The simplest quantum model for the Kibble-Zurek mechanism of topological defect production: Landau-Zener transitions from a new perspective

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It is shown that dynamics of the Landau-Zener model can be accurately described in terms of the Kibble-Zurek theory of the topological defect production in nonequilibrium phase transitions. The simplest quantum model exhibiting the Kibble-Zurek mechanism is presented. New analytical predictions concerning dynamics of the Landau-Zener model are found.

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In this paper we present a successful combination of the Kibble-Zurek (KZ) [1, 2] theory of topological defect production and quantum theory of the Landau-Zener (LZ) model [3]. Both theories play a prominent role in contemporary physics. The KZ theory predicts production of topological defects (vortices, strings) in the course of nonequilibrium phase transitions. This prediction applies to phase transitions in liquid ^{4}He and ^{3}He, liquid crystals, superconductors, ultracold atoms in optical lattices [4, 5], and even to cosmological phase transitions in the early Universe [1, 2]. The Landau-Zener theory has even broader applications. It has already become a standard tool in quantum optics, atomic and molecular physics, and solid state physics. The list of important physical systems governed by the LZ model grows. For instance, recent investigations point out that the smallest quantum magnets, Fe_8 clusters cooled below 0.36K, are successfully described by the LZ model [6].

This paper constructs the simplest quantum model whose dynamics remarkably resembles dynamics of topological defect production in nonequilibrium second order phase transitions. The model is built on the basis of LZ theory and allows us to study the KZ mechanism of topological defect production in a truly quantum case. Such a quantum insight into the KZ theory was up to now inaccessible except for the recent study of KZ theory in optical lattices filled with ultracold atoms [5]. In addition, we present a simple, intuitive, and accurate description of LZ model dynamics. In particular, we predict existence of modified exponential transition probabilities when time evolution starts in the neighborhood of an anticrossing.

For the rest of the paper it is essential to introduce briefly the KZ theory. Consider a pressure quench that drives liquid ^{4}He from a normal phase to a superfluid one at a finite rate. Suppose the transition point is crossed at time $t = 0$, while the time evolution starts at $t \ll 0$. As long as the liquid is far away from the transition point its time evolution is adiabatic. In other words, the relaxation time scale τ, which tells how much time the system needs to adjust to new thermodynamic conditions, is small enough. As the transition is approached the critical slowing down occurs, i. e. $\tau \to \infty$, so that at the instant $-\hat{t}$ the system leaves adiabatic regime and enters an impulse one where its state is effectively frozen. The time $\hat{t}$ is called the freeze-out time and was introduced by Zurek [2]. As the quench proceeds after crossing the transition point, the relaxation time scale decreases. At the instant $\hat{t}$, the system goes back into an adiabatic regime. The freeze-out time is determined by the equality: $\tau(\hat{t}) = \hat{t}$ [2]. For the case of liquid ^{4}He one finds $\tau = \tau_0/|\varepsilon|$, where τ_0 is a constant, while ε is called the relative temperature. The latter measures the distance of the liquid from a transition point being at $\varepsilon = 0$, i. e. $\varepsilon(t = 0) = 0$. Physically changes of pressure translate into changes of ε. It is further assumed that pressure changes are such that $\varepsilon = t/\tau_Q$, where τ_Q is a quench timescale. Simple calculation immediately leads to: $\hat{t} = \sqrt{\tau_Q\tau_0}$. Such a nonequilibrium phase transition leads to appearance of topological defects, e. g. vortices, whose density can be determined, up to a quench-independent factor, by system's properties at the freeze-out instant $-\hat{t}$.

