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Doublon relaxation in the Bose-Hubbard model

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Decay of a high-energy double occupancy state, doublon, in a narrow-band lattice requires creation of a coherent many-particle excitation. This leads to an exponentially long relaxation time of such a state. We show that, if the average occupation number is sufficiently small, the corresponding exponent may be evaluated exactly. To this end we develop the quasiclassical approach to calculation of the high-order tree-level decay amplitudes.

Recent experiments with cold atomic gases in optical lattices [1] allowed to create realizations of Hubbard model with high degree of control over the main parameters, the bandwidth W and the on-site interaction U . In addition to exploring rich equilibrium phase diagram [2], a rapid time variation of the parameters allows to prepare atomic systems in highly excited states suitable for studies of the far from equilibrium dynamics of this strongly correlated system. The most prominent high-energy excitations are repulsively bound doubly occupied sites called doublons [3]. They were recently observed in experiments with both bosonic [3] and fermionic [4] atoms. The dynamical properties of doublons were considered in recent publications [5–7].

In experiments doublon energy $U_d = U + W$ stays between the first and second Bloch bands, which allows to consider the single band Hubbard model. In the absence of other particles doublon is the stable excitation with a very heavy mass [3]. If other particles with the average occupation ρ_0 are present, they offer a possibility for doublon to decay by transferring its interaction energy to the kinetic energy of single-particle excitations. In the interesting limit $\nu = U_d/W \gg 1$, the number of such final state excited particles $n \geq \nu$ is very large. Similar multi particle production process is encountered in many physical situations, from liquid helium [8] to high energy physics [9, 10]. Given a high degree of control typical for the experiments on cold atomic gases, the experiments on doublon decay can bring useful insight on these phenomena.

Calculation of the relaxation rate requires therefore analyzing very high orders of the perturbation theory in the inter-particle interactions. Such an analysis for nearly half-filled fermionic model was recently performed in Ref. [5], which found that the decay rate scales as $\tau^{-1} \propto \exp\{-\alpha \nu \ln \nu\}$, where α was found to be approximately 0.8.

In this letter we show that if the problem admits a small parameter – the average filling factor $\rho_0 \ll 1$, the leading exponential scaling of the decay rate may be found exactly. We use the Bose-Hubbard version of the model for the illustration. Our approach allows one to

calculate generating function of *all* n -particle tree-level threshold (i.e. such that $\nu = n$) amplitudes. Such a generating function is shown to obey *classical* equation of motion for the coupled doublon and particle fields. Luckily this equation admits an analytic solution, which yields exact expression for the tree-level amplitudes. The use of the tree approximation is justified as long as $\rho_0 \nu < \gamma_D$, where $\gamma_D = e^{-3}(\pi/2e)^{D/2}$ and D is spatial dimensionality of the lattice. The similar approach was developed in high-energy physics for calculation of the threshold amplitudes for $1 \rightarrow n$ and $2 \rightarrow n$ deep inelastic scattering processes [9, 10].

If $\rho_0 \ll \gamma_D$, the window of parameters $1 \ll \nu < \gamma_D/\rho_0$ exists where the loop diagrams may be neglected as carrying extra small factors ρ_0 and only tree diagrams contribute to the decay rate. They may be effectively summed up with the quasiclassical procedure, described below, leading to the doublon decay rate

$$\frac{1}{\tau} \propto \frac{W\nu^2}{\hbar\rho_0^2} \exp \left\{ -\nu \ln \left[\frac{\gamma_D}{\rho_0\nu} \left(\frac{2}{D} \ln \frac{\gamma_D}{\rho_0\nu} \right)^{\frac{D}{2}} \right] \right\}. \quad (1)$$

The pre-exponential factor is affected by the loop diagrams and is beyond the accuracy of the quasiclassical calculation. The factor $[(2/D) \ln(\gamma_D/\rho_0\nu)]^{D/2}$ originates from spreading wavepacket of excited particles in D spatial dimensions [11]. Apart from this factor, the result in Eq. (1) reminds Landau expression for the multi-quanta excitation of a nonlinear zero-dimensional oscillator [12].

