NANOSYSTEMS:
PHYSICS, CHEMISTRY, MATHEMATICS

Abdullaev J.I., et al. *Nanosystems: Phys. Chem. Math.*, 2026, **17** (2), 179–186.
http://nanojournal.ifmo.ru
DOI 10.17586/2220-8054-2026-17-2-179-186

Original article

Critical mass ratio and phase transition in three-particle lattice systems: comparison of bosonic and fermionic cases

Janikul I. Abdullaev[1,a], Abdumalik I. Eshniyozov[2,b], Mikhail V. Dolgopolov[3,c]

[1]Samarkand State University, Samarkand, Uzbekistan

[2]Gulistan State University, Gulistan, Uzbekistan

[3]Samara State Technical University, Samara, Russian Federation

[a]jabdullaev@mail.ru, [b]eshniyozovabdumalik75@gmail.com, [c]mvdolg@yandex.com

Corresponding author: M. V. Dolgopolov, mvdolg@yandex.ru

PACS 02.30.Tb

ABSTRACT We study three-particle Schrödinger operators on the two-dimensional lattice $\mathbb{Z}^2$ and show that a critical mass ratio $\gamma_c \approx 2.75194$ governs the existence of a bound trimer in the fermionic $2+1$ configuration (two identical fermions and a third particle). For $\gamma < \gamma_c$ there is a topological prohibition (Pauli suppression) of a three-body bound state, whereas for $\gamma > \gamma_c$ a doubly degenerate eigenvalue emerges below the essential spectrum with the strong-coupling asymptotics $z(\gamma,\lambda) = -\lambda + e_0(\gamma) + O(\lambda^{-1})$. Within a unified framework based on the Birman–Schwinger principle and strong-coupling asymptotic analysis, we compare this behaviour with the bosonic case of three identical particles, where two bound states exist below the essential spectrum and the ground-state energy satisfies $z_1^s(\mu) = -3\mu + C_2 + O(\mu^{-1})$. The resulting second-order phase transition with respect to the mass ratio γ is relevant for the design of experiments on fermionic trimers in optical lattices and for modelling excitonic complexes and defect-bound states in two-dimensional nanomaterials, where the critical value γ_c serves as a design guideline for the observability of three-body bound states. We also outline a modified three-particle lattice model with two competing interaction channels, for which the Birman–Schwinger analysis naturally leads to a Landau-type scenario of a first-order phase transition in the space of trimer bound states. In the bosonic case we prove a strong-coupling theorem describing the existence and asymptotics of trimer bound states, while in the fermionic $2+1$ case we establish a spectral phase-transition theorem that identifies an explicit critical mass ratio γ_c separating the trimer and non-trimer regimes.

KEYWORDS three-particle Schrödinger operator, lattice systems, bound states, bosons, fermions, critical mass ratio, phase transition, Birman–Schwinger principle.

ACKNOWLEDGEMENTS The first author is grateful to the Foundation for Fundamental Research of the Republic of Uzbekistan for financial support of the research (grant no. AL – 922 41 04 685)

FOR CITATION Abdullaev J.I., Eshniyozov A.I., Dolgopolov M.V. Critical mass ratio and phase transition in three-particle lattice systems: comparison of bosonic and fermionic cases. *Nanosystems: Phys. Chem. Math.*, 2026, **17** (2), 179–186.

1. Introduction

The study of few-particle bound states on quantum lattices is of fundamental interest both for mathematical physics and for applications in quantum simulation, condensed-matter physics, and nanotechnology; see, for example, Refs. [1–3]. Experiments with ultracold atoms in optical lattices make it possible to realize controllable quantum systems with tunable interaction parameters and geometry, which calls for precise theoretical predictions of their spectral properties.

In recent years, substantial progress has been made in the analysis of three-particle Schrödinger operators on lattices; see, e.g., [4–6]. In parallel, the spectral theory of lattice Schrödinger operators with a finite number of isolated levels has been actively developed: in particular, Ref. [7] establishes the existence of a maximal number of isolated eigenvalues for a broad class of lattice Schrödinger operators. The present work continues this line of research by turning to three-particle systems that exhibit critical phenomena with respect to the mass ratio. At the same time, the problem of critical behavior in fermionic systems with mass imbalance has remained insufficiently explored. In particular, it has been unclear whether there exists a threshold value of the mass ratio that separates qualitatively different regimes of existence of bound states. A related question of independent interest is whether suitable modifications of a multi-particle lattice model (for instance, by adding an external field or an additional interaction channel) can give rise to a first-order phase transition accompanied by a discontinuous rearrangement of the three-particle spectrum.

In this work, we perform a comparative analysis of the spectral properties of two principal classes of three-particle systems on a two-dimensional lattice: (i) three identical bosons and (ii) a fermionic $2+1$ configuration (two identical

TABLE 1. Position of the present work within the landscape of lattice few-body models.