We consider time dependent Hamiltonian

$$\frac{1}{2}\begin{pmatrix} \Delta\cdot t & \omega_0 \\ \omega_0 & -\Delta\cdot t \end{pmatrix} \tag{1}$$

written in the basis of time independent states $|1\rangle$ and $|2\rangle$. Eigenstates of (1) have the form

$$\begin{bmatrix} |\uparrow(t)\rangle \\ |\downarrow(t)\rangle \end{bmatrix} = \begin{pmatrix} \cos(\theta(t)/2) & \sin(\theta(t)/2) \\ -\sin(\theta(t)/2) & \cos(\theta(t)/2) \end{pmatrix} \begin{bmatrix} |1\rangle \\ |2\rangle \end{bmatrix},$$

where $\cos(\theta) = \varepsilon/\sqrt{1+\varepsilon^2}$, $\sin(\theta) = 1/\sqrt{1+\varepsilon^2}$, $\theta \in [0,\pi]$, $\varepsilon = \Delta\cdot t/\omega_0$. As in LZ theory $\Delta, \omega_0 > 0$ are constant parameters. The level structure of (1) is depicted in Fig. 1a, while the gap equals $\sqrt{\omega_0^2 + (\Delta\cdot t)^2}$.

Topological defects can be introduced into the LZ model in the following way. Suppose the state $|1\rangle$ corresponds to a vortex state being an eigenstate of angular momentum operator: $\hat{L}_z|1\rangle = n|1\rangle$ $(n = \pm1, \pm2, \ldots)$, while the state $|2\rangle$ satisfies $\hat{L}_z|2\rangle = 0$. System's wave function can be written as $|\Psi\rangle = a|1\rangle + b|2\rangle$ $(|a|^2 + |b|^2 = 1$, $\langle i|j\rangle = \delta_{ij})$. We propose to identify the density of topological defects with the average value of angular momentum: $\langle\Psi|\hat{L}_z|\Psi\rangle = n|a|^2$ [7]. For the rest of discussion we define normalized to unity density of defects as [8]

$$\mathcal{D}_n := \langle\Psi|\hat{L}_z|\Psi\rangle/n = |\langle\Psi|1\rangle|^2. \tag{2}$$

In general, one can expect that the state with $a, b \neq 0$ contains $|n|$ vortices of unit circulation because vortices with multiple topological charge are presumably unstable against such splitting- see [9] for an example. Suppose now that the system undergoes adiabatic time evolution from the ground state of (1) at $t \to -\infty$ to the ground state of (1) at $t \to \infty$. Therefore, the state of the system undergoes the "phase transition" from $|1\rangle$ to $|2\rangle$, i. e. from a vortex-defected "phase" to a vortex-free one. If time evolution fails to be adiabatic, which is usually the case, the final state of the system is a superposition of states $|1\rangle$ and $|2\rangle$ so that the final density of topological defects becomes non-zero. We will show that the KZ-like theory predicts surprisingly correctly vortex density (2) as a function of a transition rate only.

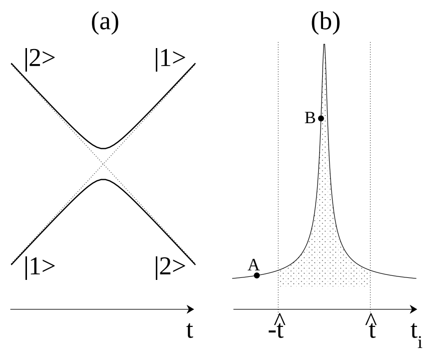

FIG. 1: Plot (a): energy levels of the Hamiltonian (1). Dotted line: $\omega_0 = 0$ case. Plot (b): inverse of the gap as a function of time. The dotted part corresponds to the impulse regime.

Analogs of relaxation timescale, relative temperature and quench timescale are identified as follows. As known from the adiabatic approximation, inverse of the gap determines how long the system follows adiabatically changes of the Hamiltonian in the course of time evolution. Therefore, we propose to consider it as a quantum mechanical equivalent of the relaxation timescale introduced above: we set $\tau = 1/\sqrt{\omega_0^2 + (\Delta \cdot t)^2}$ [10]. The equivalent of the relative temperature ε, i. e. a dimensionless distance of the system from anticrossing, is $\Delta \cdot t/\omega_0$. As a quench timescale τ_Q we take ω_0/Δ, while ω_0 we identify with $1/\tau_0$. Finally, we arrive at

$$\tau = \frac{\tau_0}{\sqrt{1+\varepsilon^2}} \quad , \quad \varepsilon = \frac{t}{\tau_Q}. \tag{3}$$

For $|\varepsilon| \gg 1$ expressions (3) are identical as those introduced above in the context of topological defect production in liquid ^{4}He, which will be commented below.

