Dynamics of localized states in extended supersymmetric quantum mechanics with multi-well potentials

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Abstract

In this paper we propose a self-consistent approach to the description of temporal dynamics of localized states. This approach is based on exactly solvable quantum mechanical models with multi-well potentials and their propagators. States of Hamiltonians with multi-well potentials form a suitable basis for the expansion of wave packets with different shapes and localization degrees. We also consider properties of the tunneling wave packets, taking into account all states of Hamiltonians with symmetric and asymmetric potentials. The study of the dynamics of initially localized states shows that application of the two-state approximation for the description of tunneling is considerably limited, especially for systems which have several states in the under-barrier region, as for example in modern superconducting quantum interference devices and traps for cold atoms.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Being one of the most exciting manifestations of the wave properties of particles, tunneling seemed to be a paradoxical prediction of quantum mechanics. Historically, the theory of the nuclear $\alpha$-decay was the first study of tunnel transitions [1], caused by bonding between nuclear resonances and continuous spectrum. Explanation of the intermolecular rearrangement of the ammonium spectrum [2] due to the tunnel splitting of vibrational spectra opened the era of study of tunneling in multi-well potentials [3]. This problem became even more important in view of interpretation of the observed tunneling phenomena in condensed matter [4, 5], and in particular in the Josephson junctions [6]. Currently, investigations of tunneling processes are mostly related to the study of the Bose–Einstein condensate in different types of traps [7, 8].
Theoretical analysis of tunneling in double-well potentials is mostly performed within the two-mode approximation [3]. Important characteristics of this approach are the difference of energies of the ground state and of the first excited state ($\Delta = E_1 - E_0$), as well as their wavefunctions. Values of $\Delta$ define, in particular, revival times of the wave packets (WPs). This approximation explains general properties of tunneling, but it is unable to give interpretations of many subtle effects. Analysis of processes in multi-well potentials is complicated, since most of the models use phenomenological or piecewise potentials (e.g., building from the rectangular wells and barriers, or from parabola), which are far from the real potentials. Spectra and wavefunctions in such potentials are unknown, that supposes the numerical analysis of their properties in consequent studies. It is important to note that there exist exactly solvable models with multi-well potentials [9–12], which could be used for the description of tunneling processes.

Going beyond the two-mode approximation reveals interesting features of the dynamics of localized states. In particular, characteristics of tunneling strongly depend on the shape of the potential, and demonstrate a non-regular behavior which realized in bouncing increasing the probability of the localization of the WP in a certain well [13–16]. These features become even more striking upon the initial localized state squeezing.

In quantum mechanics (QM) the time evolution of WPs is described by propagators, in which the contribution of the entire spectrum of the considered Hamiltonian is taken into account. However, only a few models, mostly with one-well potentials, are known to have analytical expressions for propagators. To build propagators for exactly solvable quantum mechanical models with double-well potentials, one could use the same approach as in [11, 17, 18] and construct new propagators from the known ones.

The aim of this paper is to describe the dynamics of localized states in multi-well potentials within the self-consistent approach. It is based on constructing exactly solvable quantum mechanical models with multi-well potentials having the preassigned energy value of the tunneling doublet. The corresponding Hamiltonians lead to a closed analytical expression for propagators which describe the temporary dynamics of localized states. We use multi-well potentials obtained in the framework of $N = 4$ SUSY QM [12] and describe the dynamics of WPs with corresponding propagators, calculated by use of the approach of [11, 17, 18].

The remaining structure of this paper is as follows. In section 2 we briefly discuss the construction of exactly solvable models in the framework of $N = 4$ SUSY QM [12] and give expressions for Hamiltonians with both symmetric and asymmetric potentials, and wavefunctions, obtained from the initial model of harmonic oscillator (HO). In section 3 we obtain the expressions for propagators in these models using the approach of [11, 17, 18]. Using the Hamiltonian of HO as the initial one, we obtain the explicit expressions for propagators in models with multi-well potentials. In section 4 we use the obtained potentials and corresponding propagators for the non-perturbative analysis of the dynamics of localized states in both symmetric and asymmetric potentials, and for different types of WPs. In section 5 we summarize the obtained results and discuss some topics related to the considered problems and further developments.

2. $N = 4$ SUSY QM and multi-well potentials

Extended $N = 4$ SUSY QM [19–21] is equivalent to second-order polynomial supersymmetric quantum mechanics (SUSY QM) (reducible case) [22, 23] and assumes the existence of
complex operators of supersymmetries $Q_2(\hat{Q}_1)$ and $Q_2(\hat{Q}_2)$, through which the Hamiltonians $H_{\sigma_1}^{\sigma_2}$ can be expressed. The Hamiltonian of $N = 4$ SUSY QM has a form ($\hbar = m = 1$):

\[
H_{\sigma_1}^{\sigma_2} = \frac{1}{2}(p^2 + V_{\sigma_1}(x) + \sigma_3^{(1)}V_{\sigma_2}(x)) = \frac{1}{2}(p^2 + V_1(x) + \sigma_3^{(2)}V_1(x)),
\]

where $W(x)$ is a superpotential and $\sigma_3^{(i)}$—matrices, which commute with each other and have eigenvalues $\pm 1$, $\sigma_3^{(1)} = \sigma_3 \otimes 1$, $\sigma_3^{(2)} = 1 \otimes \sigma_3$. Supercharges $Q_i$ of extended SUSY QM form an algebra:

\[
\{Q_i, \bar{Q}_k\} = 2\delta_{ik}H, \quad \{Q_i, Q_k\} = \{\bar{Q}_i, \bar{Q}_k\} = 0, \quad i, k = 1, 2
\]

\[
Q_i = \sigma_3^{(i)}(p + i\lambda_{i+1}(x)), \quad \bar{Q}_i = \sigma_3^{(i)}(p - i\lambda_{i+1}(x)),
\]

where $V_1(x) \equiv V_1(x)$, $\sigma_4^{(1)} = \sigma_4 \otimes 1$, $\sigma_4^{(2)} = 1 \otimes \sigma_4$. Hamiltonian and supercharges act on four-dimensional internal space and Hamiltonian is diagonal on vectors $\psi(x, E)$, where $\sigma_1, \sigma_2$—eigenvalues of $\sigma_3^{(1)}$, $\sigma_3^{(2)}$. Supercharges $Q_i(\bar{Q}_i)$ act as lowering (raising) operators for indexes $\sigma_1, \sigma_2$. It is convenient to represent the structure of Hamiltonian and connection between wavefunctions in a diagram form:

\[
\begin{align*}
\psi^-(x, E) & \overset{Q_1}{\leftrightarrow} \psi^+(x, E) \\
Q_1 & \quad \bar{Q}_1 & \quad Q_2 \\
\psi^-(x, E) & \overset{Q_2}{\leftrightarrow} \psi^+(x, E)
\end{align*}
\]