We consider Bose-Hubbard model on a D -dimensional cubic lattice

$$H = -J \sum_{(i,j)} c_i^\dagger c_j + \frac{U}{2} \sum_i c_i^\dagger c_i^\dagger c_i c_i \quad (2)$$

where (i, j) denote nearest neighbor sites. The first term in the Hamiltonian, H_0 describes the hopping between adjacent sites and creates a band of the delocalized single particle states of the width $W = 4JD$ proportional to the tunneling amplitude J [1, 2]. Its dispersion relation is symmetric around zero energy $\epsilon_{\mathbf{k}} = -2J \sum_{\mu=1}^D \cos k_\mu$, where $-\pi < k_\mu \leq \pi$ is the quasimomentum within the

first Brillouin zone, measured in units of the inverse lattice spacing a . In the optical lattice, the lattice spacing is given by the half of the laser wave length, while the on-site repulsion U is proportional to the bulk s -wave scattering length a_s [1, 2], which in turn can be tuned experimentally in the wide range by taking advantage of Feshbach resonance phenomenon.

The zero-temperature phase diagram of this model consists of the superfluid and the Mott-insulator phases [1, 13]. The Mott insulator is characterized by an integer occupation number ρ_0 at each site and a finite energy gap for the quasiparticle excitations. On the other hand, the compressible superfluid phase is characterized by the presence of the Bose condensate with a noninteger average occupation ρ_0 . We restrict ourselves with the latter scenario at $\rho_0 \ll 1$.

Among the momentum content $c_{\mathbf{k}}$ of the bosonic fields a special role is played by the field $c_0(t) = \sqrt{\rho_0} e^{-i\mu t}$, representing the condensate with the chemical potential $\mu = -W/2$. We shall also separate the field $c_\pi(t)$, describing quantized particles with the energy $\epsilon_\pi - \mu = W$ at the very top of the Bloch band. To proceed we pass to a coherent state functional representation for the evolution operator e^{iHt} and decouple the interaction term in Eq. (2) with the help of the Hubbard-Stratonovich transformation

$$\frac{U}{2} \bar{c}_i c_i c_i c_i = \frac{\bar{d}_i d_i}{2U} - \frac{1}{2} (\bar{c}_i, c_i) \begin{pmatrix} 0 & d_i \\ \bar{d}_i & 0 \end{pmatrix} \begin{pmatrix} c_i \\ \bar{c}_i \end{pmatrix}, \quad (3)$$

introducing the auxiliary field $d_i(t)$ which describes the doublon. We now perform Gaussian integration over bosonic fields $c_{\mathbf{k}}$ with $\mathbf{k} \neq 0, \pi$, using the free propagator $G_{\mathbf{k}}(\epsilon) = (\epsilon - \epsilon_{\mathbf{k}})^{-1}$, and expand the resulting action to the second order in the d -fields [14]. This leads to the doublon Lagrangian

$$\mathcal{L}_d = \frac{1}{2} \sum_{\mathbf{q}} \bar{d}_{\mathbf{q}}(\epsilon) [U^{-1} - \mathcal{C}(\epsilon, \mathbf{q})] d_{\mathbf{q}}(\epsilon), \quad (4)$$

where $\mathcal{C}(\epsilon, \mathbf{q})$ is the Cooper polarization given by

$$\mathcal{C}(\epsilon, \mathbf{q}) = i \sum_{\mathbf{k}, \bar{\epsilon}} G_{\mathbf{k}+\mathbf{q}}(\epsilon - \epsilon') G_{-\mathbf{k}}(\epsilon') = \sum_{\mathbf{k}} \frac{1}{\epsilon - \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{-\mathbf{k}}}. \quad (5)$$

The poles of the doublon propagator, i.e. $\mathcal{C}(\epsilon, \mathbf{q}) = U^{-1}$, determine its dispersion relation $\epsilon = \epsilon_d(\mathbf{q})$. In the limit $U \gg J$ one may expand the denominator on the right hand side of Eq. (5) to the second order to find [3]

$$\epsilon_d(\mathbf{q}) \approx U + \frac{8J^2}{U} \sum_{\mu=1}^D \cos^2 \frac{q_\mu}{2} + O(J^4/U^3). \quad (6)$$

