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Abstract

A numerical variational strategy for approximating quantum eigenstates and eigenvalues using an expansion in a basis of Morlet functions is presented. Because the work domain has a finite size, the Morlet basis is non-orthonormal. The variational problem naturally leads to a generalized eigenvalue problem rather than to an ordinary diagonalization of the Hamiltonian matrix. The corresponding formulation includes the overlap matrix on a reduced-subspace. The autonomous variational procedure defines the range of the active basis in each iteration. The adaptive subspace enrichment is based on residual vectors and three convergence criteria are tested simultaneously. The energies and wavefunctions are calculated for four different potentials obtaining results that are in excellent agreement with the numerical exact solutions.

Introduction

Localized functional representations provide a useful framework for the numerical treatment of quantum-mechanical eigenvalue problems [1]. In particular, Morlet functions combine spatial localization with oscillatory structure and multiscale resolution, making them potentially suitable for representing wavefunctions with nontrivial nodal and oscillatory patterns [2].

The objective considered here is to construct approximations to the eigenstates and eigenvalues of a one-dimensional time-independent Hamiltonian by expanding them in a basis constructed with the discrete Morlet wavelet (DMW) family [3].

The approximate wavefunctions and their corresponding energies can then be compared with a reference solution in order to assess both the quality of the wavefunctions and the accuracy of the energies. Three independent convergence criteria are applied.

An issue becomes particularly important: while the DMW is an orthogonal basis set in $\mathbb{R}$, the domain is bounded for any numerical implementation. Then, the orthogonality is lost. This a key point that requires careful consideration within the numerical strategy. Furthermore, overall phase control is taken into account throughout the iterative procedure. Finally, an approach to reduce computational cost by exploiting the parity properties of the potential and solutions is proposed.

Problem Formulation

By considering a one-dimensional time-independent Hamiltonian of the form [4]

$$\hat{H} = \hat{T} + V(x), \tag{1}$$

with stationary eigenstates satisfying

$$\hat{H}\psi_n(x) = E_n\psi_n(x), \text{ with } n = 1, ..., N_{modes}, \tag{2}$$

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the objective is to find an expansion of the $\psi_n(x)$ in terms of a (minimal) proper set of DMW, which also ensures an accurate energy spectrum:

$$\psi_n^{(N_T)}(x) = \sum_{p=1}^{N_p}\sum_{q=1}^{N_q} c_{pq}^n \ \mu_{pq}(x) = \sum_{j=1}^{N_T} c_j^n \ \mu_j(x), \tag{3}$$

where $\mu_{pq}(x)$ denotes a DMW set (or dictionary) and c_{pq} is the corresponding weight coefficient for the pq direction in the nth state. $N_T = N_p \times N_q$ is the total number of elements in the expansion, and j is only a reduced index, $j \equiv pq$.

Explicitly, the DMWs are [3]

$$\mu_{pq}(x) = A^{p/2} \ \mathcal{M}(A^p x - Bq), \tag{4}$$

with

$$\mathcal{M}(x) = C(\xi_0) \ \left(e^{i\xi_0 x} - e^{-\xi_0^2/2}\right) \ e^{-x^2/2}, \tag{5}$$

being the mother Morlet wavelet. $\mathcal{M}(x)$ is normalized in the sense $||\mathcal{M}||_2 = 1$ with a normalization constant which is dependent on the oscillating parameter, $\xi_0 > 0$:

$$C\left(\xi_0\right) = \pi^{-1/4}\left(1 + e^{-\xi_0^2} - 2e^{-\frac{3}{4}\xi_0^2}\right)^{-1/2}. \tag{6}$$

In Eq. 4 A, $B \in \mathbb{R}$, $A > 1$ and p, $q \in \mathbb{Z}$. For practical reasons, it is generally assumed that $A = 2$ and $B = 1$. p is a scale parameter that changes in a general sense the oscillatory behavior of the DMW and q is a translational parameter that controls the localization. For a time-independent Hamiltonian with real potentials, it is possible to retain only the real part of the DMW. Hereinafter this will be the case.

The Hamiltonian matrix in the DMW basis $W \equiv \{\mu_j\}$ is (Dirac notation is used):

$$H_{ij}^W = \langle \mu_i | \hat{H} | \mu_j \rangle, \ i, j = 1, ..., N_T, \tag{7}$$

and the matrix eigenvalue Schrödinger (Sch.) equation is

$$H^W c = Ec, \tag{8}$$

where c is the coefficients matrix and E is vector column with the energy eigenvalues. Besides, if μ denotes the matrix whose columns contains the basis functions, the approximated eigenvectors Ψ^W becomes

$$\Psi^W = \mu c. \tag{9}$$

In order to find the best approximation to the exact result, an autonomous variational procedure is implemented. The autonomous stage constructs its variational subspace without using (numerical) exact eigenstates to determine that subspace. The numerical solution can still be used afterwards to compare variationally converged wavefunctions and energies. Thus, *autonomous* means autonomous with respect to the exact eigenstates, but not independent of the Hamiltonian, the spatial grid, or the Morlet original set.