Work	System	Dim.	Key feature
Two-particle lattice models [11]	dimer	$d = 2, 3$	threshold effects, monotonicity
Three-fermion models on $\mathbb{Z}$ [12]	trimer	$d = 1$	strong-coupling discrete spectrum
Fermionic 2+1 trimer (this work)	trimer	$d = 2$	critical γ_c, spectral phase transition
2+1 fermions [8]	trimer	$d = 3$	repulsive contact, critical $\gamma_s(K), \gamma_{as}(K)$

fermions and a third particle of a different nature). Employing a unified methodological framework based on the Birman–Schwinger principle and asymptotic analysis in the strong-coupling regime, we uncover fundamental differences induced by the quantum statistics of the particles. We prove a strong-coupling theorem for bosonic trimers and a spectral phase-transition theorem for the fermionic 2+1 trimer with an explicit critical mass ratio γ_c.

For a related three-particle 2+1 fermionic model on $\mathbb{Z}^3$ with repulsive contact interactions, Khalkhuzhaev et al. [8] introduced two critical mass ratios $\gamma_s(K)$ and $\gamma_{as}(K)$ that determine the number of eigenvalues lying to the right of the essential spectrum at strong coupling. Here we consider instead an attractive 2+1 model on $\mathbb{Z}^2$, where a single critical mass ratio γ_c controls the emergence of a low-energy trimer level below the essential spectrum and gives rise to a second-order spectral phase transition.

The application of this unified framework to concrete three-particle lattice models reveals deep structural distinctions that are entirely dictated by the underlying quantum statistics.

2. Comparative analysis of bosonic and fermionic trimers

We consider the Hamiltonian of a three-particle system on the two-dimensional lattice $\mathbb{Z}^2$ in the coordinate representation,

$$\hat{H} = \hat{H}_0 - \alpha \sum_{i<j} \hat{V}_{ij}, \tag{1}$$

where $\hat{H}_0$ is the kinetic-energy operator, $\alpha > 0$ is the coupling constant, and $\hat{V}_{ij}$ are zero-range pair potentials given by

$$(\hat{V}_{ij}\psi)(n_1, n_2, n_3) = \delta_{n_i,n_j}\, \psi(n_1, n_2, n_3).$$

The particle statistics is encoded in the choice of the Hilbert space: the symmetric subspace ℓ^2_s for bosons and the antisymmetric subspace ℓ^2_a for fermions (with respect to the coordinates of identical particles). For the fermionic $2+1$ system we introduce the mass ratio $\gamma = m_f/m_3$, where m_f is the fermion mass and m_3 is the mass of the third particle, and δ_{n_i,n_j} denotes the Kronecker delta.

2.1. Bosonic system: three identical bosons on a lattice

We consider a system of three identical bosons of unit mass on the two-dimensional lattice $\mathbb{Z}^2$. In the coordinate representation, the three-particle Hamiltonian takes the form

$$\hat{H}_\mu = \hat{H}_0 - \mu(\hat{V}_{12} + \hat{V}_{13} + \hat{V}_{23}), \qquad \hat{H}_\mu : \ell^2_s((\mathbb{Z}^2)^3) \to \ell^2_s((\mathbb{Z}^2)^3),$$

where $\mu > 0$ is the interaction strength and $\hat{H}_0$ denotes the free kinetic-energy Hamiltonian. Here $\ell^2_s((\mathbb{Z}^2)^3)$ is the subspace of square-summable symmetric functions on $(\mathbb{Z}^2)^3$, describing the states of three identical bosons on the lattice.

The Fourier transform on $\mathbb{Z}^2$ maps the coordinate-space Hamiltonian $\hat{H}_\mu$ into the momentum representation, in which the total Hamiltonian H_μ admits a direct-integral decomposition with respect to the total quasimomentum $\mathbf{K} \in \mathbb{T}^2$,

$$H_\mu = \int_{\mathbb{T}^2}^{\oplus} H_\mu(\mathbf{K})\, d\mathbf{K},$$

where, for each fixed $\mathbf{K}$, the fiber operator $H_\mu(\mathbf{K})$ acts in the symmetric subspace $L^2_s((\mathbb{T}^2)^2)$ and is given (see. [4,5]) by

$$\big(H_\mu(\mathbf{K})f\big)(\mathbf{p}, \mathbf{q}) = E_{\mathbf{K}}(\mathbf{p}, \mathbf{q}) f(\mathbf{p}, \mathbf{q}) - \mu(V_1 + V_2 + V_3) f(\mathbf{p}, \mathbf{q}), \qquad f \in L^2_s((\mathbb{T}^2)^2).$$

Here

$$E_{\mathbf{K}}(\mathbf{p}, \mathbf{q}) = \varepsilon(\mathbf{p}) + \varepsilon(\mathbf{q}) + \varepsilon(\mathbf{K} - \mathbf{p} - \mathbf{q}), \qquad \varepsilon(\mathbf{p}) = 2 - \cos p_1 - \cos p_2,$$

and

$$
\begin{aligned}
&(V_1 f)(\mathbf{p},\mathbf{q}) = \frac{1}{(2\pi)^2}\int_{\mathbb{T}^2} f(\mathbf{p},\mathbf{s})\,d\mathbf{s}, \qquad (V_2 f)(\mathbf{p},\mathbf{q}) = \frac{1}{(2\pi)^2}\int_{\mathbb{T}^2} f(\mathbf{s},\mathbf{q})\,d\mathbf{s},\\
&(V_3 f)(\mathbf{p},\mathbf{q}) = \frac{1}{(2\pi)^2}\int_{\mathbb{T}^2} f(\mathbf{s},\mathbf{p}+\mathbf{q}-\mathbf{s})\,d\mathbf{s}.
\end{aligned} \tag{2}
$$