Therefore the doublon band is narrow $W^2/2DU \ll W$. One can thus disregard the \mathbf{q} -dependence of the doublon dispersion and think of it as of infinitely heavy localized particle with the energy U . This is equivalent to the

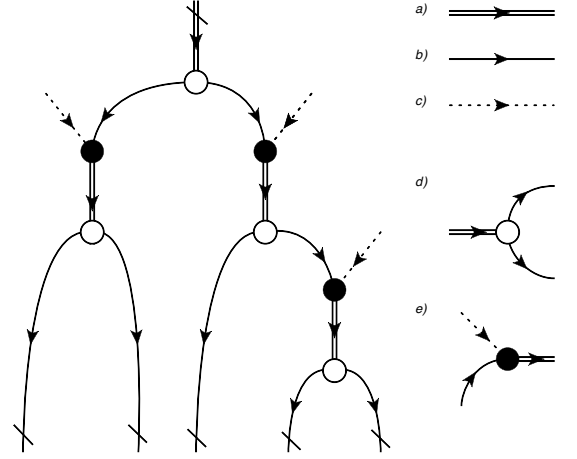


FIG. 1. An example of a tree-level diagram for the amplitude of the doublon decay in $n = 5$ particles. a) Doublon propagator $\langle d\bar{d} \rangle$; b) particle propagator $\langle c_\pi \bar{c}_\pi \rangle$; c) condensate amplitude $c_0 \propto \sqrt{\rho_0}$; d) doublon decay vertex $\bar{c}_\pi \bar{c}_\pi d$; e) particle interaction with the condensate vertex $\bar{d} c_0 c_\pi$. Crossed lines denote the mass-shell particles.

approximation where one takes $\mathcal{C}(\epsilon, \mathbf{q}) \approx \mathcal{C}(\epsilon, \pi) = \epsilon^{-1}$. Hereafter we suppress site or momentum index of the doublon, assuming it to be localized and infinitely heavy.

In the absence of the condensate, $\rho_0 = 0$, the doublon is absolutely stable, which is reflected in the presence of the true pole in its Green function, cf. Eq. (4), at $\epsilon \approx U$. Interaction with the condensate results in the doublon self-energy $\Sigma(\epsilon)$. Its imaginary part taken at the mass-shell is the doublon decay rate $1/2\tau = \text{Im}\Sigma(U)$, which is the focus of this letter. With the help of the vertex $\bar{c}_\pi \bar{c}_\pi d$, cf. Eq. (3), the doublon initially decays onto two virtual particles with momenta close to the boundaries of the Brillouin zone. Each of the created particles may collide with the condensate and with the help of the vertex $\bar{d} c_0 c_\pi$ create more virtual doublons, the latter again decay, *etc.* This process, depicted in Fig. 1, continues until the initial doublon energy (counted from the chemical potential) $U_d = U - 2\mu = U + W$ is transferred into the kinetic energy of $n \geq U_d/W$ real particles. The corresponding decay rate is given by the Golden Rule

$$\frac{1}{\tau} = \sum_{n > U_d/W} \frac{2\pi}{\hbar} \sum_{\mathbf{p}_1, \dots, \mathbf{p}_n} |\mathcal{A}_n|^2 \delta \left(U_d - \sum_{l=1}^n (\epsilon_{\mathbf{p}_l} - \mu) \right), \quad (7)$$

$$\mathcal{A}_n(U_d; \mathbf{p}_1, \dots, \mathbf{p}_n) = \langle \mathbf{p}_1, \dots, \mathbf{p}_n | c_\pi^\dagger c_\pi^\dagger d | d \rangle,$$

where $\langle \mathbf{p}_1, \dots, \mathbf{p}_n |$ is the final n -particle excited state of the *interacting* gas and $|d\rangle$ is the initial state with the single doublon and rest of the gas in the condensate.