Overlap Matrix and Generalized Eigenvalue Problem

In any practical implementation, it is necessary to bound and discretize the space domain Ω. Thus, the spatial $N-$grid will be a vector

$$X = [x_1, ...x_N] \tag{10}$$

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This unavoidable constraint implies transforming the basis set into a non-orthonormal one. That is, the basis functions generally do not satisfy

$$\langle \mu_i | \mu_j \rangle_\Omega = \delta_{ij}. \tag{11}$$

In other words, the overlap matrix is not zero and it is defined by

$$S^W_{ij} = \langle \mu_i | \mu_j \rangle_\Omega = \int_\Omega \mu_i^*(x) \mu_j(x)\, dx. \tag{12}$$

Then, the non-orthonormal basis leads to the generalized eigenvalue problem

$$H^W c = E\ S^W c. \tag{13}$$

This is the appropriate Galerkin formulation when the basis carries a nontrivial metric [5]. S^W is not merely a numerical correction: it is an essential component of the variational geometry of the problem.

Reduced-Subspace Formulation

Now, a procedural question to address is how to select the optimal number of DMW functions to represent the wavefunctions. Firstly, a large number of Morlet functions is considered. This overabundant set is the dictionary. Then, a strategy to reduce the work subspace is implemented.

Let N be the number of spatial grid points and N_T the total number of DMW functions. The dictionary matrix

$$\boldsymbol{\mu} \in \mathbb{R}^{N \times N_T}$$

stores one sampled DMW per column. A function is marked valid when its (discrete) norm in the Ω domain exceeds a predetermined threshold, excluding functions whose support is effectively outside the computational domain. Thus, the initial active set, A, consists of M valid functions, selected from the dictionary. This is a simple initialization and does not use the exact eigenstates. An adaptive mechanism is used to expand the active set until convergence is reached.

Restricting the full projected Hamiltonian H^W and overlap matrix S^W to these indices gives

$$H^A = (H^W)_{A,A}, \qquad S^A = (S^W)_{A,A}, \qquad H^A, S^A \in \mathbb{R}^{M \times M}.$$

Then, the reduced variational problem is:

$$H^A c_n = E_n S^A c_n. \tag{14}$$

Although the reduced problem is now established, a key numerical issue warrants attention. The active basis could still include nearly linearly dependent functions (or nearly parallel directions). This implies great values on the elements of the S^A and consequently, very low (or nearly zero within the numerical error) eigenvalues. To eliminate ill-conditioned basis functions, firstly the code diagonalizes the active overlap matrix and the set of eigenvalues $\{s_1, s_2, ..., s_M\}$ is obtained. To do this diagonalization the overlap matrix is written as:

$$S^A = U\ \Lambda\ U^T. \tag{15}$$

Here U is an $M \times M$ orthogonal matrix. Its columns are the normalized eigenvectors of the real symmetric matrix S^A, and $\Lambda = \mathrm{diag}(s_1, \ldots, s_M)$ contains the corresponding eigenvalues. Ideally, $U^T U = I_M$. Each column of U describes a direction in the active coefficient space; the associated eigenvalue measures the overlap norm of that direction.

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As very small overlap eigenvalues indicate directions that are linearly dependent -or nearly dependent- on the sampled grid, the code retains only eigenvalues satisfying

$$s_i > \epsilon_s s_{\max}, \qquad \epsilon_s = 10^{-10}, \qquad s_{\max} = \max_i s_i. \tag{16}$$

This condition redefines the effective active range, r. If $r \leq M$ eigenvalues survive, a new $U_r \in \mathbb{R}^{M\times r}$ containing the corresponding columns of U, and $\Lambda_r \in \mathbb{R}^{r\times r}$ is the diagonal matrix of retained eigenvalues. Therefore, the full matrix U is $M \times M$, while U_r is $M \times r$.

