

where the tunnelling rates

$$J_{ij}=-\int dx W(\boldsymbol{x}-\boldsymbol{x}_i)\left(\frac{p^2}{2m}+V_{\mathrm{latt}}(\boldsymbol{x})+V_{\mathrm{ext}}(\boldsymbol{x})\right)W(\boldsymbol{x}-\boldsymbol{x}_j)\,,$$

while

$$U_{ijkl}=g\int dx W(\boldsymbol{x}-\boldsymbol{x}_i)W(\boldsymbol{x}-\boldsymbol{x}_j)W(\boldsymbol{x}-\boldsymbol{x}_k)W(\boldsymbol{x}-\boldsymbol{x}_l)$$

describe the collisions. For sufficiently deep lattices, and V_{ext} being either slowly changing or much smaller than V_{latt} additional simplifications are possible. first of all particles interact mostly only if they are at the same site, the U_{ijkl} integral becomes site independent. The diagonal terms J_{ii} yield the energy ε_i at site i, which may be well approximated by $V_{\mathrm{ext}}(\boldsymbol{x}_i)$. In the off-diagonal terms, describing the tunnelling, the dominant V_{latt} term is kept only; We note also that, due to localisation properties of Wannier functions, the tunnelling to nearest neighbours is dominant. The resulting integral is site-independent and is denoted as J. In this way we arrive at the standard Bose–Hubbard model Hamiltonian:

$$H=-J\sum_{\langle i,j\rangle}\hat{a}_j^{\dagger}\hat{a}_i+\frac{U}{2}\sum_{i=1}\hat{n}_i(\hat{n}_i-1)+\sum_{i=1}\varepsilon_i\hat{n}_i\,, \tag{4}$$

where $\hat{n}_i=\hat{a}_i^{\dagger}\hat{a}_i$.

The interaction constant U, for given atomic species, depends weakly on the lattice height through changing spacial extensions of Wannier functions. On the other hand the tunnelling rate J strongly depends on the lattice depth. Thus varying the lattice depth (changing the corresponding laser intensity) once can modify J/U ratio in a broad range. The energies at different sites ε_i may be modified in a controlled way. Typically the cloud of atoms is kept in an additional optical or magnetic trap; then ε_i's may reflect the harmonic (or other) binding energy. Additional perturbation (*e.g.* the disorder treated later on) further affects ε_i values.

The behaviour of the system as J/U is varied has been extensively discussed in a number of papers, see, *e.g.*, [13]. Consider first the homogeneous case $\varepsilon_i = 0$. For vanishing U the tunnelling dominates, particles are delocalized over the whole lattice realizing the so called superfluid state. The ground state of N particles may be expressed as $|\Psi_{\rm SF}\rangle \propto \sum_i \hat{a}_i^\dagger)^N|{\rm vac}\rangle$. In the opposite limit of vanishing tunnelling $J/U \to 0$ is is clear that due to the interactions (the bosons repel each other) they tend to distribute themselves as evenly as possible among sites. If the ratio of number of particles N to number of sites M is commensurate the so called Mott insulator state may be formed, realising (in $J = 0$ limit) a Fock state at each site. A Mott insulator is characterised by a gap in the excitation spectrum. It is easy to convince oneself that, in $J = 0$ limit, the gap, $\Delta_{\rm g}$ is equal to U as this is the energy cost to move one particle to already occupied site. For increasing J the gap decreases vanishing at the point when transition to superfluid phase occurs. Thus changing the ration of J/U one may realise the quantum phase transition [3] between the insulator and the superfluid state. This has been proposed for cold atoms [2] and soon realized experimentally [4, 14].

The experimental realisation of the quantum phase transition is somewhat subtle since atoms are kept in an additional trap. In effect the density of atoms changes across the trap being largest at the centre. Even in ideal case one looses then "pure" quantum phase transition behaviour, rather a crossover between different phases is observed [15]. Thus in some areas of the trap one may observe (for sufficiently deep optical lattice) a characteristic integer filling of sites, while in the transition areas superfluid phase exists. This has been also exemplified in dynamical (mean field) simulations [16] as shown in Fig. 1.