Construction of isospectral Hamiltonians in the framework of $N = 4$ SUSY QM is based on the fact that four Hamiltonians are combined into supermultiplet $H_{\sigma_1}^{\sigma_2}$. Nevertheless, it should be noted that due to symmetry $\sigma_1 \leftrightarrow \sigma_2 - H_{\sigma_1}^{\sigma_2} \equiv H_{-\sigma_1}$, only three of them are nontrivial. The procedure of constructing isospectral Hamiltonians, when the ground state is removed from the initial Hamiltonian, is treated in [21, 24] in detail. The expressions for a nonlinear oscillator were obtained in [25]. The procedure of constructing the nonlinear oscillator Hamiltonian of [25] consists in two steps. On the first step the ground state of the HO spectrum is removed. But it is recovered on the second step, and with the superpotential, expressed in terms of the general solution to the Ricatti equation. This completely coincides with the procedure of constructing isospectral Hamiltonians within $N = 4$ SUSY QM, and the obtained expressions in [21, 24] match the corresponding expressions of [25]. Therefore, the proposed [25] procedure of constructing the nonlinear oscillator Hamiltonian is the concrete realization of obtaining isospectral Hamiltonians in $N = 4$ SUSY QM.

We will consider the construction of isospectral Hamiltonians by addition of states below the ground state of the initial Hamiltonian. Let us consider the auxiliary equation:

\[
H\varphi(x) = \varepsilon\varphi(x).
\]

As initial let us take one of the Hamiltonians

\[
H_{\sigma_1}^{\sigma_2} = \frac{1}{2}(p - i\sigma_1 V_2(x))(p + i\sigma_1 V_2(x)) + \varepsilon
\]

\[
= \frac{1}{2}(p - i\sigma_2 V_1(x))(p + i\sigma_2 V_1(x)) + \varepsilon,
\]

\[
(2.4)
\]
dependence on these parameters. The new state with excited states is preserved (for a discrete spectrum). Using the second representation which by definition has normalized wavefunction. Normalization of wavefunctions of factorization energy \( \psi \) \( \lambda \), \( H \) and \( H - \varepsilon \) are the same. When fixing operator \( H_{\sigma_1}^\varepsilon \), the form of \( W(x) \) depends on the choice of factorization energy \( \varepsilon \), thereby the Hamiltonians \( H_{\sigma_1}^\varepsilon, H_{-\sigma_1}^\varepsilon, H_{-\sigma_2}^\varepsilon \) also have nontrivial dependence on \( \varepsilon \).

When \( \varepsilon < E_0 \) (where \( E_0 \) is the ground state energy of the initial Hamiltonian), the auxiliary equation (2.3) has two linear independent solutions \( \psi_i(x, \varepsilon), i = 1, 2 \), which are nonnegative and have the following asymptotic behavior [11]: when \( x \to -\infty \) \( \psi_1(x) \to +\infty \) (\( \psi_2(x) \to 0 \)), and when \( x \to +\infty \) \( \psi_2(x) \to 0 \) (\( \psi_1(x) \to +\infty \)), i.e. with appropriately chosen constants the general solution has the form \( \psi(x, \varepsilon, c) = (\psi_1(x, \varepsilon) + c\psi_2(x, \varepsilon)) \) and has no zeros on all axis. Thus, the function \( \hat{\psi}(x, \varepsilon, c) = \frac{\psi(x, \varepsilon, c)}{\psi(x, \varepsilon, N)} \) is finite and can be normalized at every concrete choice of \( \varepsilon \) and \( c \). Let us note that with concrete values of \( \varepsilon \) and \( c \), \( \psi(x, \varepsilon, c) \) can have local extrema. In this case the natural choice of the initial Hamiltonian is \( H^+ \) or \( H^- \) (which are identical due to symmetry of \( H_{\sigma_1}^\varepsilon \) under \( \sigma_1 \leftrightarrow \sigma_2 \)). Then superpotential has the form [21]:

\[
W(x, \varepsilon, \lambda) = -\frac{1}{2} \ln \left( 1 + \lambda \int_{t_1}^x dx \sqrt{\hat{\psi}^2(t, \varepsilon, c)} \right)
\]  

(5.5) with two new arbitrary parameters \( \lambda, x_1 \), but last of them is inessential, because it gives an additional contribution to \( W(x) \). All Hamiltonians that form a supermultiplet have nontrivial dependence on these parameters.

To consider the connection between Hamiltonians from supermultiplet, let us take \( H_+ \) as initial. Denoting as \( \psi_+^\varepsilon(x, E) = E\psi_+^\varepsilon(x, E) \) and using the first representation of Hamiltonian \( H_{\sigma_1}^\varepsilon \), we obtain the following relation between \( H_-, \psi_-(x, E) \) and initial expressions:

\[
H_-^\varepsilon = H_+^\varepsilon + \frac{d^2}{dx^2} \ln \hat{\psi}(x, \varepsilon, c),
\]

\[
\psi_-(x, E_i) = \frac{1}{\sqrt{2(E_i - \varepsilon)}} \frac{W(\psi_+^\varepsilon(x, E_i), \psi(x, \varepsilon, c))}{\psi(x, \varepsilon, c)} N^{-1} \hat{\psi}(x, \varepsilon, c).
\]  

(7.1)