The transformation

$$T = U_r\ \Lambda_r^{-1/2} \qquad T \in \mathbb{R}^{M\times r}, \tag{17}$$

whitens the overlap metric:

$$T^T S^A T = I_r. \tag{18}$$

The reduced Hamiltonian in these coordinates is

$$H_r = T^T H^A\ T, \qquad H_r \in \mathbb{R}^{r\times r}. \tag{19}$$

The code solves

$$H_r d_n = E_n d_n \tag{20}$$

and transforms back to active-basis coefficients:

$$c_n = T d_n. \tag{21}$$

Once the corresponding coefficient vectors are reconstructed, the approximate wavefunctions are

$$\psi_n^M(x) = \sum_{j=1}^{M} c_j^n \mu_j(x), \text{with } n = 1, ..., N_{modes}. \tag{22}$$

in where the coefficient are redefined so that the reconstructed states were normalized.

$$\int_\Omega |\psi_n^M(x)|^2\, dx = 1. \tag{23}$$

This normalization is required for a direct comparison with normalized reference eigenstates and for the evaluation of overlap-based quantities such as the fidelity. Additionally, as the states are defined up to global phase, the code also align the sign of each real state with its previous-iteration counterpart.

Convergence and Adaptive Variational Subspace Enrichment

The convergence in the iterative process is controlled in three properties simultaneously: the energy eigenvalues, the wavefunctions and the discrete Sch. equation. A meaningful iterative improvement should not merely repeat the same diagonalization. Instead, the variational subspace could be enriched from information contained in the current approximation. It means that if the three convergence criteria are not reached, the scheme adss in next iteration new DMWs to the active set.

If at any $k-$iteration, $M^{(k)}$ denotes the number of active functions and $A^{(k)}$ the active set of indexes, the adaptative rule is the following:

1. The procedure starts with an arbitrary number $M^{(0)}$ of active DMW selected from the reduced dictionary.

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2. After the diagonalization scheme described in the preceding section, the residuals of the Sch. equation and their corresponding norms are calculated:

$$R_n^{(k)}(x) = H\psi_n^{M^{(k)}}(x) - E_n^{(k)}\psi_n^{M^{(k)}}(x) \tag{24}$$

$$\left\|R_n^{(k)}\right\|_2 = \left(\int_\Omega \left|R_n^{(k)}\right|^2 dx\right)^{-1/2} \tag{25}$$

Then, the global relative residual is used to check convergence:

$$\eta_n^{(k)} = \frac{\left\|R_n^{(k)}\right\|_2}{\left\|H\psi_n^{M^{(k)}}\right\|_2 + |E_n^{(k)}|\left\|\psi_n^{M^{(k)}}\right\|_2} \tag{26}$$

A nonzero relative residual measures the failure of the approximate state to satisfy the eigenvalue equation.

3. For each μ_j belonging to the dictionary, but not used in the current $k-$iteration, is calculated and assigned a score:

$$q_j = \max\left|\langle\mu_j|R_n\rangle\right|, \text{ with } n = 1, ..., N_{modes}. \tag{27}$$

4. The three convergence criteria are checked:

   (a) The energy eigenvalues criterion:

$$|E_n^{(k)} - E_n^{(k-1)}| < \varepsilon_E, \tag{28}$$

   (b) The wavefunction quality: At this point, the quantum fidelity is used

$$F_n^{(k)} = |\langle\psi_n^{M^{(k)}}|\psi_n^{M^{(k-1)}}\rangle|^2 \tag{29}$$

   $0 \leq F_n \leq 1$ and the convergence criteria is

$$1 - F_n^{(k)} < \varepsilon_F. \tag{30}$$

   (c) The approximation on the discretization of the Sch. equation

$$\eta_n^{(k)} < \varepsilon_R. \tag{31}$$

   To stop the iteration procedure, the three convergence criteria must be satisfied simultaneously for all the modes.

5. If any of the criteria fails, a predetermined number of DMW with greater scores are added to the active set, the dimension of the basis pass from $N \times M^{(k)}$ to $N \times M^{(k+1)}$, and the procedure to conform the reduced space described in the precedent paragraph starts again.

The essential feature is that successive iterations enlarge or improve the approximation space rather than repeatedly solving the same fixed finite-dimensional problem. Energy accuracy, wavefunction fidelity, and the approximation to Sch. equation should nevertheless be regarded as complementary diagnostics.