In the following we consider dynamics of the LZ model described by the Schrödinger equation: $i\frac{d}{dt}|\Psi\rangle = \hat{H}|\Psi\rangle$, with $\hat{H}$ given by (1). We assume that time evolution starts from a ground state of (1) at some $t = t_i$ and lasts till $t_f \to +\infty$. The quantity of interest will be density of defects (2) at the end of time evolution, which is in fact the probability of finding the system in the excited eigenstate at t_f. From the KZ perspective we propose to classify time evolutions into two non-trivial schemes:

A: $t_i < -\hat{t}$: the point A in Fig. 1b. The evolution is adiabatic from t_i till $-\hat{t}$, then impulse from $-\hat{t}$ to $\hat{t}$, and finally adiabatic from $\hat{t}$ to t_f,

B: $t_i \in [-\hat{t}, \hat{t}]$: the point B in Fig. 1b. From t_i to $\hat{t}$ the evolution is impulse, while from $\hat{t}$ to t_f adiabatic.

The statement that the evolution is impulse means that the system's wave function changes by the overall phase factor only. All these assumptions are, of course, approximate and heuristic as the whole KZ theory is, and our aim is to find how good they work in the LZ system. The only quantity that is still unknown is the instant $\hat{t}$. It is found from the equation originally proposed by Zurek in the context of classical phase transitions [2]

$$\tau(\hat{t}\,) = \alpha\hat{t}, \tag{4}$$

and modified by us by a factor $\alpha = \mathcal{O}(1)$, i. e. the only free parameter of our theory *independent* of τ_Q and τ_0. The solution of (4) reads

$$\hat{\varepsilon} = \varepsilon(\hat{t}\,) = \frac{1}{\sqrt{2}}\sqrt{\sqrt{1+\frac{4}{x_\alpha^2}} - 1}, \quad x_\alpha = \alpha\frac{\tau_Q}{\tau_0}. \tag{5}$$

The first observation shows that for fast transitions, i. e. $x_\alpha \to 0$ at τ_0 being fixed, one gets $\hat{t} = \sqrt{\tau_0\tau_Q/\alpha}$. Therefore we recover, up to $\mathcal{O}(1)$ factor, the well known result [2]. It happens because in the fast transition limit $\hat{\varepsilon} \gg 1$ and then $\tau(\hat{\varepsilon}) \approx \tau_0/\hat{\varepsilon}$, which is the same as in the theory of dynamics of quantum phase transitions in liquid ^{4}He [2]. This observation further supports similarities of our model to KZ systems.

For the first application of our theory we consider the situation when time evolution starts far away from the anticrossing - a generic **A** scheme case. Taking $|\Psi(t_i)\rangle = |\downarrow(t_i)\rangle$ as an initial system's wave function, and assuming limits $t_i \to -\infty$ and $t_f \to \infty$, one easily gets the following final density of topological defects

$$\mathcal{D}_n = |\langle\Psi(t_f)|1\rangle|^2 \approx |\langle\uparrow(\hat{t}\,)|\downarrow(-\hat{t}\,)\rangle|^2 = \frac{\hat{\varepsilon}^2}{1+\hat{\varepsilon}^2}. \tag{6}$$

Derivation of (6) uses the following relations: $|\langle\uparrow(t_f)|\Psi(t_f)\rangle| \approx |\langle\uparrow(\hat{t}\,)|\Psi(\hat{t}\,)\rangle| \approx |\langle\uparrow(\hat{t}\,)|\Psi(-\hat{t}\,)\rangle| \approx |\langle\uparrow(\hat{t}\,)|\downarrow(-\hat{t}\,)\rangle|$. Substitution of (5) into (6) gives

$$\mathcal{D}_n = \frac{2}{\mathcal{P}(x_\alpha)} \quad , \quad \mathcal{P}(x_\alpha) = x_\alpha^2 + x_\alpha\sqrt{x_\alpha^2+4} + 2. \tag{7}$$

Expanding $\mathcal{D}_n$ into a series one gets for fast transitions

$$\mathcal{D}_n = \exp(-x_\alpha) + \mathcal{O}\left(x_\alpha^3\right), \tag{8}$$

which is an exact result up to $\mathcal{O}\left(x_\alpha^3\right)$ terms if the constant α is chosen as $\pi/2$ [3]. Notice that $\alpha = \mathcal{O}(1)$ as assumed in (4). In the adiabatic limit ($x_\alpha \to \infty$), Eq.