The dynamical mean field analysis of (4) is based on the time-dependent variational principle [17]. The dynamical equations are obtained minimising

$$\langle G(t)|\, i\hbar\,\frac{\partial}{\partial t} - H(t) + \mu\hat{N}|G(t)\rangle\,, \tag{5}$$

with $H(t)$ being the time dependent Hamiltonian. This time dependence is implicit in the dependence of U, J as well as ε_i in (4) on the lattice depth

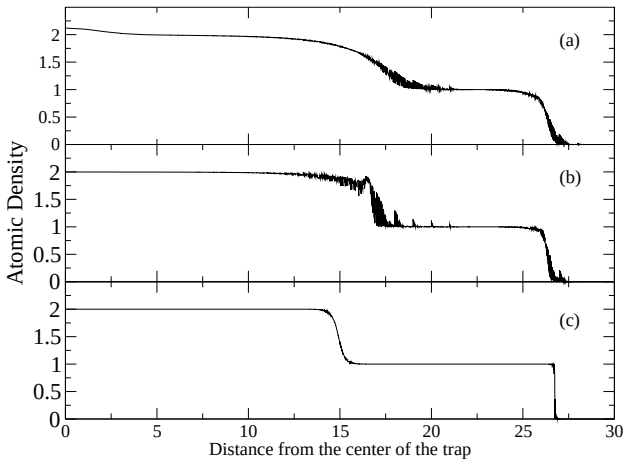

Fig. 1. Atomic density (on-site filling factor) in a trap as simulated for realistic experimental conditions of [4] experiment. Panel (a) shows the dynamical mean field final state for experimental conditions, panel (b) the situation for a more optimal lattice turn on, while panel (c) represents the mean field ground state for a deep lattice. For further discussion see text.

that is changed in a controlled way. The chemical potential μ becomes also time dependent when system parameters are varied. $|G(t)\rangle$, the variational wave function takes a standard Gutzwiller-type form

$$|G\rangle = \prod_{i=1}^{M} \left(\sum_{n=0}^{n_m} f_n^{(i)} |n\rangle_i \right) . \tag{6}$$

with $f_n^{(i)}(t)$ now being time-dependent. One thus neglects all possible entanglement between different M sites of the lattice; n_m is a maximal bosonic occupation at a given site. The very same approach has been successfully applied recently to the formation of molecules [17, 18], the treatment of the disordered optical lattices [6] as well as for determining the phase diagram in Bose–Fermi mixtures [19].

The minimisation of (5) yields the set of first order differential equations for $f_n^{(i)}(t)$:

$$i\frac{d}{dt} f_n^{(i)} = \left[\frac{U}{2} n(n-1) + n(\varepsilon_i - \mu) \right] f_n^{(i)} - J \left[\Phi_i^{\star} \sqrt{n+1} f_{n+1}^{(i)} + \Phi_i \sqrt{n} f_{n-1}^{(i)} \right] , \tag{7}$$

where $\Phi_i = \sum_{\langle j \rangle} \langle G(t)|a_j|G(t)\rangle$ (the sum, as indicated by subscript in brackets is over the nearest neighbours only). The nice feature of the evolution resulting from equations (7) is that the average number of particles $N = \langle \hat{N} \rangle$

is an exact constant of the motion [17]. This large set of equations is solved numerically to mimic as precisely as possible the experiment [4], for details see [16].

The simulations suggests that at the original conditions of the experiment [4] significant excitations occurred and insulator phase has been reached in part of the atomic sample only. For slightly slower lattice turn on, however, the insulator phase is reached in a significant part of the trap, as shown in the panel (b). It is worth stressing that the simulations (see [16] for all the details) have been performed within the mean field approximation only, exact dynamical calculations for the conditions of the experiment are impossible. Importantly also, later experiments [14] used longer times (and different geometries) ensuring the formation of the Mott insulator from the superfluid initial state. It seems now, therefore, to be a quite accepted fact that experiments [4, 14] are clear demonstrations of quantum phase transitions in necessarily finite experimental systems.

The additional experimental evidence for the existence of the insulator Mott phase is the resonance at energy U (and its multiplicities) observed in absorption studies of the condensate in the deep lattice [4]. Such a resonance is a clear indicator of the importance of the interaction energy term in the Hamiltonian (4) and of the presence of the gap (with size U) in the excitation spectrum, the gap expected for the Mott insulator.

3. The effect of disorder, strong interactions

The presence of disorder may strongly affect the behaviour of atoms in optical lattices. In the Bose–Hubbard model the problem was studied in detail by Fisher *et al.* [13]. The existence of a novel insulating phase, the Bose glass has been postulated. The transition from Mott insulator to the superfluid was argued to occur only via this third phase. The Bose glass, as opposed to Mott insulator, has no gap in the excitation spectrum and has a finite compressibility. There is no superfluid fraction — the corresponding wave function is localised.

Assume a disorder leads to some distribution of offset energies ε_i's, say, ε_i is randomly distributed in $[-\Delta/2, \Delta/2]$ interval. Then, if the gap is Δ_{g} without the disorder, it may decrease to $\Delta_{\mathrm{g}} - \Delta$. Increasing J/U we decrease Δ_{g}, reaching the limiting situation of $\Delta_{\mathrm{g}} = \Delta$ when the gap disappears. It is argued [13] that this limit gives the offset for the Bose glass phase.