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Hamiltonian parity advantage

When the potential is symmetric with respect to the origin, $V(x) = V(-x)$, the Hamiltonian commutes with the parity operator $\hat{\mathcal{P}}$,

$$(\hat{\mathcal{P}}\psi)(x) = \psi(-x), \qquad [\hat{H}, \hat{\mathcal{P}}] = 0. \tag{32}$$

Consequently, the eigenstates will have alternatively well defined parity

$$\psi^{(+)}(-x) = \psi^{(+)}(x), \qquad \psi^{(-)}(-x) = -\psi^{(-)}(x), \qquad \langle\psi^{(+)}|\psi^{(-)}\rangle = 0. \tag{33}$$

This feature is an advantage for the numerical calculation presented here. The DMW family has a pair of symmetric translation indices q and $-q$ for each scale index p. A $\mu_j = \mu_{pq}$ has a reflected one $\mu_{j'} = \mu_{p-q}$, and the problem can be separated between even and odd sets.

$$\mu_j^{(+)}(x) = \frac{\mu_j(x) + \mu_{j'}(x)}{\sqrt{2}}, \tag{34}$$

$$\mu_j^{(-)}(x) = \frac{\mu_j(x) - \mu_{j'}(x)}{\sqrt{2}}. \tag{35}$$

Thus, the problem is decoupled in two orthogonal subspaces, $A^{(+)}$ and $A^{(-)}$ represented by the even and odd reconstruction of the active basis. The functions with $q = 0$ are added at the $A^{(+)}$ subset.

For symmetric potentials and active basis closed respect to reflections, the initial basis with $M^{(0)}$ functions have to be centered in the translational indexes, and the adaptative scheme must incorporate pairs of reflected DMW. Lastly, the autonomous variational scheme is applied for even and odd subspaces separately. Upon reaching convergence, even and odd eigenvalues and eigenvectors are sorted in increasing order

$$\{(E_n, c_n)\} = \mathrm{sort}_E\left(\{(E_+, c_+)\} \cup \{(E_-, c_-)\}\right). \tag{36}$$

The order is not assigned alternating even and odd solutions. It is determined by the energies resulting of the each independent calculation.

The code takes advantage of the parity only for symmetric potentials, for any other case, it solves the diagonalization by using the whole space.

Results

The variational scheme is applied on two examples and their variants: the standard square potential and the double square well potential and their softened versions. The oscillating parameter ξ_0 is fixed in 1.0. This value in a trade-off between confined and free systems. A discussion on this topic can be seen in [6]. A detail on the parameters used in the numerical calculations are summarized in the appendix.

Figures [1] and [2] show the results for the first four modes for the square and the softened square potential, and in the figures [3] and [4] the corresponding results for the double quantum well are shown. For comparison, the variational solutions are plotted alongside with the numerical output of the discretization of the Sch. equation. In panel (a), the wavefunctions are shifted according the corresponding energy eigenvalue. There is a remarkable agreement with the reference and perfectly the even-odd sequence is reached. In the (b)-panel the probability densities given by the square modulus of the wavefunctions are graphed. The localization and spatial distribution of the particle described by these densities are very well represented. The (c)-panel is a heatmap for the meaningful coefficients participating in the Morlet expansion of the ground state. The (d)-panel show how the quantum fidelity tends to one for each mode. A

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mark for the $F = 0.99$ is labeled. In the (e)-panel the evolution of the eigenvalues throughout the iterative process are plotted. Finally, the (f)-panel shows the convergence parameters. Here is also included the η_{int}, which is the same as η but restricting the integration domain in Eq. (25) only for $x-$values where the potentials are attractive.

Discussion and conclusions

The overall results are very encouraging. It is clear that the Morlet family, and the discrete version in particular, are a very good basis to reproduce solutions of the time-independent Hamiltonian. An autonomous variational procedure was implemented in order to reach the better size of the truncated basis set. Because the spacial domain is necessarily restricted to a finite size, the set of DMW becomes non-orthogonal, the overlap assume a role of a new metric and the diagonalization scheme take account this issue. Besides, and adaptative sequence looking for the better size of the basis set in which the effective range grows in each iteration until the convergence is achieved. The residuals between the eigenfunctions of given iteration and the DMW not used in the expansion are used as control parameter to include more functions to the active basis in the next iteration. Three criteria are checked simultaneously: eigenvalues, eigenfunctions and the discretization on the Sch. equation. Besides, the parity of the potentials is taking as a advantage to optimize the numerical calculation.

This scheme becomes a very robust tool to represent quantum states able to accounts particle confinement in arbitrary attractive potentials and it is a starting point to analyze more complex problems in higher dimensions.