Consider now a special situation where the doublon energy happens to be slightly below the n -particle creation threshold $U_d \lesssim nW$. In this case all n final

particles must be very close to the top of the band. One may thus approximate their dispersion relation as $\epsilon_{\mathbf{p}_l} - \mu = W - (\mathbf{p}_l - \pi)^2/2m^*$, where $m^* = (2J)^{-1}$ is the effective mass. The corresponding phase volume for the decay process

$$\mathcal{V}_n = \sum_{\mathbf{p}_1, \dots, \mathbf{p}_n} \delta\left(U_d - \sum_{l=1}^n (\epsilon_{\mathbf{p}_l} - \mu)\right) = \frac{[(nW - U_d)/4\pi J]^{\frac{Dn}{2}}}{\Gamma\left(\frac{Dn}{2}\right) (nW - U_d)} \quad (8)$$

depends very strongly on the deviation $nW - U_d > 0$ from the threshold. On the other hand, the corresponding matrix element $\mathcal{A}_n(U_d; \mathbf{p}_1, \dots, \mathbf{p}_n)$ appears to be a smooth function of U_d . This implies that in the vicinity of the threshold it may be substituted by a constant $\mathcal{A}_n \approx \mathcal{A}_n(nW; \pi, \dots, \pi)$. Indeed, once the doublon energy is fixed at the n -particle threshold $U_d = nW$, all final state particles must be at the top of the band, i.e. in the same quantum state with $\mathbf{p} = \pi$. Therefore only $\mathbf{p} = \pi$ state (along with the condensate $\mathbf{p} = 0$) may ever appear as a real particle, while the rest of (already integrated out) states are purely virtual. As a result the decay rate of the doublon with the energy U_d is given by

$$\frac{1}{\tau(U_d)} = \frac{2\pi}{\hbar} \sum_{n > U_d/W} |\mathcal{A}_n|^2 \mathcal{V}_n(U_d). \quad (9)$$

The crack of the matter thus is to evaluate the threshold amplitudes \mathcal{A}_n .

If the doublon energy U_d is not too large the leading contribution to the amplitude comes from the *tree-level* diagrams, i.e. those which do not include loops. Indeed for the same number of the final state mass-shell particles n , a loop diagram involves a higher order of the perturbation theory than a corresponding tree one. Such tree level diagrams are generated by repeated Wick contractions of the two types of vertices $\bar{c}_\pi \bar{c}_\pi d$ and $\bar{d} c_0 c_\pi$. The Hermitian conjugated vertices participate only in the loop diagrams. As a result, the tree level amplitudes are generated by the following Lagrangian

$$\mathcal{L} = \frac{1}{2} \bar{d} \left[\frac{1}{U} - \frac{1}{\epsilon} \right] d + \bar{c}_\pi \left(i\partial_t - \frac{W}{2} \right) c_\pi - \frac{1}{2} \bar{c}_\pi \bar{c}_\pi d - \bar{d} c_\pi c_0, \quad (10)$$

where the condensate field possesses a classical expectation value $c_0(t) = \sqrt{\rho_0} e^{iWt/2}$. Since the tree-generating Lagrangian is linear in annihilation fields $c_\pi(t)$ and $d(t)$, the functional integration over these fields enforces equations of motion for the corresponding creation components $\bar{c}_\pi(t)$ and $\bar{d}(t)$. To avoid the time non-local operator $1/\epsilon$ let us define an auxiliary dimensionless field $\bar{\sigma} = \bar{d}/\epsilon$, i.e. $\bar{d}(t) = -i\partial_t \bar{\sigma}(t)$. It is also convenient to shift the energies for the condensate to be at zero by the gauge transformation $\bar{c}_\pi \rightarrow \bar{c}_\pi e^{-iWt/2}$ and $\bar{\sigma} \rightarrow \bar{\sigma} e^{-iWt}$. Taking then variation of the Lagrangian (10) with respect to c_π and d , one obtains the following equations of