2.2. Fermionic system: two identical fermions and a third particle

We consider a system of two identical fermions of unit mass and a third particle of mass m (a $2+1$ configuration) on the two-dimensional lattice $\mathbb{Z}^2$. Let $\ell^2\big((\mathbb{Z}^2)^3\big)$ denote the Hilbert space of square-summable functions of three lattice sites $\boldsymbol{n} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) \in (\mathbb{Z}^2)^3$, and let

$$\ell^2_a\big((\mathbb{Z}^2)^3\big) \subset \ell^2\big((\mathbb{Z}^2)^3\big)$$

be its antisymmetric subspace with respect to the exchange of the fermionic coordinates $\mathbf{n}_1 \leftrightarrow \mathbf{n}_2$.

In the coordinate representation, the three-particle Hamiltonian is given by

$$\widetilde{H}_{\gamma,\lambda} = \hat{H}_0 - \lambda\big(\hat{V}_{13} + \hat{V}_{23}\big), \qquad \widetilde{H}_{\gamma,\lambda} :\, \ell^2_a\big((\mathbb{Z}^2)^3\big) \to \ell^2_a\big((\mathbb{Z}^2)^3\big),$$

where $\lambda > 0$ is the strength of the contact interaction and $\gamma{:=}m_f/m_3$ is the mass ratio (the ratio of the fermion mass to the mass of the third particle). Here ℓ^2_a denotes the antisymmetric subspace of ℓ^2 corresponding to the two identical fermions.

Passing to the momentum representation and fixing the total quasimomentum $\mathbf{K} = \mathbf{0}$, we arrive at the fiber Schrödinger operator

$$H_{\gamma,\lambda}(\mathbf{0}) = H_{\gamma,0}(\mathbf{0}) - \lambda\big(V_1 + V_2\big), \qquad H_{\gamma,\lambda}(\mathbf{0}) :\, L^2_a((\mathbb{T}^2)^2) \to L^2_a((\mathbb{T}^2)^2),$$

where $L^2_a((\mathbb{T}^2)^2)$ is the antisymmetric subspace in momentum space obtained as the image of $\ell^2_a((\mathbb{Z}^2)^2)$ under the three-particle Fourier transform,[1] and V_1 and V_2 are partial integral operators describing the contact interaction of the fermions with the third particle (see (2)). The operator $H_{\gamma,0}(\mathbf{0})$ acts as multiplication by the dispersion function

$$E_\gamma(\mathbf{p},\mathbf{q}) = \varepsilon(\mathbf{p}) + \varepsilon(\mathbf{q}) + \gamma\,\varepsilon(-\mathbf{p}-\mathbf{q}) = \varepsilon(\mathbf{p}) + \varepsilon(\mathbf{q}) + \gamma\,\varepsilon(\mathbf{p}+\mathbf{q}).$$

Remark. Due to the unitary equivalence $H_{\gamma,\lambda}(\mathbf{K}) \cong H_{\gamma,\lambda}(-\mathbf{K})$ via the transformation $f(\mathbf{p},\mathbf{q}) \mapsto f(-\mathbf{p},-\mathbf{q})$, it suffices to consider the total quasimomentum $\mathbf{K}$ in a fundamental domain of $\mathbb{T}^2$ modulo this involution. In this work we focus on the case $\mathbf{K} = 0$, which captures the essential spectral features; the extension to $\mathbf{K} \neq 0$ follows similar lines and will be addressed elsewhere.

2.3. General comments and development

The main analytical tool is the Birman–Schwinger principle [9, 10]. For energies z that are outside the essential spectrum of the operators $H_\mu(\mathbf{0})$ and $H_{\gamma,\lambda}(\mathbf{0})$, the corresponding eigenvalue problems

$$H_\mu(\mathbf{0})\psi = z\psi, \qquad H_{\gamma,\lambda}(\mathbf{0})\varphi = z\varphi$$

are reduced to fixed-point problems for compact self-adjoint Birman–Schwinger operators $B_\mu(z)$ and $B_{\gamma,\lambda}(z)$, respectively:

$$\psi \neq 0,\ H_\mu(\mathbf{0})\psi = z\psi \iff B_\mu(z)\psi^* = \psi^*, \qquad \varphi \neq 0,\ H_{\gamma,\lambda}(\mathbf{0})\varphi = z\varphi \iff B_{\gamma,\lambda}(z)\varphi^* = \varphi^*.$$

Moreover, for z below the bottom of the essential spectrum, the number of eigenvalues of $H_\mu(\mathbf{0})$ (respectively, $H_{\gamma,\lambda}(\mathbf{0})$) lying below z coincides with the number of eigenvalues of $B_\mu(z)$ (respectively, $B_{\gamma,\lambda}(z)$) that exceed one.