The new state with \( E = 0 \) (with energies measured from \( \varepsilon \)) appears in Hamiltonian, which by definition has normalized wavefunction. Normalization of wavefunctions of excited states is preserved (for a discrete spectrum). Using the second representation \( H_{\sigma_1}^\varepsilon = \frac{1}{2}(p - i\sigma_2 V_{\sigma_1}(x))(p + i\sigma_2 V_{\sigma_1}(x)) + \varepsilon \) and identity \( H_+^\varepsilon = H_-^\varepsilon \), the relation between \( H_+^\varepsilon, \psi_+^\varepsilon(x, E) \) and initial Hamiltonian and wavefunctions can be obtained:

\[
H_+^\varepsilon = H_+^\varepsilon + \frac{d^2}{dx^2} \ln \left( \frac{\psi(x, \varepsilon, c)}{1 + \lambda \int_{x_1}^x dx \sqrt{\hat{\psi}^2(t, \varepsilon, c)}} \right)
\]

\[
\psi_+^\varepsilon(x, E_i) = \frac{1}{\sqrt{2(E_i - \varepsilon)}} \left( \frac{1}{dx} \hat{\psi}(x, \varepsilon, c) + \frac{d}{dx} \ln \left( \frac{\psi(x, \varepsilon, c)}{1 + \lambda \int_{x_1}^x dx \sqrt{\hat{\psi}^2(t, \varepsilon, c)}} \right) \right) \psi_+^\varepsilon(x, E_i).
\]  

(8.1)
It is important to mention that normalization of wavefunction $\psi_\pm(x, E = 0)$, as in the case of one-well potentials, can always be performed at any $\bar{\psi}(x, \varepsilon, c)$ and $\lambda$ using the following expression in normalization condition:

$$
\frac{N^{-2}_\lambda \bar{\psi}^2(x, \varepsilon, c)}{(1 + \lambda N^{-2} \int_{-\infty}^{\infty} d\bar{\psi}^2(t, \varepsilon, c))^2} = -\frac{N^{-2}_\lambda}{\lambda N^{-2} \int_{-\infty}^{\infty} d\bar{\psi}^2(t, \varepsilon, c)}
$$

which easily gives the relation between normalization constants: $N^{-2}_\lambda = (1 + \lambda)N^{-2}$. Normalization of $\psi_\pm(x, E)$ is the same as for $\bar{\psi}(x, \varepsilon, c)$.

To calculate integrals entering the superpotential (2.5), and normalization constants of wavefunctions of additional states $\psi_\pm(x, E = 0)$, $\psi_\pm(x, E = 0)$, it is useful to apply the expression derived in [26]. Let $y_1$ and $y_2$ be two linear independent solutions of a homogeneous second-order differential equation, then

$$
\int_{x}^{x} \frac{W[y_1, y_2]}{(A_1 y_1(t) + A_2 y_2(t))^2} dt = \frac{1}{A_1^2 + A_2^2} \left[ \frac{(A_2 y_1(x) - A_1 y_2(x))}{A_1 y_1(x) + A_2 y_2(x)} \right]
$$

where $W[y_1, y_2] = y_1 y_2' - y_1' y_2$ is Wronskian, which is independent of $x$ for the second-order differential equation, reduced to a canonical form, as the Schrödinger equation, and thus could be passed from integral. This expression is very useful for calculation of the integrals in the above given expressions. First of all, it is natural to put $x_1 = -\infty$ in expression (2.5) of superpotential. Therefore

$$
N^{-2} \int_{-\infty}^{x} \frac{dt}{(\varphi_1(t, \varepsilon, c) + c \varphi_2(t, \varepsilon, c))^2} = -\frac{N^{-2}}{(1 + c^2) W[\varphi_1, \varphi_2]} \left[ \Delta(x, \varepsilon, c) - \Delta(-\infty, \varepsilon, c) \right]
$$

$$
N^{-2} = \frac{1}{(1 + c^2) W[\varphi_1, \varphi_2]} \left[ \Delta(+\infty, \varepsilon, c) - \Delta(-\infty, \varepsilon, c) \right]
$$

$$
\Delta(x, \varepsilon, c) = \frac{c \varphi_1(x, \varepsilon, c) - \varphi_2(x, \varepsilon, c)}{\varphi_1(x, \varepsilon, c) + c \varphi_2(x, \varepsilon, c)}.
$$

Let us consider the case of $c = 1$. This allows to avoid the unnecessary awkwardness, but nevertheless, reveal the fundamental features of Hamiltonians and wavefunctions of $N = 4$ SUSY QM, using only general properties of the solutions of auxiliary equation when $\varepsilon < E_0$. Using relations considered above, it is easy to obtain the expression for superpotential up to constant term:

$$
W(x, \varepsilon, \lambda) = -\frac{1}{2} \ln \left( 1 + \lambda N^{-2} \int_{-\infty}^{x} \frac{dt}{(\varphi_1(x, \varepsilon, \lambda) + \varphi_2(x, \varepsilon, \lambda))^2} \right)
$$

$$
= -\frac{1}{2} \ln \left( \frac{\varphi_1(x, \varepsilon, \lambda) + \Lambda(\varepsilon, \lambda) \varphi_2(x, \varepsilon, \lambda)}{\varphi_1(x, \varepsilon, \lambda) + \varphi_2(x, \varepsilon, \lambda)} \right)
$$

$$
\Lambda(\varepsilon, \lambda) = \frac{\Delta(+\infty, \varepsilon, 1) - \lambda - (\lambda + 1) \Delta(-\infty, \varepsilon, 1)}{\Delta(\infty, \varepsilon, 1) + \lambda - (\lambda + 1) \Delta(-\infty, \varepsilon, 1)}.
$$