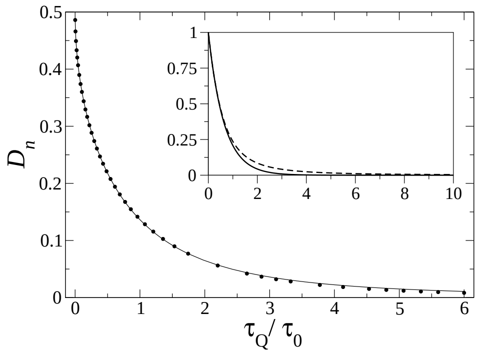

FIG. 2: Density of defects for the system whose evolution starts at the anticrossing center. Solid line prediction (10), dots- numerical data. The parameter $\alpha = 0.77$ was found from fit of (10) to numerics. Inset: exact vs. approximate density of defects when $t_i \to -\infty$. Solid line exact result $\exp(-\pi\tau_Q/2\tau_0)$, dashed line Eq. (7) with $\alpha = \pi/2$.

(7) predicts $\mathcal{D}_n = \mathcal{O}(1/x_\alpha^2)$ instead of exponential decay, which does not affect results much due to very small value of $\mathcal{D}_n$ in that regime- see inset of Fig. 2.

The best performance for fast transitions can be understood as follows. The derivation of (6) requires assumption that in the time interval $[-\hat{t}, \hat{t}\,]$ the state of the system does not change essentially. The smaller is this time interval the better is this assumption. From (3) and (5) one easily finds that $\hat{t}/\tau_0$ grows monotonically with x_α. Indeed, $\hat{t}/\tau_0$ equals $\sqrt{x_\alpha}/\alpha$ for $x_\alpha \to 0$ and increases to $1/\alpha$ for $x_\alpha \to \infty$. Therefore it is not surprising that our predictions work better for fast transitions.

Now we would like to discuss the situation when time evolution begins at the anticrossing center, $t_i = 0$, which is a generic **B** scheme situation. As $t_f \to \infty$ one gets

$$\mathcal{D}_n = |\langle\uparrow(\hat{t}\,)|\downarrow(0)\rangle|^2 = \frac{1}{2}\left(1 - \frac{1}{\sqrt{1+\hat{\varepsilon}^2}}\right), \qquad (9)$$

where we put $|\Psi(0)\rangle = |\downarrow(0)\rangle = -\frac{\sqrt{2}}{2}|1\rangle + \frac{\sqrt{2}}{2}|2\rangle$, and assumed that $|\langle\uparrow(t_f)|\Psi(t_f)\rangle| \approx |\langle\uparrow(\hat{t})|\Psi(\hat{t}\,)\rangle| \approx |\langle\uparrow(\hat{t}\,)|\Psi(0)\rangle|$. Combining (5) and (9) one gets

$$\mathcal{D}_n = \frac{1}{2}\left(1 - \sqrt{1 - 2/\mathcal{P}(x_\alpha)}\right), \qquad (10)$$

with x_α and $\mathcal{P}(x_\alpha)$ defined in (5) and (7). The agreement of this expression with results of numerical calculations is remarkable as depicted in Fig. 2. It is even better than in the previous case when we considered the evolution starting far away from the avoided crossing. We attribute it to the fact that now the frozen part takes less time, i. e. $\hat{t}$ instead of $2\hat{t}$, and to the absence of the approximation that the initial stage of evolution is adiabatic.