motion

$$(-i\partial_t - W) \bar{c}_\pi = \sqrt{\rho_0} (-i\partial_t - W) \bar{\sigma}; \quad (11)$$

$$(-i\partial_t - U_d) \bar{\sigma} = U \bar{c}_\pi \bar{c}_\pi. \quad (12)$$

The solution we seek may be written as a series of positive powers of $z(t) = e^{iWt}$. For example $\bar{c}_\pi(t) = \sum_{n=1}^{\infty} \alpha_n z^n$, where α_n represent the tree diagrams starting with one virtual particle and ending up with n mass-shell particles, each having the energy W (thus the factor e^{inWt}). The proper normalization is thus $\alpha_1 = 1$. Similarly $\bar{\sigma}(t) = \sum_{n=1}^{\infty} \beta_n z^n$, generates tree diagrams which start from the doublon and end up with n mass-shell particles, Fig. 1. Since the doublon must decay at least on two particles, the normalization is $\beta_1 = 0$.

The properly normalized solution of Eq. (11) is thus

$$\bar{c}_\pi = e^{iWt} + \sqrt{\rho_0} \bar{\sigma}. \quad (13)$$

Expressing $\bar{\sigma}$ and employing Eq. (12), one finds

$$(i\partial_t + U_d) \bar{c}_\pi + U \sqrt{\rho_0} \bar{c}_\pi^2 = U e^{iWt}. \quad (14)$$

This equation describes a weakly non-linear high frequency U_d oscillator, which is forced with the low frequency $W \ll U_d$ driving force. The non-linearity generates higher harmonics of the applied force, bringing the oscillator into the exact resonance if $U_d/W = n$ is an integer. One expects thus the solution to have a pole $(nW - U_d)^{-1}$, reflecting the resonance condition. This pole represents the Green function of the incoming doublon at the threshold energy $\epsilon = nW$. Since we are interested in the self-energy $\Sigma(nW)$ rather than the Green function itself, we need to focus only on the residue of the corresponding pole. The latter is a function of time given by a series in powers of z . The threshold amplitude \mathcal{A}_n is proportional to the coefficient in front of $z^n = e^{inWt}$ term of this series. Indeed, it is exactly the term $z^n \bar{z}^n = e^{inW(t-t')}$ in $\langle \bar{d}(t) d(t') \rangle$, which generates the proper delta-function in Eq. (7) upon the Fourier transform.

Equation (14) is of Riccati type, which may be transformed into the linear second order differential equation by the substitution $\bar{c}_\pi = i\partial_t v / (U \sqrt{\rho_0} v)$. Changing also the variable $t \rightarrow z$ and using $\nu = U_d/W$, one finds

$$z \partial_z^2 v - (\nu - 1) \partial_z v - \sqrt{\rho_0} (\nu - 1)^2 v = 0. \quad (15)$$

The exact solution of Eq. (15) is given in terms of the Bessel functions

$$v(z) = (bz)^{\nu/2} \left\{ C_1 \Gamma(1 - \nu) I_{-\nu}(2\sqrt{bz}) + (-1)^\nu C_2 \Gamma(1 + \nu) I_\nu(2\sqrt{bz}) \right\}, \quad (16)$$

where $b = \sqrt{\rho_0} (\nu - 1)^2$, and C_1 and C_2 are free integration constants. As explained above, we look for the resonant poles of the form $z^n/(n - \nu)$ at integer values

of ν . It is easy to see that they may come only from the first term on the r.h.s. of Eq. (16), which reads as

$$v(z) = C_1 \Gamma(1 - \nu) \sum_{k=0}^{\infty} \frac{(bz)^k}{k! \Gamma(k + 1 - \nu)}. \quad (17)$$

The pole structure can be made explicit by rewriting the coefficient of z^k in the form

$$\frac{\Gamma(1 - \nu)}{\Gamma(k + 1 - \nu)} = \frac{1}{(k - \nu)(k - 1 - \nu) \dots (1 - \nu)}. \quad (18)$$