We emphasize that a key ingredient of our analysis is the detailed spectral information available for the two-particle lattice operator. In particular, the properties of the discrete spectrum of the two-particle Schrödinger operator on $\mathbb{Z}^d$ and its dependence on the total quasimomentum $\mathbf{k}$ have been studied in detail in [11], where the monotonicity of the eigenvalue branches $z_n(\mathbf{k})$ with respect to the components of $\mathbf{k}$ and bounds on the number of levels below the essential spectrum were established. In the present work, these results are used at a conceptual level to justify the robustness of two-particle threshold states, which enter the kernel of the Birman–Schwinger operator associated with the three-particle problem.

A related Birman–Schwinger type reduction combined with a finite-rank principal part has recently been employed for a different lattice few-body model, namely a system of three identical fermions on the one-dimensional lattice with nearest-neighbour attraction; in that setting, the discrete spectrum at strong coupling was analysed in [12], while the essential spectrum and further extensions to systems of identical particles were explicitly meant in the subsequent development, including in this research article. Although the underlying operator and statistics differ from our 2+1 model, these works are methodologically close to our approach and provide complementary examples of how the Birman–Schwinger framework can be used to control the discrete spectrum of multi-particle lattice Schrödinger operators.

[1]The original coordinate-space Hilbert space is three-particle, while after fixing the center-of-mass quasimomentum the effective dimension is reduced.

As a natural generalization of the model (1), we consider a three-particle Hamiltonian with two competing interaction channels,

$$H_{\gamma,\lambda,\beta}(\mathbf{0}) = H_{\gamma,0}(\mathbf{0}) - \lambda \sum_{i<j} V_{ij}^{(0)} + \beta \sum_{i<j} V_{ij}^{(1)}, \tag{3}$$

where $V_{ij}^{(0)}$ describes a contact attractive interaction, while $V_{ij}^{(1)}$ accounts for a more long-ranged interaction between the particles (for instance, of Coulombic or polaronic type). For the Hamiltonian (3), the Birman–Schwinger operator $B_{\gamma,\lambda,\beta}(z)$ typically develops several qualitatively distinct eigenvalue branches associated with different spatial structures of trimer states (a localized versus an "extended" trimer). In the language of Landau's phenomenological theory, this leads to an effective potential for the order parameter η of the form

$$\mathcal{F}(\eta;\gamma,\lambda,\beta) = a(\gamma,\lambda,\beta)\,\eta^2 + b(\gamma,\lambda,\beta)\,\eta^4 + c(\gamma,\lambda,\beta)\,\eta^6 + \dots, \tag{4}$$

where the signs of the coefficients a, b, c are determined by the spectral characteristics of $B_{\gamma,\lambda,\beta}(z)$. In the regime $b < 0$, $c > 0$, two competing local minima $\eta = \eta_{1,2}$ emerge, and variations of the parameters (γ, λ, β) may induce an abrupt transition between them, corresponding to a first-order phase transition in the space of three-body bound states, in full agreement with the general principles of Landau's phenomenological theory of first- and second-order phase transitions [13, 14].

In the strong-coupling regime ($\mu \to \infty$ for the bosonic system and $\lambda \to \infty$ for the fermionic one), the operators $B_\mu(z)$ and $B_{\gamma,\lambda}(z)$ admit an asymptotic decomposition into a principal finite-rank part and a remainder of small norm. A spectral analysis of the principal part then yields precise asymptotics of the eigenvalues and provides conditions for the existence of bound states.

3. Main results

3.1. System of three identical bosons

For a system of three identical bosons with strong zero-range attraction ($\mu \to \infty$) in the sector of zero total quasimomentum, we obtain the following result.

Theorem 3.1 (Strong-coupling trimers in the bosonic case)**.** *For all sufficiently large $\mu > \mu_0$, the three-boson Schrödinger operator $H_\mu(\mathbf{0})$ has exactly two bound states below the essential spectrum. The ground-state energy admits the asymptotic expansion*

$$z_1^s(\mu) = -3\mu + C_2 + O(\mu^{-1}), \qquad \mu \to \infty,$$

where C_2 is a constant determined by the Green function of the free Hamiltonian. The first excited state $z_2^s(\mu)$ is a threshold resonance with the asymptotics

$$z_2^s(\mu) = -\mu + \mathrm{const} + O(\mu^{-1}), \qquad \mu \to \infty.$$

Thus, in the bosonic case bound states exist for arbitrarily weak and strong interactions, and their number and asymptotic behavior are governed purely by geometric and symmetry considerations.

3.2. Fermionic $2{+}1$ system

For the fermionic $2{+}1$ configuration, the picture is fundamentally different. The antisymmetry of the wave function under the exchange of the two identical fermions imposes strong constraints on the possibility of forming a bound state.