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Appendix: Principal matrix dimensions

The calculations were done with a discretization of $N = 2001$ points in the space domain, and de total DMW dictionary runs from $p = -7, ..., 7$ ($N_p = 15$) and $q = -25, ..., 25$ ($N_q = 51$), $N_T = 765$, and $n_{modes} = 4$ states:

Quantity	Dimension	Meaning
μ	$N \times N_T$	Full Morlet dictionary
H^W	$N_T \times N_T$	Full projected Hamiltonian
S^W	$N_T \times N_T$	Full overlap matrix
μ_A	$N \times M$	Active Morlet functions
H^A, S^A	$M \times M$	Active matrices
U	$M \times M$	Eigenvectors of $\boldsymbol{S}_s$
U_r	$M \times r$	Retained overlap eigenvectors
T	$M \times r$	Whitening transformation
H_r	$r \times r$	Reduced Hamiltonian
c_A	$M \times n_{modes}$	Active-basis coefficients
Ψ^W	$N \times n_{modes}$	Reconstructed states

Here M is the active-basis size and $r \leq M$ is the effective rank after thresholding the overlap matrix. At the final stage, the M value is limited to 80.

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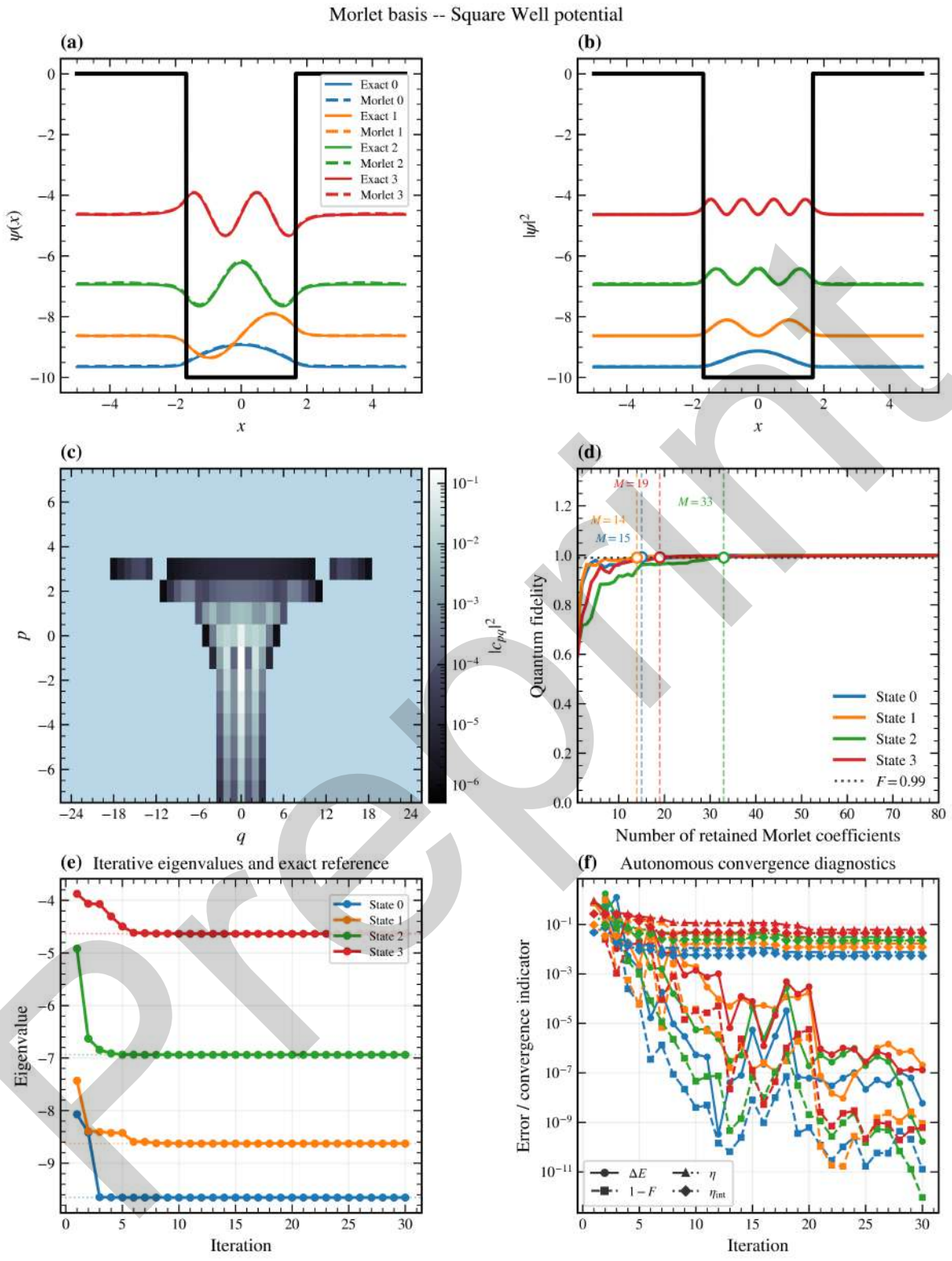


Figure 1: (a) The first four modes are shown. Solid lines represents the (exact) numerical solutions. Dashed lines are the results of the autonomous variational scheme. The wave functions are shifted according the corresponding eigenvalue (numerical or variational). (b) The same as (a) for the probability densities. (c) A heatmap for the coefficients retained for the ground state. (d) Quantum fidelity as function of the variational subspace size. Circles indicates the point where the fidelity is 0.99. (e) Evolution of the eigenvalues throughout iterative process. (f) Convergence parameters.