We can also easily calculate density of defects when time evolution starts in the impulse regime (**B** scheme), but outside the avoided crossing center. Taking $|\Psi(t_i)\rangle = |\downarrow(t_i)\rangle := -\sin(\theta_0/2)|1\rangle + \cos(\theta_0/2)|2\rangle$ we obtained

$$\mathcal{D}_n = -\frac{\cos(\theta_0)}{\sqrt{2\mathcal{P}(x_\alpha)}} + \frac{1 - \sqrt{1-2/\mathcal{P}(x_\alpha)}\sin(\theta_0)}{2}, \quad (11)$$

where $\theta_0 = \arctan(\omega_0/(\Delta \cdot t_i)) \in [0, \pi]$ measures distance of the starting point of time evolution from an avoided crossing, e. g. $\theta_0 = \pi/2$ when evolution starts from an anticrossing center and then Eq. (11) is the same as Eq. (10). Interestingly, to the best of our knowledge, the analytical expressions for the transition probability (density of defects) in this regime are absent in the literature contrary to the situation when evolution starts far away from the avoided crossing [3].

Comparison of (11) to numerics for $\tau_Q/\tau_0 \le 1.75$ and $|\theta_0 - \pi/2| \le \pi/10$ reveals satisfactory agreement- see Fig. 3 for a typical situation. For larger τ_Q/τ_0 and/or $|\theta_0 - \pi/2|$ the agreement gradually decreases, which we attribute to the fact that for these parameters the starting time moment, $t_i = \tau_Q/\tan\theta_0$, might be outside $[-\hat{t}, \hat{t}\,]$, so that the assumption that the initial stage of time evolution is impulse can be wrong. One avoids these problems when either $t_i \ll -\hat{t}$ or $|t_i| \ll \hat{t}$, i. e. when the system evolves clearly within the **A** or **B** scheme, respectively.

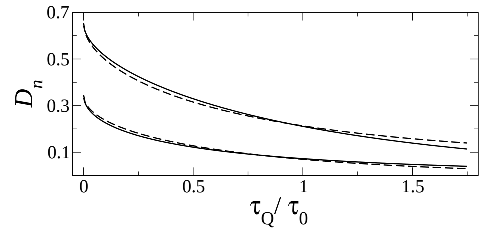

FIG. 3: Density of defects. Solid lines- numerics, dashed lines- Eq. (11) with α determined from fit. Upper (lower) curves correspond to $\theta_0 = 0.6\pi$, $\alpha = 1.06$ ($\theta_0 = 0.4\pi$, $\alpha = 0.58$).

It turns out that Eq. (11) can be significantly simplified. To this aim we propose to expand (11) in a Taylor series at $x_\alpha \to 0$, and match the series with a simple closed analytical expression up to desired order. Motivation for this procedure comes from the success of a similar calculation for the case when $t_i \to -\infty$: see Eq. (8). Notice, that as $x_\alpha \to 0$ we have $t_i \in [-\hat{t}, \hat{t}\,]$ as was assumed in derivation of (11). From a Taylor series we get

$$\begin{aligned}\mathcal{D}_n \;&=\; \sin(\theta_0/2)^2 - \sqrt{x_\alpha/4}\exp\left(-x_\alpha/4\right)\sin(\theta_0) \\ &+\; x_\alpha \cdot \cos(\theta_0)/4 + \mathcal{O}\left(x_\alpha^2\right),\end{aligned} \qquad (12)$$

where the exponential part, $\sqrt{x_\alpha/4}\exp(-x_\alpha/4)\sin(\theta_0)$, agrees with (11) up to $\mathcal{O}(x_\alpha^{7/2})$. In particular, when time evolution starts from anticrossing center ($t_i = 0, \theta_0 = \pi/2$), one gets

$$\mathcal{D}_n = 1/2 - \sqrt{x_\alpha/4}\exp(-x_\alpha/4) + \mathcal{O}(x_\alpha^{7/2}). \qquad (13)$$

As shown in Fig. 4 there is very good agreement between predictions (12,13) and numerics even for τ_Q/τ_0 of the