Theorem 3.2 (Spectral phase transition in the fermionic $2{+}1$ trimer)**.** *For the fermionic $2{+}1$ trimer on the two-dimensional lattice, there exists a critical mass ratio $\gamma_c > 0$ such that:*

(1) *If $\gamma < \gamma_c$, then for any $\lambda > 0$ (equivalently, for arbitrarily large coupling) the operator $H_{\gamma,\lambda}(\mathbf{0})$ has no bound states (has no eigenvalues) below the bottom of the essential spectrum; this follows from the fact that the critical coupling diverges as $\gamma \to \gamma_c^-$.*

(2) *If $\gamma > \gamma_c$, then there exists a threshold value $\lambda_0(\gamma)$ such that for all $\lambda > \lambda_0(\gamma)$ there appears exactly one doubly degenerate bound state with energy*

$$z(\gamma,\lambda) = -\lambda + e_0(\gamma) + O(\lambda^{-1}), \qquad \lambda \to \infty.$$

(3) *The function $\Delta E(\gamma) := z_0(\gamma,\lambda) - z(\gamma,\lambda)$ satisfies $\Delta E(\gamma) > 0$ for $\gamma > \gamma_c$, $\Delta E(\gamma) = 0$ for $\gamma \le \gamma_c$, and there exists $\nu > 0$ such that*

$$\Delta E(\gamma) \sim C\,(\gamma - \gamma_c)^\nu, \qquad \gamma \downarrow \gamma_c,$$

for some constant $C > 0$.

The critical value γ_c is determined by an integral equation that follows from the solvability condition of the Birman–Schwinger equation at the bottom of the essential spectrum:

$$\gamma_c^{-1} = \frac{1}{(2\pi)^2} \int\limits_{[-\pi,\pi]^2} \frac{(\sin q_1 + \sin q_2)^2}{4 - 2(\cos q_1 + \cos q_2)}\, dq_1 dq_2. \tag{5}$$

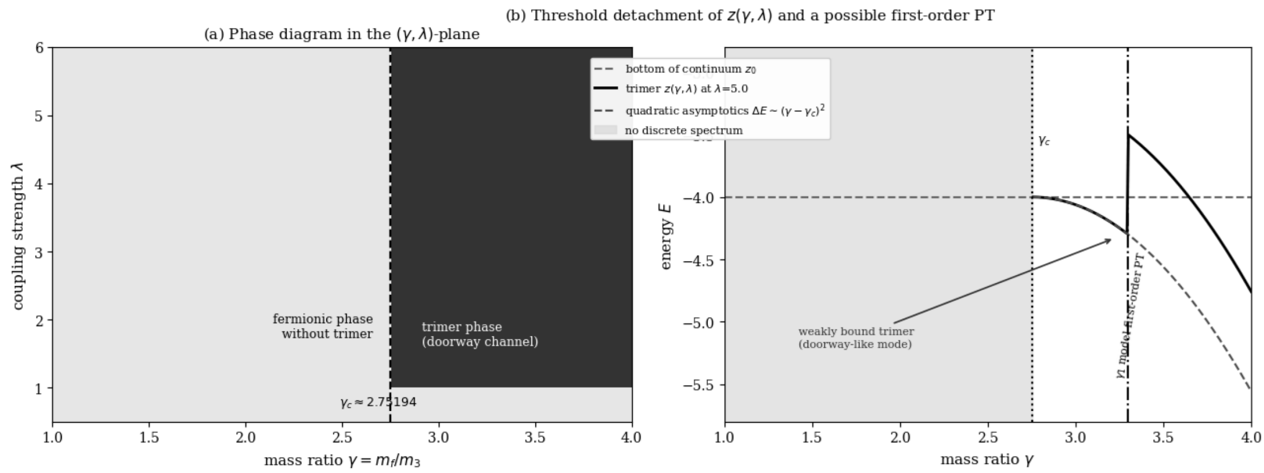

FIG. 1. (a) Schematic phase diagram in the (γ, λ)-plane for the fermionic 2+1 trimer at $\mathbf{K} = \mathbf{0}$. For $\gamma < \gamma_c$ the operator $H_{\gamma,\lambda}(\mathbf{0})$ has no three-body bound states for any λ (fermionic phase without a trimer). For $\gamma > \gamma_c$ and sufficiently large λ there exists a unique trimer bound state, corresponding to an effective doorway channel at the three-body level. (b) Trimer energy $z(\gamma, \lambda)$ at fixed sufficiently large λ near the critical mass ratio γ_c. As $\gamma \uparrow \gamma_c$ the level $z(\gamma, \lambda)$ approaches the bottom of the essential spectrum z_0, while for $\gamma > \gamma_c$ it separates from the threshold according to a quadratic law $\Delta E(\gamma) = z_0 - z(\gamma, \lambda) \sim C\,(\gamma - \gamma_c)^2$, which corresponds to a second-order phase transition in the spectral sense. The vertical line at γ_1 illustrates a possible, more intricate scenario with an additional first-order transition at larger γ, where the trimer level undergoes a discontinuous rearrangement (a model example for discussing multicritical behavior).

A numerical solution of equation (5) yields

$$\gamma_c \approx 2{,}75194 \pm 0{,}00001.$$

The transition at $\gamma = \gamma_c$ is of second order. As $\gamma \to \gamma_c^+$, the level $z(\gamma, \lambda)$ merges with the bottom of the essential spectrum, and the energy difference follows a power law $\Delta E \sim (\gamma - \gamma_c)^\nu$.

The physical mechanism behind this transition is the competition between two effects:

(1) Contact attraction, which tends to localize all three particles on the same lattice site and lower the energy of the system.