Let us note that $\Delta(\pm\infty, \varepsilon, \lambda)$, which enter the $\Lambda(\varepsilon, \lambda)$, are determined by the asymptotic behavior of solutions of auxiliary equation. Due to this, while in the case of $H_\lambda^-$, potential is determined by symmetric combination $\varphi_1(x, \varepsilon, \lambda) + \varphi_2(x, \varepsilon, \lambda)$, in the case of $H_\lambda^+$ by asymmetric $\varphi_1(x, \varepsilon, \lambda) + \Lambda(\varepsilon, \lambda) \varphi_2(x, \varepsilon, \lambda)$:

$$
H_\lambda^- = H_\lambda^+ - \frac{d^2}{dx^2} \ln(\varphi_1(x, \varepsilon, \lambda) + \varphi_2(x, \varepsilon, \lambda))
$$

$$
H_\lambda^+ = H_\lambda^+ - \frac{d^2}{dx^2} \ln(\varphi_1(x, \varepsilon, \lambda) + \Lambda(\varepsilon, \lambda) \varphi_2(x, \varepsilon, \lambda)).
$$
In some sense, potentials $\tilde{U}^-(x, \varepsilon)$ and $\tilde{U}^+(x, \varepsilon, \lambda)$ are form invariant [27], i.e. potentials and wavefunctions transform to each other by changing of parameters and their spectra are identical and this holds independently of the choice of the initial Hamiltonian. Moreover, the form of $\tilde{U}^+(x, \varepsilon, \lambda)$ can change, when varying $\varepsilon$, as well as $\lambda$. Relations (2.10) and (2.11) are also useful for the derivation of exact form of wavefunctions $\psi^-(x, E)$ and $\psi^+(x, E)$.

$$H^- = H^+ - \frac{d^2}{dx^2} \ln(\psi_1(x, \varepsilon) + \psi_2(x, \varepsilon)),$$

$$\psi^-(x, E) = \frac{1}{\sqrt{2(E_0 - \varepsilon)}} W[\psi^-(x, E_0), \psi(x, \varepsilon, 1)],$$

$$\psi_0^-(x, E = 0) = \frac{N^{-1}}{\psi(x, \varepsilon, 1)} \frac{\psi_1(x, \varepsilon) - \psi_2(x, \varepsilon)}{\psi(x, \varepsilon) + \psi_2(x, \varepsilon)}$$

(2.14)

Thus, expression for wavefunctions $\psi^+(x, E)$ results from a similar expression for $\psi^-(x, E)$ by the substitution $\psi_1(x, \varepsilon) + \psi_2(x, \varepsilon) \to (\psi_1(x, \varepsilon) + \Lambda(\varepsilon, \lambda) \psi_2(x, \varepsilon))$. In particular, the normalization constant for $\psi^+(x, E = 0)$ can be easily obtained from a corresponding expression for $\psi^-(x, E = 0)$.

In what follows, we will use the Hamiltonian of HO as the initial Hamiltonian. Thus, the solutions to the auxiliary equation are parabolic cylinder functions $\phi_{1,2}(\xi, \bar{\varepsilon}) = D_\nu(\sqrt{2}\xi), \phi_{1,2}(\xi, \bar{\varepsilon}) = D_\nu(-\sqrt{2}\xi)$ and the Wronskian becomes $W[\phi_1, \phi_2] = \frac{2\sqrt{\pi\omega}}{\Gamma(-\nu)}$ [28], where $\Gamma(-\nu)$ is the gamma function, $\xi = \sqrt{\omega} x, \nu = -\frac{1}{2} + \frac{1}{4} = -\frac{1}{2} + \bar{\varepsilon}$, parameter $\lambda$ is restricted to be $\lambda > -1$:

$$\phi_1(\xi, \bar{\varepsilon}, 1) = D_\nu(\sqrt{2}\xi) + D_\nu(-\sqrt{2}\xi).$$

(2.15)

Note that $\Delta(\pm\infty, \varepsilon, \lambda)$, entering $\Lambda(\varepsilon, \lambda)$, are determined by the asymptotes of the solutions $\phi_1(\xi, \bar{\varepsilon}), \phi_2(\xi, \bar{\varepsilon})$. The ground state wavefunction of $H^-$ is

$$\psi^-(x, E = 0) = \frac{N^{-1}}{(D_\nu(\sqrt{2}\xi) + D_\nu(-\sqrt{2}\xi))} = \frac{N^{-1}}{\psi(\xi, \bar{\varepsilon}, 1)}, \quad N^{-2} = \frac{2\sqrt{\pi\omega}}{\Gamma(-\nu)},$$

(2.16)

and wavefunctions of excited states are determined by (2.14), where $\psi^+(x, E_n) = (\xi^n)! \frac{1}{\sqrt{2\xi^n}} D_\nu(\sqrt{2}\xi), n = 0, 1, 2, \ldots$ are the wavefunctions of HO. The potential of the Hamiltonian $H^-(p, x) = \omega(\frac{p^2}{2} + (\frac{\xi^2}{4} - \bar{\varepsilon}) - \frac{\psi_1^2}{\psi_2^2} \ln \psi_1(\xi, \bar{\varepsilon}, 1))$ (see figure 1) is defined by the symmetric combination of solutions $\psi_1(x, \varepsilon) + \psi_2(x, \varepsilon)$, while the potential of $H^+$ is defined by the asymmetric combination $\psi_1(x, \varepsilon) + (\lambda + 1) \psi_2(x, \varepsilon)$, and corresponds to the family of Hamiltonians with different values of $\omega$. Hence, the ground state wavefunction of $H^+$ has the form of

$$\psi^+(x, E = 0) = \frac{N_{\lambda}^{-1}}{(D_\nu(\sqrt{2}\xi) + (\lambda + 1)D_\nu(-\sqrt{2}\xi))} = \frac{N_{\lambda}^{-1}}{\psi(\xi, \bar{\varepsilon}, \lambda + 1)},$$

$$N_{\lambda}^{-2} = \frac{2(\lambda + 1) \sqrt{\pi\omega}}{\Gamma(-\nu)}.$$  

(2.17)

It should be noted that in terms of a dimensionless variable $\xi$, the only way to vary the form of the potential is to vary $0 < \bar{\varepsilon} < 1/2$ and $-1 < \lambda$. In the case of natural units $x$, additionally, the form of the potential (in particular, the position of local minima) can be changed by variation of $\omega$. Multi-well structure of the obtained potential becomes more striking when $\frac{\Delta_{\varepsilon}}{E_0} \ll 1$.
3. Time evolution of states in $N = 4$ SUSY QM

In many cases tunneling is considered within the two-mode approximation. It allows to describe density oscillations and revival times for WPs, but this approach fails, for example, in reproducing the dependence of the WP dynamics on the shape of the potential and the coherence breaking [14]. For instance, to correctly describe the dynamics of squeezed WPs initially localized in one of the minima, one has to take into account not only the ground and first excited states, but also higher excited states. Contribution of these states increases with the squeezing of WP, and is also significant in potentials with low barriers, as for example in superconducting quantum interference devices (SQUIDs) and in cold atoms traps.