Can this phase be realized in the cold atom setting? This relies on the possibility to create an appropriate disorder in the optical lattice. At least two possibilities exist [6, 20]. One can add an additional random optical potential using *e.g.* speckle radiation imagined on the atomic sample. The second possibility is to add an additional weak optical lattice with a different period. If corresponding wavelengths are incommensurate, a quasi periodic

variation of ε_i along lattice sites is generated. This is not a truly random solution but one should keep in mind that the typical atomic samples are quite limited in size, to several tens of the effective lattice sites in a given direction [4, 14]. For such a sample both a truly random and a sufficiently quasi periodic sequence should lead to similar observations.

We have verified that this is indeed the case making a dynamical mean field simulation in a two-dimensional lattice [6] following the procedure described above, Eq. (7). The question remains how to detect the appearance of the Bose glass phase. In our numerical experiment two stages were present. First the lattice was adiabatically turned on for *incommensurate* filling. In fact we assumed that the ratio of number of atoms N to number of sites M to be fixed at $\eta = N/M = 0.75$. The system remains then in the superfluid state, but the condensate fraction (*i.e.* the largest eigenvalue of the single particle density matrix) decreases to about 30% (see the inset in Fig. 2) from the original close to unity value. This is a manifestation of entering the strong interaction regime, where Mott insulator is expected at integer filling. In fact we reach U/J of the order of 70 for the considered case of Na atoms.

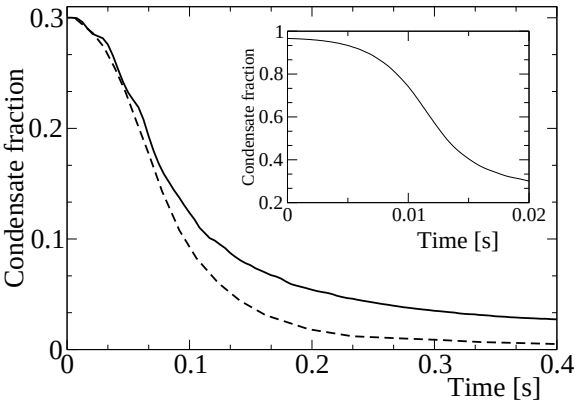

Fig. 2. Condensate (superfluid) fraction shown as a solid (dashed) line as a function of time when the disorder in the lattice is dynamically turned on. The disorder is due to incommensurate second lattice with the ratio of the primary and secondary lattice $q = 1.338$. The inset shows the first stage of the process — the turn on of the primary lattice. The lattice has 40×40 sites.

In the second state a quite weak secondary laser beams are turned on. The ratio of primary to secondary wavelength $q = 1.338$ (corresponding to say nd:YAG and Ti:sapphire lasers) is incommensurate. The secondary laser is quite weak with the resulting optical potential being a weak perturbation only of the effect due to the primary beams. The secondary beams are turned on very slowly to assure that the system remains adiabatically in the ground

state. Still the condensate fraction rapidly drops to almost a zero value (it remains at 2% level due to the finite size as well as mean field approximate calculations). Even a more dramatic is a drop in the so called superfluid fraction, see the dashed line in Fig. 2. The latter can be determined by studying the sensitivity of the system to the change of boundary conditions [6, 21]. Due to the presence of the disorder superfluidity is lost and the system lands in a localised, insulating state — the Bose glass phase. Similar behaviour is observed for rapidly changing random speckle potential [6].

The suggestion of [6] has been taken up experimentally [22]. As usual, the experimental realization differs significantly. In particular the experiment is performed with a set of one-dimensional tubes, the atoms are confined by very strong beams in the perpendicular direction. Within each tube the weak secondary beam is superimposed on top of the strong one creating the lattice, as described above. Since there is no direct way to measure the condensate (or superfluid) fraction, the experiment measures the absorption profiles. Recall that the excitation spectra in the Mott phase exhibit a resonant structures which may be associated with the presence of the gap. When the disorder is turned on, the excitation spectra change. first, the corresponding peaks broaden, later for a sufficient disorder, they disappear altogether. While the authors do not consider their results as conclusive, it seems that their experiment leads to formation of Bose glass — the state of matter not observed in other than cold atoms arrangement. The remaining challenging problem is to find new characteristics which will enable an unambiguous identification of the state of atoms.

4. The effect of disorder, weak interactions

Finally let us briefly mention the case of a shallow optical lattice potential in the presence of the disorder. As mentioned in the Introduction, in that case we have to consider an effective Gross–Pitaevski description of the condensate. This case is not tractable via a tight binding model, so we mention here very shortly the current status of disorder studies.