(2) Pauli repulsion, which forbids the two identical fermions from occupying the same state and increases the kinetic energy of the system.

For small γ (light fermions) the kinetic energy of the fermions is large, and Pauli repulsion suppresses the formation of a bound state. For $\gamma > \gamma_c$ the fermion mass is sufficiently large so that their kinetic energy becomes comparable to the interaction energy, which allows a trimer bound state to form.

Geometrically, the behavior of the lowest trimer level in a neighborhood of the critical mass ratio γ_c is illustrated in Fig. 1, which shows the separation of the energy $z(\gamma, \lambda)$ from the bottom of the essential spectrum z_0 for $\gamma > \gamma_c$ and the absence of a bound state for $\gamma < \gamma_c$ (Pauli-suppressed regime). This picture is consistent with a bifurcation scenario in which the contact attraction overcomes the effective Pauli repulsion only after the critical mass ratio γ_c is reached. In Fig. 1 this bifurcation is visualized as the detachment of the trimer level $z(\gamma, \lambda)$ from the threshold z_0 for $\gamma > \gamma_c$.

The second-order phase transition described in Theorem 3.2 can be visualized both in the parameter plane (γ, λ) and via the behavior of the trimer level at the threshold. In Fig. 1, panel (a) shows the domain of existence of the fermionic trimer for $\gamma > \gamma_c$, while panel (b) illustrates the quadratic detachment of the level $z(\gamma, \lambda)$ from the bottom of the essential spectrum z_0 and the corresponding second-order character of the transition. The model parameter γ_1 highlighted in panel (b) indicates a possible scenario of more complex (multicritical) behavior, with a first-order transition at larger mass ratios.

In this context, the trimer phase for $\gamma > \gamma_c$ plays the role of an effective doorway state on the lattice, analogous to the doorway modes controlling secondary electron emission in layered materials [15].

The spectral visualizations in Fig. 1 thus emphasize the qualitative difference between the fermionic and bosonic cases and, at the same time, illustrate how the proposed methodological approach captures a model scenario of a first-order phase transition built on top of the second-order bifurcation.

Remark. The exponent ν in the asymptotic law $\Delta E(\gamma) \sim C(\gamma - \gamma_c)^\nu$ is expected to be $1/2$, characteristic of a square-root bifurcation at a threshold. A rigorous determination of ν requires a refined analysis of the Birman–Schwinger kernel near the bottom of the essential spectrum and will be addressed in a forthcoming work.

4. Discussion and conclusions

The comparative analysis carried out in this work reveals a fundamental difference between the behaviors of bosonic and fermionic three-particle lattice systems:

- Bosons. Bound states exist for arbitrarily weak interactions; their number and properties are governed by the symmetry and geometry of the system.
- Fermions (2+1). A three-body bound state exists only if the mass ratio satisfies $\gamma > \gamma_c$, which reflects a *topological prohibition* imposed by the Pauli principle.

The critical phenomenon identified in the (γ, λ) parameter space can be interpreted as a *second-order phase transition*. It is characterized by a discontinuous change in the number of bound states upon crossing the critical line $\gamma = \gamma_c$. The critical value γ_c plays the role of a *universal constant of lattice geometry* that delineates two topologically distinct phases of trimer states.

A natural direction for further work is to investigate modified three-particle Hamiltonians of the type (3), where the presence of two competing interaction channels (such as short-range attraction combined with long-range repulsion or an external field) may lead to several local minima of the effective potential (4) and, consequently, to a *first-order* phase transition between different trimer phases.

The results obtained in this paper have important implications in several contexts:

(1) Quantum simulation in optical lattices. The value of γ_c provides a concrete "design rule" for experiments aiming at the observation of fermionic trimers: one has to choose atomic species with a mass ratio exceeding the threshold 2.75194 and tune the interaction into the strong-coupling regime (large λ), in which the asymptotics of $z(\gamma, \lambda)$ is realized.

(2) Condensed-matter physics. Similar three-particle models arise in the description of bound defect complexes in semiconductors and excitonic complexes in two-dimensional materials. The mechanism based on the competition between attraction and statistical constraints can manifest itself in these systems as well.

(3) Mathematical physics. This work demonstrates the efficiency of combining the Birman–Schwinger principle with asymptotic analysis for studying the spectral properties of discrete multi-particle operators. For two-particle systems, a closely related approach to the spectral structure and its parametric monotonicity was developed in [11], and here it is extended to the three-particle case with a critical phenomenon in the mass ratio. In Ref. [7], the existence of a maximum number of isolated eigenvalues of lattice Schrödinger operators under variations of the interaction parameters is analyzed, providing a natural two-particle analog of the three-body phase transitions studied in the present work. From a mathematical point of view, Theorem 3.2 gives the first example of a three-particle lattice system in which a critical value of a parameter (the mass ratio) produces a bifurcation of the discrete spectrum with an explicitly computable critical constant γ_c, while Theorem 3.1 describes the complementary strong-coupling behaviour in the purely bosonic case.

Promising directions for future research include:

- extending the present approach to systems with mixed statistics (Bose–Fermi mixtures);
- studying the influence of the lattice dimension and geometry on the critical value γ_c;
- analyzing the dynamical properties and stability of trimer states;
- relating the microscopic results obtained here to macroscopic phase diagrams of lattice models.