The time evolution of the Gaussian WP $\Phi(x) = \left(\frac{2R}{\pi}\right)^{1/4} \exp\left(-\frac{1}{2} (x - x_0)^2 e^{2R}\right)$ (here $R$ is the squeezing parameter) initially localized in $x = x_0$ is determined by [29]

$$\Phi(x, t) = \int_{-\infty}^{+\infty} K(x, t; x_0, 0) \Phi(x_0) \, dx_0,$$

$$K(x, t; x_0, 0) = \sum_{n=0}^{\infty} \psi^+_{\sigma_n}(x, E_n) \psi^+_n(x_0) e^{-iE_n t}.$$

(3.1)

Here $K(x, t; x_0, 0)$ is the propagator, which sufficiently describes the dynamics of localized states in potentials of arbitrary complexity.

Currently, only a few exactly solvable models with analytic expressions of the propagator $K(x, t; x_0, 0)$ are known [30]. Usually, their Hamiltonians have one-well potentials. The construction of new models and their propagators on the basis of propagators of exactly solvable models with one-well potentials is proposed in [11, 17, 18]. Main ideas of this approach are outlined in [11, 17, 18], so we will briefly discuss the procedure of the construction of propagators in $N = 4$ SUSY QM, starting from exactly solvable model with the confinement potential.

Let us denote propagators, corresponding to Hamiltonians $H_{\sigma_n}^\pm$ of $N = 4$ SUSY QM, as $K_{\sigma_n}^\pm(x, t; x_0, 0)$ ($\sigma_n = \pm$). Using the form invariance of $N = 4$ SUSY QM potentials, established in [12], the expression for the propagator $K_{\sigma_n}^+(x, t; x_0, 0)$ could be obtained. Supposing the presence in the $H_{\sigma_n}^-$ spectrum the only discrete levels, the expression of $K_{\sigma_n}^+(x, t; y, 0)$ has the following form:

$$K_{\sigma_n}^+(x, t; y, 0) = \sum_{n=0}^{\infty} \psi^+_{\sigma_n}(x, E_n) \psi^+_n(y, E_n) e^{-iE_n t} + \frac{N^{-2}_{\sigma_n}}{\varphi(x, \bar{\varepsilon}, \Lambda) \varphi(y, \bar{\varepsilon}, \Lambda)} e^{-i\varepsilon t}.$$

(3.2)
On account of the relation of the wavefunctions $\Psi^+(x, E_n)$ with the original wavefunctions $\psi^+(x, E_n)$

$$
\Psi^+(x, E_n) = \frac{1}{\sqrt{2 (E_n - \varepsilon)}} L_x \psi^+(x, E_n),
$$

(3.3)

as well as an apparent property of the propagator

$$
\psi^+(x, E_n) e^{-i E_n t} = \int_{-\infty}^{+\infty} K^+_n(x, t; z, 0) \psi^+(z, E_n) \, dz,
$$

(3.4)

we obtain the relation of $K^+_n(x, t; y, 0)$ to the propagator of the original exactly solvable model

$$
K^+_n(x, t; y, 0) = \frac{1}{2L_x L_y} \int_{-\infty}^{+\infty} dz K^+_n(x, t; z, 0) \frac{N^{-2} e^{-i rt}}{\psi(x, e, \Lambda) \psi(y, e, \Lambda)},
$$

(3.5)

The Green function $G_n^+(z, y, e) = \sum_{\nu=0}^{\infty} \frac{\psi_n(z, E_n) \psi_n(y, E_n)}{E_n - e}$ can be presented in terms of solutions to the Schrödinger equation with energy $e$:

$$
G_n^+(z, y, e) = -\frac{2}{W(f_1, f_2)} \left( f_1(x, e) f_2(y, e) \theta(y - x) + f_2(y, e) f_1(x, e) \theta(x - y) \right).
$$

According to our notation, $f_1(x, e) = \psi_1(x, e)$, $f_2(x, e) = \psi_2(x, e)$. Acting with the operator $L_y$ and simplifying the expression, the propagator becomes

$$
K^+_n(x, t; y, 0) = -\frac{1}{\psi(y, e, \Lambda)} L_x \left[ \Lambda(e, \lambda) \int_{-\infty}^{y} dz K^+_n(x, t; z, 0) \psi_2(z, e) \right. \
\left. - \int_{y}^{\infty} dz K^+_n(x, t; z, 0) \psi_1(z, e) \right] + \frac{N^{-2} \Lambda^{-2} e^{-i rt}}{\psi(x, e, \Lambda) \psi(y, e, \Lambda)}.
$$

(3.6)

Choosing the Hamiltonian of HO as $H^+_n$, we obtain $\psi_1(\xi, \tilde{e}) = D_\nu(\sqrt{\tilde{e}})$, $\psi_2(\xi, \tilde{e}) = D_\nu(-\sqrt{\tilde{e}})$, $\Lambda(e, \lambda) = (1 + \lambda)$, and $K^+_n(x, t; y, 0)$ becomes [30]

$$
K^+_n(x, t; y, 0) = \left( \frac{\omega e^{-i r (\frac{1}{2} + n)}}{2 \pi \sin \omega t} \right)^{1/2} \exp \left\{ \frac{i \omega}{2 \sin \omega t} \left[ (x^2 + y^2) \cos \omega t - 2xy \right] \right\},
$$

(3.7)

where $t = t + \tau, n \in N_0, 0 < \tau < \frac{\pi}{2n}$. The factor $e^{-i r (\frac{1}{2} + n)}$ ensures correct behavior of the propagator for all values of time $t$. Expressions (2.16), (2.17), (3.1), (3.6) and (3.7) are the basic expressions to study the dynamics of localized states both in symmetric and asymmetric potentials. At the same time, this approach takes into account all the states, which form the localized state $\Phi(x, 0)$. $K^+_n(x, t; y, 0)$ could be obtained from (3.6) by substitution $\Lambda(e, \lambda) = 1$ and corresponds to a symmetric potential.