With no interactions, at least in the one-dimensional case, the tight-binding model with random on-site energies is equivalent to the Anderson model. As such we expect the ground state to be exponentially localised. Similar situation is expected by continuity for weak interactions. Yet three independent experiments performed in Florence [23], Orsay [24] and Hanover [25] have brought surprising, at first glance, results. In the presence of a random speckle-like light induced potential the fragmentation of the condensate was observed. However, the partial localisation observed was classical in nature. The results could be understood via localisation of the condensate at the bottoms of potential wells. Similarly, the inhibition of transport [24] could be explained as due to a purely classical, "under the bar-

rier" reflection. A detailed analysis of experimental conditions [26] revealed that two effects are vital for interpreting the results. Firstly, the random speckle-like potential, due to its origin, is slowly varying as compared *e.g.*, to the condensate healing length [24]. It thus provides a smooth modulation of the potential.

The other important effect is due to the interactions. The effective potential in the nonlinear Gross–Pitaevskii equation takes a form

$$V_{\text{eff}}(x) = \frac{x^2}{2} + V_0 \cos^2(kx) + V_{\text{dis}}(x) + gN|\phi(x)|^2 \,, \tag{8}$$

where the first term describes the harmonic trap, the condensate is kept in, the second the periodic lattice, the third the disorder, while the last term is proportional to interaction strength g, compare (1) as well as to the density of the condensate (we assume $\phi(x)$ to be square normalised to unity so N, the number of atoms appears explicitly in the effective potential). Observe that (at least for most interesting repulsive interactions, *i.e.* g positive) local minima of $V_0 \cos^2(kx) + V_{\text{dis}}(x)$ where the wavefunction supposedly localizes are "filled in" by the nonlinear term $gN|\phi(x)|^2$ smoothing the potential. Such a screening by nonlinearity is, in fact, a well known effect [27].

In effect, as discussed in detail elsewhere [26], the Anderson type of localisation may be possibly observed in quite weakly interacting systems only. To realize the feasible experimental setting one can either modify the interactions via the well known Feshbach resonance mechanism [28, 29], or increase significantly the size of the atomic cloud (by making the trap holding the atoms much weaker). Work in this direction is in progress in Hanover.

The question remains whether the nonlinear screening effect discussed above can not be turned into an advantage by considering attractive interactions (g negative). Then indeed the localisation will persist in the presence of the interactions. Yet, it is not due to disorder, it appears also in its absence — this is the so called bright soliton (a localised solution of nonlinear Gross–Pitaevskii equation). It survives in the presence of the disorder [30] but clearly the localisation mechanism in this case is not Anderson-like.

5. Mixtures of bosons and fermions

Atoms appear as bosons and fermions so a natural possibility seems to trap fermions or mixture of fermions and bosons. Spin-polarized (such polarized atoms are typically trapped in magneto–optical traps) fermions do not interact via s-wave collisions at low temperature due to Pauli exclusion principle but they can be cooled effectively by collisions with bosons [31]. In effect it is quite realistic to consider a mixture of bosons and fermions in a common trap or, *e.g.*, in an optical lattice. The latter, for a sufficiently

deep lattice, leads to a convenient description of the system in terms of a Fermi–Bose–Hubbard model [35]

$$H_{\rm BFH} = -J_{\rm B}\sum_{\langle ij\rangle} a_i^\dagger a_j - J_{\rm F}\sum_{\langle ij\rangle} f_i^\dagger f_j + \sum_i \left[\frac{1}{2}Un_i(n_i-1) - \mu_{\rm B}n_i - \mu_{\rm F}m_i\right] + V\sum_i n_i m_i\,, \tag{9}$$

where, $f_i^\dagger$, f_j are fermionic creation and annihilation operators, $m_i = f_i^\dagger f_i$ while V denotes the interaction between fermions and bosons and $\mu_{\rm B}$ ($\mu_{\rm F}$) is the chemical potential for bosons (fermions), similarly $J_{\rm B}$ ($J_{\rm F}$) denotes the corresponding tunnelling rates. To minimise the number of parameters of the model, we assume $J_{\rm B} = J_{\rm F} = J$. Even in the strong coupling limit $J \ll U, V$ the phase diagram of the system may be quite reach, in particular, if boson–fermion interaction is attractive (repulsive) composite fermions composed of a fermion and a boson (correspondingly, a bosonic hole) may be formed. The subject, also in the presence of the disorder, has been extensively reviewed recently [7, 36, 37] so I refer the interested reader to these sources. It is sufficient to mention that disordered mixtures allow for simulation of spin glass physics, as well as quantum percolation effects.

6. Summary

I have reviewed briefly how cold atoms placed in an optical lattice may serve as a versatile tool to mimic standard condensed matter models. This may open a novel experimental field of *controlled* studies of such models since most of the parameters may be modified at will in the cold atoms settings. In particular, one may attempt novel studies of disorder with a quite different perspective. Rather than being interested in properties "averaged over disorder", cold atoms allow for a repeated controlled studies of single realizations of the disorder. This opens up new and fascinating possibilities.

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