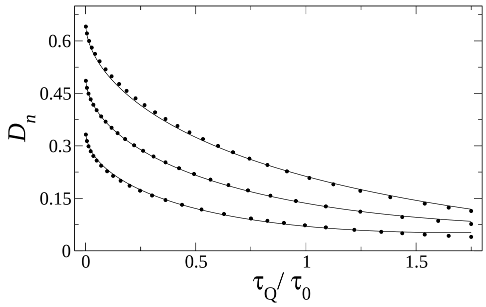

FIG. 4: Density of defects for time evolutions starting in the neighborhood of anticrossing. The curves, from top to bottom, correspond to (θ_0, α) equal to: $(0.6\pi, 0.96)$, $(0.5\pi, 0.78)$, $(0.4\pi, 0.65)$. Dots- numerical data, solid lines- fit on the basis of Eq. (12) with α being the fitting parameter.

order of 1.75 and $\theta_0 \in [0.4\pi, 0.6\pi]$. It justifies *a posteriori* our tricky simplification of (11). For larger deviations $|\theta_0 - \pi/2|$ and/or larger τ_Q/τ_0 the range of applicability of (12,13) decreases.

Several concluding remarks are in order. First of all, we have shown that the very simple LZ model successfully reproduces KZ-like dependence of topological defect density on the quench rate, although not all aspects of traditional KZ theory are present in this model. In particular, the vortices created by the KZ mechanism are subjected to short wavelength thermal fluctuations and annihilation processes [11]. We expect that absence of these processes in our theory makes the quench-independent constant α to be $\mathcal{O}(1)$ to fit correctly density of defects; compare to [11, 12] where factors $\mathcal{O}(1/10)\ldots\mathcal{O}(1/10^2)$ show up. Second, our results show that the KZ theory can provide predictions beyond the lowest non-trivial τ_Q/τ_0 order usually considered [2, 5, 11, 12]. Third, our results are directly applicable to different quantum two level systems, e. g. to the molecular magnets Fe_8 [6]. Therefore, our prediction that in addition to standard exponential transition probabilities (8) also modified exponential ones (12,13) should exist can be experimentally verified and might be helpful in interpretation of experimental data. It is also worth to mention that modified exponential dependence of defect density on the quench rate, was derived by Dziarmaga [13] in a particular 1D spin model. As an interesting extension of this work we envision application of our theory to different two level systems, e. g. to the nonlinear Landau-Zener description of a Bose-Einstein condensate in an optical lattice [14]. It is also very interesting to try to calculate exactly transition amplitudes (defect densities) for the case when evolution starts in the neighborhood of an avoided crossing, and to compare them to (10)-(13). We have not attempted this calculation to provide unbiased results coming from the KZ-like theory only.

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[8] Other definitions can be worked out when the particular form of wave functions is assumed. For an illustrative example see [9], where the knowledge of $\langle\Psi|\hat{L}_z|\Psi\rangle$ is sufficient for determination of vortex spacing.

[9] For the $n = 2$ case consider, e. g., $\langle r,\varphi|1\rangle = r^2 e^{2i\varphi} e^{-r^2/2}/\sqrt{2\pi}$, $\langle r,\varphi|2\rangle = e^{-r^2/2}/\sqrt{\pi}$ in (r,φ) cylindrical variables. Taking $|\Psi\rangle = ae^{i\gamma}|1\rangle + \sqrt{1-a^2}e^{i\chi}|2\rangle$, where $\gamma,\chi \in \mathcal{R}$ and $a \in [-1,1]$, one finds in $\langle r,\varphi|\Psi\rangle$ two vortices of unit circulation placed at (r,φ_1) and (r,φ_2): $r = (-2+2/a^2)^{1/4}$, $|\varphi_1 - \varphi_2| = \pi$- see [7].

[10] Other definitions of τ seem to be equally plausible on the heuristic level considered here, e. g. $\tau = \omega_0/[\omega_0^2 + (\Delta \cdot t)^2] \sim 1/\text{gap}^2$. We studied a few such choices of τ and found that the simplest one, $\tau \sim 1/\text{gap}$ discussed in the paper, compares the best to exact results.

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