### 4. Dynamics of localized states in multi-well potentials

In this paper we focus on the case when only a few states of the Hamiltonian with the multi-well potential are located below the barrier. This is a common situation for different physical problems, both in atomic and solid state physics. In general, the dynamics of the localized states cannot be correctly described in the traditional framework of the tunnel splitting $\Delta = E_1 - E_0$, because the initially localized state cannot be expanded as a superposition of the wavefunctions of the tunnel doublet. Higher excited states are essential in $\Phi(x, 0)$ and their contribution increases with increasing of the WP squeezing. In contrast, the approach,
where state

Let us note that study of the dynamics of the localized states (4.1) allows one to study the dynamics of localized states taking into account all states of the exactly solvable Hamiltonian, both with symmetric and asymmetric multi-well potentials. Since the spectra of all states of the exactly solvable Hamiltonian, both with symmetric and asymmetric multi-well potentials. Since the spectra of $H_-$ and $H_+$ are identical, the tunnel splittings $\Delta = E_1 - E_0$ are equal for symmetric and asymmetric potentials.

We will study the dynamics of the localized states in potentials constructed from the potential of HO (2.14)–(2.17), with the propagator (3.6), (3.7). Their expressions in the dimensionless variables are

$$K_+^\pm (\xi, \eta, 0) = -\sqrt{\frac{\alpha}{\phi(\eta, \xi, \lambda + 1)}} \frac{1}{T^2} \sum_{n=0}^{\infty} \int \frac{d\xi}{\phi(\eta, \xi, \lambda + 1)} \psi(\eta, \xi, \lambda + 1) \psi(\eta, \xi, \lambda + 1),$$

where $T = \pi n + \tau, n \in \mathbb{N}, 0 < \tau < \pi$. The propagator $K_-^\pm (\xi, T; \eta, 0)$ describing the dynamics of WPs in the symmetric potential can be obtained from (4.1) with $\lambda = 0$. Thus, expression (3.1) in the dimensionless variables reads

$$\Phi(\xi, T) = \int_{-\infty}^{+\infty} d\xi K_+^\pm (\xi, T; \xi, 0) \Phi(\xi, 0),$$

$$\Phi(\xi, 0) = \left(\frac{e^{2R}}{\pi}\right)^{1/4} e^{-\frac{(\xi - \eta_0)^2}{\sigma^2}}, \quad \sigma^2 = e^{-2R}.\quad (4.2)$$

These relations allow one to obtain the form of the WP as a function of time and spatial coordinates.

4.1. Small squeezed states

Let us note that study of the dynamics of the localized states (4.2) cannot be performed in the two-mode approximation, even when $R = 0$. A satisfactory approximation of the initially localized state $\Phi(\xi, 0)$ is achieved with taking into account eight states of the Hamiltonian $H_-$ (see line 1 in table 1). At the same time, the expansion of the initial state $\Phi(\xi, 0)$ over states of $H_-(H_+)$ is not required to compute $|\Phi(\xi, T)|$ using the exact propagator. We will compare the results of the exact calculation using (4.2) with $|\Phi(\xi, T)| = |\sum_{n=0}^{\infty} c_n \psi(\xi, \eta, n) \exp(-iE_nT)|$ to demonstrate the effectiveness of the basis of $H_-(H_+)$ in the considered problem. Figure 2 shows $|\Phi(\xi, T)|$ for the same, as in figure 1, potentials $U_-^\pm (\xi, \lambda)$ and $U_+^\pm (\xi, \lambda)$, and for the value of squeezing parameter $R = 0.35$. The latter corresponds to the weak localization. Initially (at $T = 0$), the WP is localized in the left local minimum and has the energy $E_\Phi(\Phi|H_-^\pm(p, x)\Phi|E_\Phi = 0.16$ for the symmetric potential, and $E_\Phi = 0.185$ for the asymmetric one.

Table 1. Coefficients of the expansion of the initial WP (4.2). The third (fourth) row corresponds to the initial localization of $\Phi(\xi, 0)$ in the left (right) local minimum of $U_\pm^\pm (\xi, \lambda)$.

| No. of states | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---------------|---|---|---|---|---|---|---|---|---|---|
| $\lambda = 0, R = 0$ | 0.668 | -0.664 | 0.018 | 0.017 | 0.048 | -0.146 | 0.203 | -0.184 | 0.110 | -0.031 |
| $\lambda = 0, R = 0.35$ | 0.682 | -0.692 | 0.135 | -0.082 | 0.056 | -0.069 | 0.094 | -0.090 | 0.044 | 0.015 |
| $\lambda = -0.95, r$ | 0.208 | -0.945 | 0.179 | -0.105 | 0.065 | -0.066 | 0.077 | -0.060 | 0.013 | 0.029 |
| $\lambda = -0.95, r$ | 0.941 | 0.213 | 0.038 | 0.011 | -0.007 | 0.011 | 0.066 | 0.128 | 0.153 | 0.115 |
Figure 2. Time dependence of $|\Phi(\xi, T)|$ with $R = 0.35$, initially localized in the left minimum of (a) potential $U_-(\xi)$ ($\xi_l = -2.29$) and (b) potential $U_+^+(\xi, \lambda)$ with $\lambda = -0.95$ ($\xi_l = -2.153$).

Approximation of the initial WP by states of $H_-^-$ and $H_+^+$ is mainly determined by few lower states (see table 1) which indicate the suitability of the basis. Nevertheless, despite a small contribution of higher states, they determine fine details of time evolution of WP, as we will show later. These details include specific beats caused by the interference of excited states. When the asymmetric potential is used, the expansion of the initial packet contains more terms, than in the symmetric potential (see table 1), and at the same time the contribution of states with $n > 9$ is comparable to the contribution of low-lying states.