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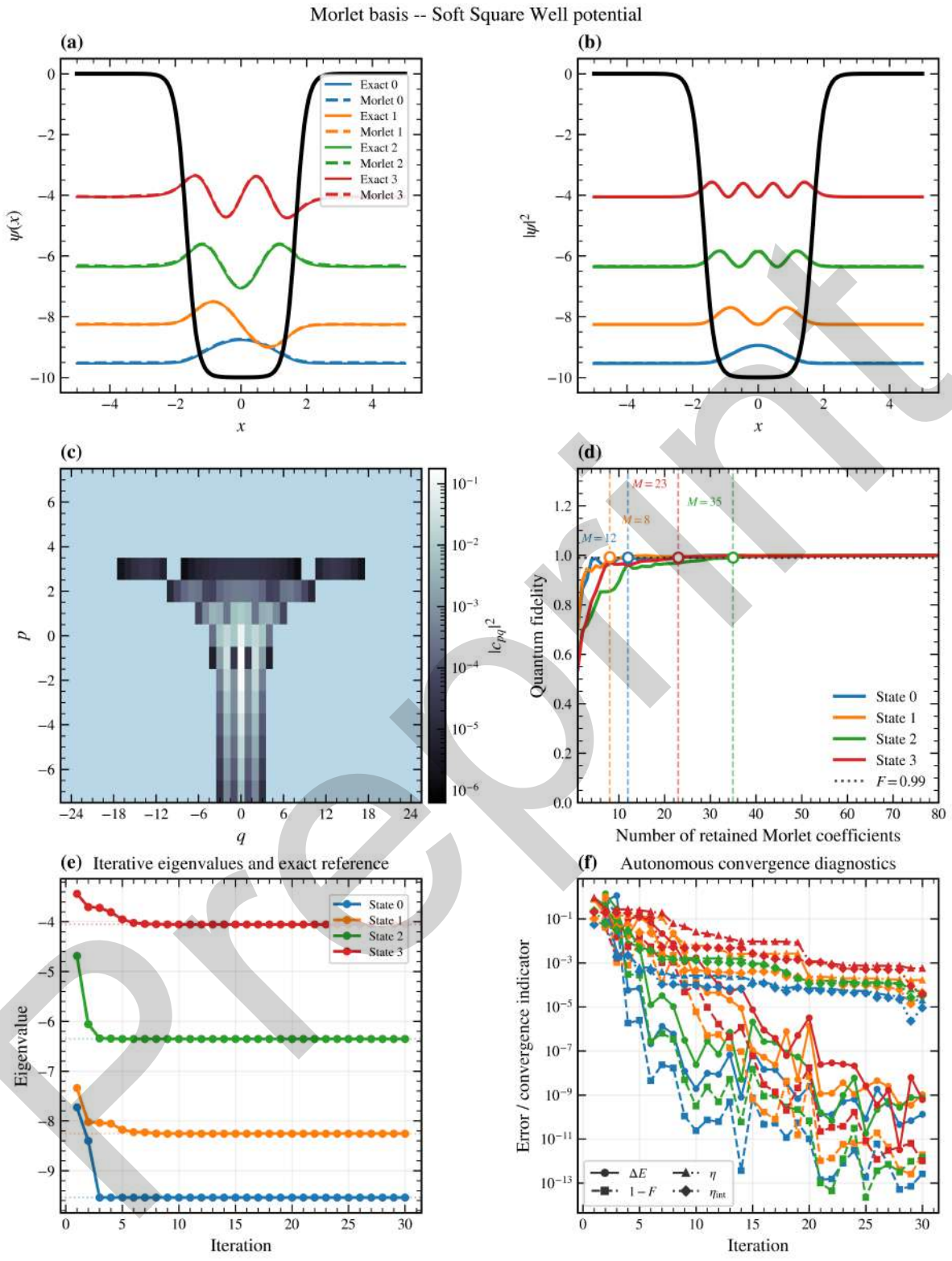


Figure 2: (a) The first four modes are shown. Solid lines represents the (exact) numerical solutions. Dashed lines are the results of the autonomous variational scheme. The wave functions are shifted according the corresponding eigenvalue (numerical or variational). (b) The same as (a) for the probability densities. (c) A heatmap for the coefficients retained for the ground state. (d) Quantum fidelity as function of the variational subspace size. Circles indicates the point where the fidelity is 0.99.(e) Evolution of the eigenvalues throughout iterative process. (f) Convergence parameters.