From the viewpoint of Landau's phenomenological theory of phase transitions [13], the mass ratio γ plays the role of a control parameter, whereas the quantity $\Delta E(\gamma) = z_0 - z(\gamma, \lambda)$ can be interpreted as an order parameter that vanishes in the limit $\gamma \to \gamma_c^+$. The behavior $\Delta E(\gamma) \sim (\gamma - \gamma_c)^\nu$ and the emergence of a doubly degenerate level below the essential spectrum for $\gamma > \gamma_c$ are characteristic of a second-order phase transition accompanied by symmetry breaking in the space of three-particle states.

4.1. Applied relevance for quantum nanosystems

The critical values obtained in this work have a direct experimental relevance for ultracold atomic systems in optical lattices. The value $\gamma_c \approx 2.75194$ provides a precise condition for the observability of fermionic trimers: one has to select combinations of atomic species such as $^6\mathrm{Li}$–$^{87}\mathrm{Rb}$ or $^{40}\mathrm{K}$–$^{133}\mathrm{Cs}$ with a mass ratio exceeding the threshold.

In condensed-matter physics, analogous three-particle models describe:

- triexciton states in monolayer WS_2 under resonant exciton–exciton attraction;
- bound defect complexes (vacancy–interstitial pairs) in MoS_2 and h-BN;
- spin-triplet states in quantum dots with a pronounced imbalance of effective masses or g-factors.

From the solid-state physics perspective, the level $z(\gamma, \lambda)$, which is separated from the essential spectrum and merges with its lower edge as $\gamma \to \gamma_c^+$, can be interpreted as an analog of a doorway state in the sense of Ref. [15], mediating the effective coupling between localized trimer configurations and the continuum of extended states. In particular, the threshold configuration corresponds to the condition

$$z(\gamma_c, \lambda) \;=\; E_{\mathrm{thr}}(\gamma_c), \qquad \det\nolimits_{\mathrm{Fred}}\big(\mathbb{I} - B_\gamma(z, \lambda)\big)\big|_{\gamma=\gamma_c, z=E_{\mathrm{thr}}(\gamma_c)} = 0,$$

which marks the onset of the trimer doorway mode at the three-body continuum threshold, where $E_{\rm thr}(\gamma)$ denotes the lower edge of the essential spectrum of the three-body Hamiltonian $H_{\gamma,\lambda}(0)$ (the three-body continuum threshold) for a given mass ratio γ.

By analogy with the three-body lattice model, where the critical mass ratio γ_c controls the emergence or disappearance of a trimer bound state, mass (isotopic) effects in real crystals manifest themselves in the spectrum of collective excitations. In particular, Ref. [16] reports the experimental observation of a negative isotopic shift of the LO phonon in 3C–SiC, revealing a universal mechanism of mass-effect dominance in cubic lattices. This indicates that controlling the masses and isotopic composition, effectively tuning $\gamma = m_f/m_3$ in our terminology, can serve as a powerful tool for engineering spectral properties in nanostructures and hybrid energy sources. In particular, isotopic engineering allows one to tailor the phonon spectrum via shifts of the form

$$\Delta\omega_{\rm LO} \;=\; \omega_{\rm LO}(M_{\rm eff}) - \omega_{\rm LO}(M_{\rm ref}),$$

where $\omega_{\rm LO}(M)$ denotes the longitudinal optical phonon frequency for a crystal with an effective mass M of the vibrating sublattice, $M_{\rm eff}$ is the mass corresponding to a given isotopic configuration, and $M_{\rm ref}$ is a chosen reference mass (e.g., corresponding to the natural isotopic composition). This is directly analogous to the way the trimer energy $z(\gamma,\lambda)$ shifts relative to the three-body continuum threshold when the effective mass ratio γ is varied across the critical value γ_c.

The monotonicity of the eigenvalues of two-particle lattice Schrödinger operators established in [11] provides a complementary mechanism for the controllable rearrangement of the energy spectrum under variations of the total quasi-momentum and lattice parameters. In particular, for the two-particle operator $H(\mathbf{k})$ on $\mathbb{Z}^3$, where $\mathbf{k} = (k_1, k_2, k_3)$ is the total quasimomentum, the paper [11] proves that the number $N(\mathbf{k})$ of eigenvalues below the essential spectrum is a nondecreasing function of each component $k_i \in [0,\pi]$, and, under additional assumptions on the interaction potential, each eigenvalue branch $z_n(\mathbf{k})$ satisfies

$$k_i^{(1)} \le k_i^{(2)} \quad\Longrightarrow\quad z_n\big(k_1,\dots,k_i^{(1)},\dots,k_3\big) \;\ge\; z_n\big(k_1,\dots,k_i^{(2)},\dots,k_3\big),$$

for fixed remaining components k_j, $j \ne i$. Here $z_n(\mathbf{k})$ denotes the n-th discrete eigenvalue of $H(\mathbf{k})$ and $N(\mathbf{k})$ is the total number of such eigenvalues, in the appropriate Brillouin-zone ordering, which allows one to shift bound levels spectrally by tuning the total quasimomentum $\mathbf{k}$ and the lattice geometry. Together with the mass- and isotope-controlled effects discussed above, this forms a robust toolbox for the spectral engineering of nanoscale quantum devices based on optical and solid-state lattices.