Thus, the temporal dynamics of WP (figure 2) demonstrates slow tunnel transition of under-barrier states and fast oscillations of over-barrier states. In the case of a symmetric potential, the evolution of $|\Phi(\xi, T)|$ (figure 2(a)) has the striking oscillatory nature: the portion of the initial $\Phi(\xi, 0)$ which tunnels to the right minimum of $U_-(\xi)$ is quite large and reaches its maximum at $T \simeq E_{1}^{2\pi} / (E_1 - E_0) \approx 300$, while at $T \simeq T_{\text{rev}}$ the WP is completely restored at the left minimum of $U_-(\xi)$. At the same time, the contribution of higher excited states to $|\Phi(\xi, T)|$ is relatively small and leads only to small ‘beats’. Completely different dynamics is observed, when the WP is initially localized in one of the minima of $U_+^+(\xi, \lambda)$ (figure 2(b)). The portion of the WP which tunnels to another local minimum is small, since in the left local minimum of $U_+^+(\xi, \lambda)$ (at $\xi_l = -2.153$) the largest contribution to $\Phi(\xi, 0)$ comes from the first excited state of $H_+^+$ with the wavefunction being very small in the right well. It means that this state contributes only a small portion to the tunnel transition amplitude. The similar situation is observed, when the WP is localized at the right local minimum ($\xi_r = 2.755$) of $U_+^+(\xi, \lambda)$. In this case the ground state wavefunction of $H_+^+$, which is small in the left well, contributes mostly to $\Phi(\xi, 0)$. In some sense the WP is trapped within the initial well. The mechanism of such partial trapping of WP is simple: if one of the under-barrier states mostly contributes to $\Phi(\xi, 0)$, then its wavefunction is small in another well, that means it has a small contribution to the tunnel transition to another well. Other under-barrier states give small contributions to tunneling due to their small portion in the formation of $\Phi(\xi, 0)$. Nevertheless, the contribution of over-barrier states is larger than that in the symmetric potential, and it leads to large beats.

The phenomenon of partial trapping is more obvious when the initial WP is uniformly distributed among the local minima ($\xi_L$, $\xi_R$) of the asymmetric potential $U_+^+(\xi, \lambda)$, e.g.

$$\Phi(\xi, 0) \approx \left( \frac{\sigma^{-2}}{4\pi} \right)^{1/4} \frac{e^{-\frac{\xi^2 - \xi_l^2}{2\sigma^2}} + e^{-\frac{\xi^2 - \xi_r^2}{2\sigma^2}}}{\sqrt{1 + e^{-\frac{1}{2\sigma^2}(\xi_l^2 - \xi_r^2)}}}, \quad \sigma^2 = e^{-2R}. \quad (4.3)$$
The dynamics of tunneling of the initial $\Phi(\xi, 0) (4.3)$ differs in different local minima of $U_+^+ (\xi, \lambda)$ (figure 3).

Figure 3 shows that the portion of WP $\Phi(\xi, T)$ behaves differently in different wells of $U_+^+ (\xi, \lambda)$. In the left minimum, for example, $|\Phi(\xi, T)|$ clearly oscillates, but at the same time the dynamics of $|\Phi(\xi, T)|$ in the right minimum is more complicated. To analyze it, we give the time dependence of the square of the WP in minima of the left ($\xi_l = -2.153$) and the right ($\xi_r = 2.755$) wells (figure 4).

It is important to note that in the left well, WP oscillates and is completely restored after the time interval $T_{\text{rev}} = \frac{2\pi (E_1 - E_0)}{2\pi} \approx 300$. At the same time, the fraction of the WP in the right well increases at $0 < T < 150$, while $|\Phi(\xi, T)|$ is completely changed due to the tunneling from the left well. Moreover, when the value of time is close to $T \sim 150$, the strong squeezing of the packet occurs, and under increasing of $T$ $|\Phi(\xi, T)|$ decreases and reaches its initial value. It looks like partial ‘confining’ of the portion of WP inside the right well. Thus, in one of the minima (the left one), the tunneling dynamics possesses the oscillatory nature, while in another minimum the partial ‘trapping’ of a part of WP occurs.
Another important characteristic of the WP tunneling dynamics is the probability to find WP in a certain well, \( P_l(T) \) for the potential \( U^{+}(\xi, \lambda) \) and the initial localized state (4.3). \( P_l(T) \) is a quantitative characteristic of the localized state dynamics, and it can be revealed that a packet with the same distribution evolves in different local minima of \( U^{+}(\xi, \lambda) \) in a different way. The probability to find the packet in the right well initially increases due to the tunnel transitions from the left well, and then returns to the initial value during the time \( T_{\text{rev}} = \frac{2\pi}{|E_1 - E_0|} \approx 300. \) Meanwhile, a portion of the WP in the right well, which tunnels to the left well \( U^{+}(\xi, \lambda) \), is much smaller than in the reverse transitions, and the dynamics has typical oscillatory nature in the left well. This indicates that the partial trapping of the packet occurs in the deeper well, and typical oscillatory dynamics is kept in the left well \( U^{+}(\xi, \lambda) \).

The initial state of the WP \( \Phi(\xi, 0) \) (4.3) could be sufficiently approximated by ten states of the Hamiltonian \( H^{-} \) (see table 2); thus, the proposed basis is effective enough for the description of localized states. Distributions like (4.3) are typical in the study of the macroscopic tunneling of the Bose–Einstein condensate. Let us note that \( |\Phi(\xi, T)| \) calculated according to (4.2) coincides, with a good accuracy, with \( |\Phi(\xi, T)| = \sum_{n=0}^{\text{max}} c_n \psi_{(-,+)}^{(-,+)}(\xi, E_n) \exp(-iE_nT) | \) where \( c_n \) are chosen according to table 2.

![Figure 5. \( P_l(T) \) for the initial packet \( \Phi(\xi, 0) \) (4.3) with \( R = 0.35. \)](image)

### Table 2. Coefficients of the expansion of initial WP (4.3).

| No. of states | 0  | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|--------------|----|----|----|----|----|----|----|----|----|----|
| \( \lambda = 0 \) | 0.976 | 0.165 | 0.110 | 0.058 | 0 | −0.061 |
| \( \lambda = -0.95 \) | 0.813 | −0.517 | −0.067 | 0.042 | −0.039 | 0.101 | 0.049 | 0.117 | 0.101 |

4.2. Large squeezed states

When the degree of the WP localization increases, the number of states, which significantly contribute to \( \Phi(\xi, 0) \), also increases. Let us consider the case when the initially localized state is located at one of the minima of the symmetric potential and in the deeper minimum of the asymmetric potential. When \( R = 1.5 \), the WP with the center at \( \xi_0 = -2.29 \) is sufficiently approximated by 20 states of the Hamiltonian \( H^{+} \) (for a symmetric potential). The similar localized state with the center located at \( \xi_0 = 2.755 \) needs 25 states of \( H^{+} \) for accurate approximation (for an asymmetric potential). Although the ground and the first excited states give the leading contribution to the expansion of WPs, the contribution of higher states is still
significant. It can be directly seen from the temporal dynamics of the initially localized states (figure 6).