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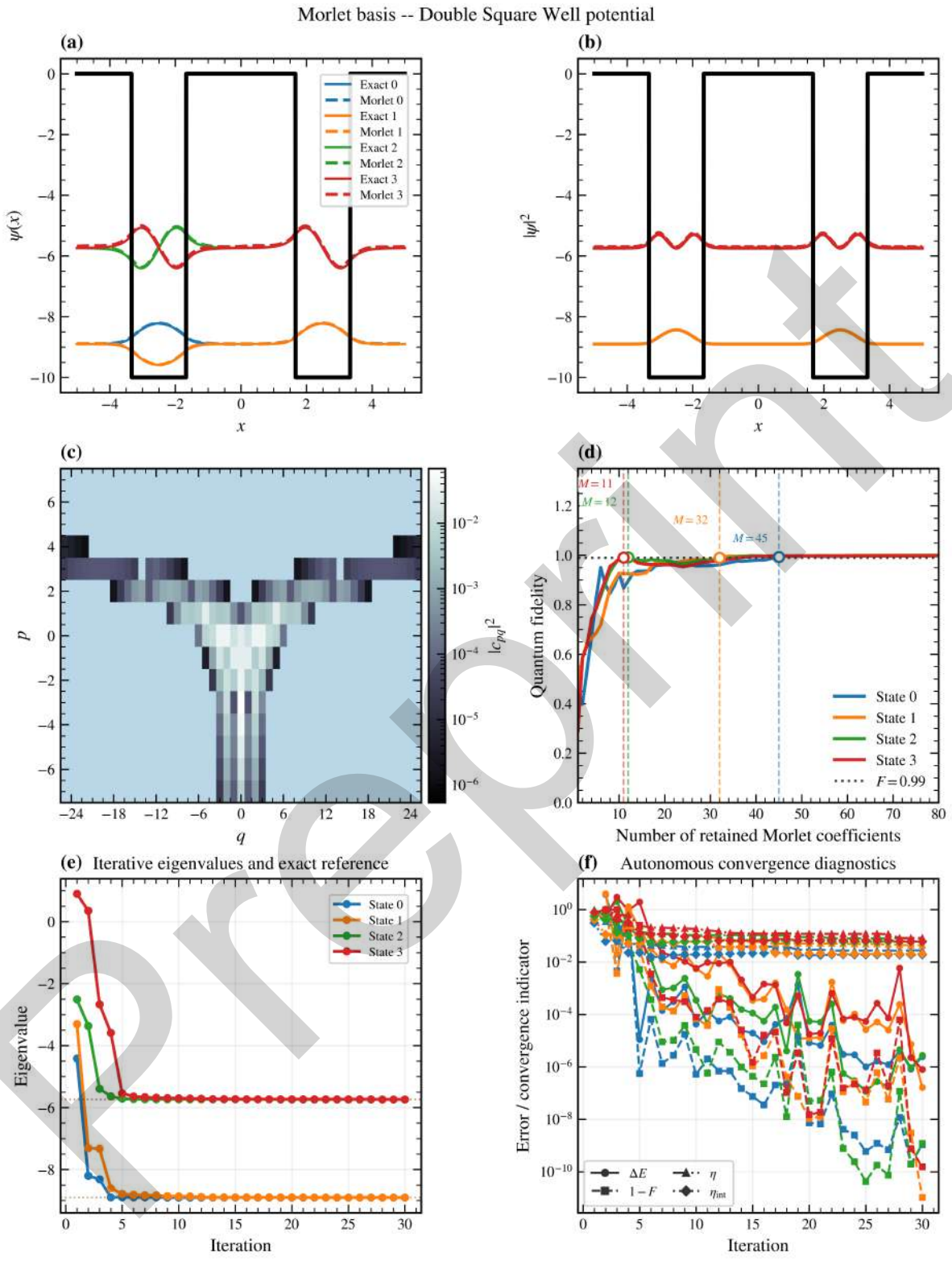


Figure 3: (a) The first four modes are shown. Solid lines represents the (exact) numerical solutions. Dashed lines are the results of the autonomous variational scheme. The wave functions are shifted according the corresponding eigenvalue (numerical or variational). (b) The same as (a) for the probability densities. (c) A heatmap for the coefficients retained for the ground state. (d) Quantum fidelity as function of the variational subspace size. Circles indicates the point where the fidelity is 0.99.(e) Evolution of the eigenvalues throughout iterative process. (f) Convergence parameters.