The proposed two-channel Hamiltonian opens a route toward realizing a first-order phase transition between distinct trimer phases, offering a microscopic realisation of Landau's phenomenological scenario in a few-body lattice system.

References

[1] Bloch I., Dalibard J., Zwerger W. Many-body physics with ultracold gases. *Rev. Mod. Phys.*, 2008, **80**(3), P. 885–964.

[2] Gross C., Bloch I. Quantum simulations with ultracold atoms in optical lattices. *Science*, 2017, **357**(6355), P. 995–1001.

[3] Atabaev B.G., Chepurnov V.I., Arutyunov N.Yu., Dolgopolov M.V., Juraev Kh.N., Radzhapov S.A. Rapid 3D defect mapping in SiC betavoltaics via positron annihilation tomography. *Physica Status Solidi (RRL) - Rapid Research Letters*, 2026, **20**(1), e202500356.

[4] Abdullaev Zh.I. Finiteness of discrete spectra for nontrivial values of the full quasi-momentum in the system of three bosons on a lattice. *Russian Math. Surveys*, 2007, **62**(1), P. 175—177.

[5] Lakaev S.N., Khalmukhamedov A.R., Khalkhuzhaev A.M. Bound states of the Schrödinger operator of a system of three bosons on a lattice. *Theoret. Math. Phys.*, 2016, **188**(1), P. 36–48.

[6] Muminov Z.I., Aktamova V.U. The point spectrum of the three-particle Schrödinger operator for a system comprising two identical bosons and one fermion on $\mathbb{Z}$. *Nanosystems: Physics, Chemistry, Mathematics*, 2024, **15**(4), P. 438–447.

[7] Lakaev S.N., Latipova D.A., Akhmadova M.O. On the existence of the maximum number of isolated eigenvalues for a lattice Schrödinger operator. *Nanosystems: Physics, Chemistry, Mathematics*, 2025, **16**(6), P. 737–748.

[8] Khalkhuzhaev A.M., Khayitova Kh.G., Khujamiyorov I.A. On the spectrum of the Schrödinger operator for a three-particle system on a lattice. *Uch. Zap. Kazan. Univ. Ser. Fiz.-Mat. Nauki*, (2025), **167**(3), P. 547–565.

[9] Birman M.Sh. On the spectrum of singular boundary-value problems. *Mat. Sb.*, 1961, **55(97)**(2), P. 125–174.

[10] Klaus M., Simon B. Coupling constant thresholds in nonrelativistic quantum mechanics. I. Short-range two-body case. *Ann. Phys.*, 1980, **130**(2), P. 251–281.

[11] Abdullaev J.I., Khalkhuzhaev A.M., Usmonov L.S. Monotonicity of the eigenvalues of the two-particle Schrödinger operator on a lattice. *Nanosystems: Physics, Chemistry, Mathematics*, 2021, **12**(6), P. 657–663.

[12] Abdullaev J.I., Ergashova S.H. Discrete Spectrum of the Schrödinger Operator of a System of Three Fermions on a One Dimensional Lattice. *Complex Anal. Oper. Theory*, 2025, **19**(6), P. 136.

[13] Landau L.D. On the theory of phase transitions. In: *Collected Papers of L. D. Landau*. Ed. by D. ter Haar. Pergamon Press, Oxford, Gordon & Breach, 1965, P. 193–216.

[14] Landau L.D., Lifshitz E.M. *Statistical Physics*. Part 1. Course of Theoretical Physics, Vol. 5. Pergamon Press, 1980.

[15] Niggas A., Hao M., Richter P., Simperl F., Blödorn F., Cap M., Kero J., Hofmann D., Bellissimo A., Burgdörfer J., Seyller T., Wilhelm R.A., Libisch F., Werner W.S.M. Identifying Electronic Doorway States in Secondary Electron Emission from Layered Materials. *Phys. Rev. Lett.*, 2025, **135**(16), 166401.

[16] Dolgopolov M.V., Chipura A.S. Negative isotopic shift of the LO phonon in 3C-SiC: A universal mechanism of mass effect dominance in cubic crystals. *JETP Lett.*, 2025, **122**(8), P. 500–506.

Submitted 1 February 2026; accepted 18 March 2026

Information about the authors:

Janikul I. Abdullaev – Samarkand State University named after Sharaf Rashidov, 15, University bul., Samarkand, 140129, Uzbekistan; ORCID 0009-0003-3315-8357; jabdullaev@mail.ru

Abdumalik I. Eshniyozov – Gulistan State University, 4th block of flats, Gulistan, 120100, Uzbekistan; ORCID 00009-0001-9357-5828; eshniyozovabdumalik75@gmail.com

Mikhail V. Dolgopolov – Samara State Technical University, 244, Molodogvardeyskaya st., Samara, 443100, Russian Federation.; ORCID 0000-0002-8725-7831; mvdolg@yandex.com

Conflict of interest: the authors declare no conflict of interest.