At integer $\nu = n$ it contains poles for $k = n, n + 1, \dots$. The resonant time dependence z^n is provided only by the pole with the lowest value $k = n$. Other pole terms contribute to the decay processes with more than n outgoing particles and are neglected. Notice also that at $z \rightarrow 0$ one has $\bar{c}_\pi = -(W/U\sqrt{\rho_0})z\partial_z \ln v = z + O(z^2)$, which provides the proper normalization of the generating function for tree diagrams. The appropriate term in the expansion of $\bar{c}_\pi(z)$ takes the form $[\bar{c}_\pi]_n z^n / (n - \nu)$, where the coefficient

$$[\bar{c}_\pi]_n = (-1)^n \frac{(n - 1)^{2n-1} \rho_0^{\frac{n-1}{2}}}{[(n - 1)!]^2}. \quad (19)$$

is evaluated at $\nu = n$. Recalling that $\bar{\sigma}(z) = (\bar{c}_\pi - z)/\sqrt{\rho_0}$, Eq. (13), while the doublon field is $\bar{d}(z) = Wz\partial_z \bar{\sigma}(z)$, one finds for the n -particle threshold amplitude $\mathcal{A}_n = \sqrt{n!} [\bar{d}]_n$

$$\mathcal{A}_n = W\sqrt{n!} (-1)^n \frac{(n - 1)^{2n} \rho_0^{\frac{n}{2}-1}}{[(n - 1)!]^2}, \quad (20)$$

where the proportionality coefficient $\sqrt{n!}$ originates from the $n!$ ways of pairing n final on mass-shell \bar{c}_π -particles in the doublon self-energy.

The total decay rate of the doublon is calculated by summing up over all open decay channels according to Eq. (9). Substituting explicit expressions for the decay amplitude Eq. (20) and the phase volume Eq. (8), we obtain the decay rate in form of the asymptotic series

$$\frac{1}{\tau} = \frac{2\pi W}{\hbar \rho_0^2} \sum_{n>\nu} \frac{n(n - 1)^{4n} (n - \nu)^{\frac{Dn}{2}-1}}{\Gamma(\frac{Dn}{2}) \Gamma^3(n)} \left(\frac{D^{D/2} \rho_0}{\pi^{D/2}} \right)^n. \quad (21)$$

To sum up the series one employs Stirling formula for gamma functions, substitutes summation by the integration and performs the latter in the stationary point approximation. As a result, one obtains the expression (1) for the doublon decay rate.

Controlling experimental parameters it is possible to form an initial state with a known fraction of single-occupied sites. Measuring the decay rate of doublons similarly to Ref. [4] will produce an experimental check of our theory and extend its results beyond leading tree approximation [15].

In conclusion, the decay of doublon is accompanied by creation of a many-particle excitation. In a certain range of parameters, dictated by a small filling factor, such process is described by tree-level diagrams. If this is the case, it is amenable to the semiclassical evaluation close in spirit to Ref. [12]. We performed this calculation for the Bose-Hubbard model in the superfluid phase and determined exactly the leading terms in the decay rate exponent. While our calculations are performed at zero temperature, the results are expected to be valid as long as $T \lesssim J$, such that majority of bosons occupy states which are close to the bottom of the band.

It remains to be seen if the method and the results can be adopted to the Fermi-Hubbard model, treated in Ref. [5] by other means. Another exciting question left for the future research is spatial diffusion of the doublon (due to stochastic recoil momenta from emission of virtual particles) as well as the role of the trap confinement.

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- [14] The higher orders of the expansion represent interactions between different double occupied sides. They may be therefore safely neglected if concentration of double occupancies is sufficiently low.
- [15] One may argue that the most general scaling form of the decay time is given by $\ln \tau = \rho_0^{-1} h_D(x)$, where $x = \rho_0 \nu$.

The dimensionless function $h_D(x)$ is known in high energy physics as a “Holy Grail” function [9]. The semiclassical methods allow to evaluate it in the limit $x \ll 1$, cf. Eq. (1). There are arguments (see Ref. [9]) that it either saturates, or grows extremely slowly at $x \gtrsim 1$.