The dynamics in the symmetric potential is complex, and the process of the barrier crossing cannot be even called tunneling. Such dynamics could be observed in the case of the coherent tunneling breaking in periodically driven systems [23, 24], e.g. the contribution of the over-barrier states completely mimics the tunneling of the under-barrier states. Nevertheless, the revival time of WPs is still $T_{\text{rev}} = \frac{2\pi}{|E_1 - E_0|} \approx 300$ according to the two-mode approximation. For the asymmetric potential, the portion of the WP outside of the deeper minimum is small and its structure is complex enough. At the same time, the WP in the global minimum squeezes at timescales $T \sim \frac{\pi}{2\varphi}$ and restores at $T = T_{\text{rev}}$.

This phenomenon could be illustrated by the probability to find the particle in a certain well $P_{l(r)}(T) = \int_{x \in l(r)\text{well}} |\Phi(x, T)|^2 \, dx$ (figure 7). Large amplitudes of beats give the evidence for the substantial contribution from the over-barrier states to the dynamics of WPs. As it was mentioned above, during the evolution in the symmetric potential, a substantial part of the WP leaves the left well and returns to the initial value at the timescale $T_{\text{rev}}$. Meanwhile, the portion of the WP in the right well of the asymmetric potential varies insignificantly, that tells on the partial trapping of the WP.

Figure 6. Time dependence of $|\Phi(\xi, T)|$ for initial packet with $R = 1.5$, localized in (a) left minimum of potential $U_1^- (\xi)$ ($\xi_l = -2.29$) and in (b) right minimum of $U_1^+ (\xi, \lambda)$, $\lambda = -0.95$ ($\xi_l = -2.153$, $\xi_r = 2.755$).

Figure 7. $P_{l(r)}(T)$ for the initial WP $\Phi(\xi, 0)$ with $R = 1.5$ initially localized in (a) left minimum of the symmetric potential and in (b) right minimum of the asymmetric potential.
5. Conclusions

In this paper we propose the approach to study of the dynamics of initially localized states, which is based on the exactly solvable quantum mechanical problems with multi-well potentials and on the corresponding exact propagators. Using the Hamiltonian of the harmonic oscillator as a basis one, we obtain, in frameworks of $N = 4$ SUSY QM, new Hamiltonians with multi-well potentials, both symmetric and asymmetric, together with the corresponding propagators. The study of the dynamics of the initially localized states demonstrates that the application of the two-mode approximation to the description of tunneling is very restricted, especially for systems with only few states in the under-barrier region. Such condition is typical for modern SQUIDs and cold atoms traps. So, even the non-squeezed wave packet ($R = 0$) cannot be adequately approximated by wavefunctions of the ground and the first excited states.

It is important to note that the states of Hamiltonians $H_-^-$ and $H_+^+$ are well suited as the basic states to expand the localized states $\Phi(\xi, 0)$. Usually, ten states are enough for a good approximation of $\Phi(\xi, T)$ in the sufficiently wide range of the squeezing parameter $R$. This can be confirmed by a good agreement between $|\Phi(\xi, T)| = \left| \sum_{n=0}^{\text{max}} c_n \psi^{(-, +)}_n(\xi, E_n) \exp(-iE_nT) \right|$ and the results of calculations by use of the exact propagator. In contrast to [13–16], where tunneling is compared in symmetric and asymmetric potentials, the spectra of Hamiltonians $H_-^-$ and $H_+^+$ are similar in our approach. Moreover, the shape of the potentials may be varied by the variation of $\bar{\varepsilon}$ and $\lambda$.

The dynamics of WP contains slow tunneling of under-barrier states and fast beats, due to over-barrier states, and has a regular character, in contrast to [13, 15, 16]. It happens since the over-barrier states have the spectrum of the initial Hamiltonian of HO (i.e. the equidistant spectrum) and the states interfere with each other. The revival time of the wave packet is equal to $T_{\text{rev}} = \frac{2\pi}{(E_1 - E_0)}$, that coincides with revival time predicted by the two-mode approximation. When the squeezing parameter is low ($R = 0.35$), the amplitude of beats is relatively small, since the number of excited states contributing to WP is low. In the symmetric potential a part of the WP which is formed by tunneling of the under-barrier states is smooth enough.

In the asymmetric potential the dynamics of WP, initially localized in one of the minima of $U_+^+(\xi, \lambda)$, has a number of distinctive features. In particular, the partial trapping of WP in the initial well and the suppression of tunneling to another well are observed. This phenomenon occurs independently on the well initially containing the WP. When the initial state is uniformly distributed between both wells of $U_+^+(\xi, \lambda)$, this phenomenon is observed for the deeper well; thus, the tunneling rate from the deeper well to the other well is smaller than the rate of reverse transitions. When the squeezing parameter $R$ increases, beats, caused by the over-barrier states, increase and mimic the contribution of slow tunneling of the under-barrier states. In some sense, it could be considered as the destruction of tunneling of the initially highly localized wave packet.

The proposed approach to dynamics of localized states is based on exactly solvable Hamiltonian models with multi-well potentials, in which only few levels are situated below the barrier. Increasing the number of under-barrier states is possible by subsequently applying the procedure of adding additional levels below of the initial ground state. In the considered formulation of $N$-fold SUSY QM [11, 34, 35], this procedure is equivalent to rearrangement of the initial Hamiltonian spectra. The corresponding propagators can be obtained within the approach of [11, 17, 18]. The case of potential with three local minima, two lateral and the deepest central one, is of special interest. Such a model can be applied for studying the resonant tunneling phenomenon [36, 37] in smooth potentials. The tunneling regime can be varied with changing the level location in the central minimum. In addition, it is possible to construct
a trap model with a finite number of cells taking into account both discrete and continuous spectra. Such a model could be useful in studying dynamical features of the Bose–Einstein condensate [38, 39].

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