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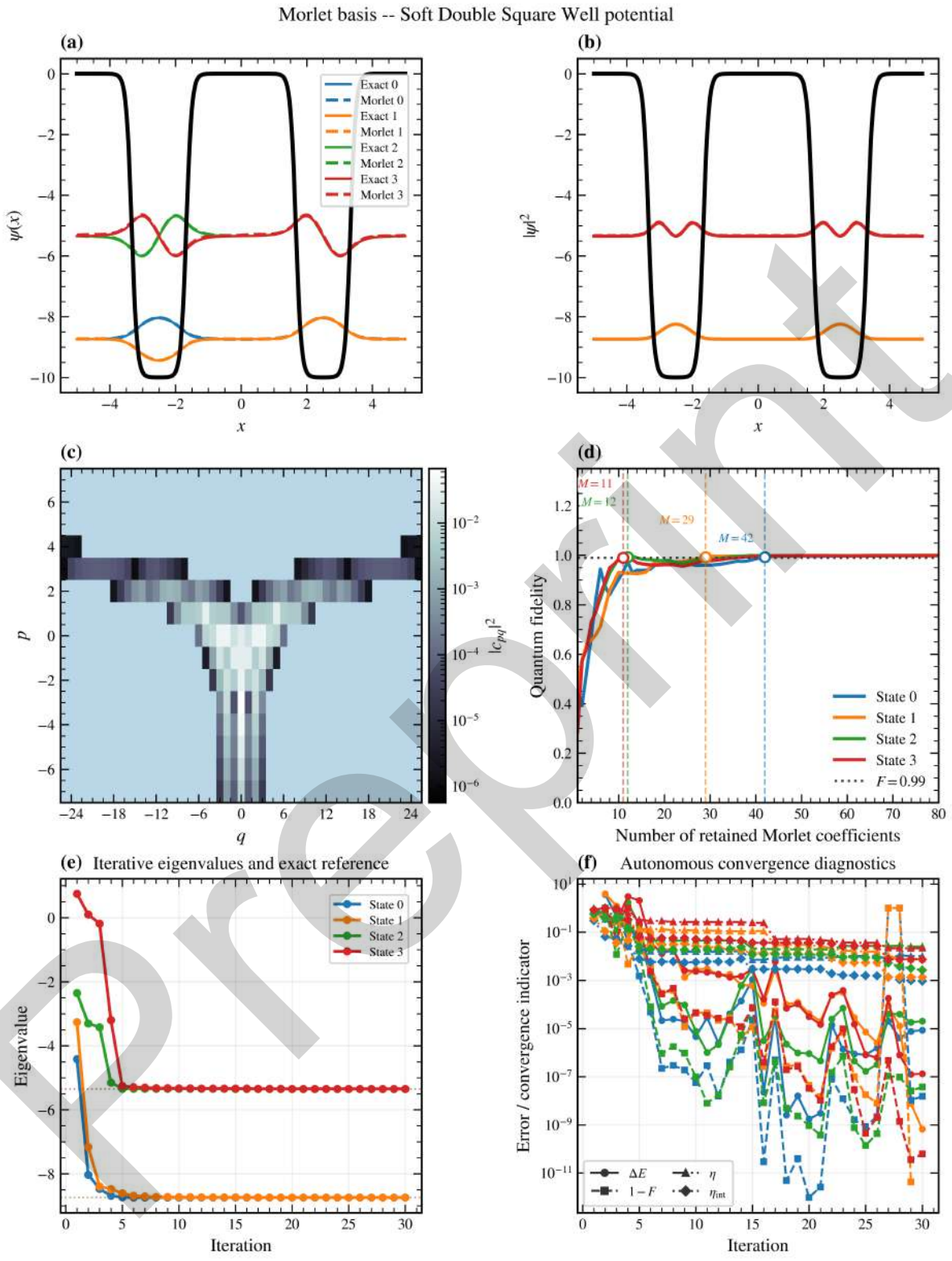


Figure 4: (a) The first four modes are shown. Solid lines represents the (exact) numerical solutions. Dashed lines are the results of the autonomous variational scheme. The wave functions are shifted according the corresponding eigenvalue (numerical or variational). (b) The same as (a) for the probability densities. (c) A heatmap for the coefficients retained for the ground state. (d) Quantum fidelity as function of the variational subspace size. Circles indicates the point where the fidelity is 0.99.(e) Evolution of the eigenvalues throughout iterative process. (f) Convergence parameters.

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