

Excited eigenstates from a two-species random walk

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Macroscopically, the population density function of random walk models can satisfy self-contained dynamics and exhibit unexpected order. Here, we show how a two-species random walk model that includes diffusion, probabilistic absorption of walkers mediated by a potential function, cross-species annihilation, and normalization of the population density can be implemented semianalytically (by propagating the population density directly instead of simulating individual walkers) to yield steady states that precisely match eigenstates of the Hamiltonian with the corresponding potential function. Key parameters of the random walk model, namely, the absorption coefficient and the diffusion displacement variance, are constrained by establishing an explicit correspondence between the model and imaginary-time propagation of the Schrödinger equation for small time steps. To enforce convergence toward a targeted excited state—rather than merely the ground state—we implement a sparse and periodic orthogonalization where components of the population density proportional to lower-energy eigenstates are removed. This adjustment is sufficient to ensure that the population density propagates within the subspace orthogonal to the span of the lower-energy states, while still converging toward the target state. The model is tested in one- and two-dimensional cases, for different potential functions and different energy levels. The model converges to steady states whose energy uncertainty extrapolates to zero in the limit of vanishing time step, and comparison with theoretical eigenfunctions yields error norms ranging from 10^{-3} to 10^{-11} . Beyond the application to Hamiltonian eigenvalue problems, this work gives insight into the emergence of nontrivial macroscopic observables based on microscopic, stochastic dynamics.

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I. INTRODUCTION

The collective behavior of microscopic, stochastic, and interacting constituents can often lead to macroscopic order, where self-contained laws and dynamics emerge [1–3]. At the macroscopic scale, observables can be insensitive to changes in a system's microscopic rules—so-called sloppy directions in the high-dimensional parameter space [4]. As a result, a variety of systems exhibit a many-to-one mapping between their collective, microscopic dynamics, and the observables that emerge at the macroscopic level. It is thus to be expected that the emergent features of complex systems are generally robust, rather than a mere manifestation of microscopic details, and that they offer a reliable framework for investigation. These aspects of complex systems arise, for instance, in the study of random walk models and their associated macroscopic behavior [4]. Of particular relevance to the work presented here is a line of research whose aim is to provide a microscopic, statistical basis to the emergence of macroscopic observables governed by partial differential equations [5–13].

The classical, paradigmatic case of such reasoning dates back to Einstein [14], where he showed that the probability density for the position of single particles undergoing random motion satisfies the diffusion equation, and can thus be associated with the macroscopic concentration field. Other seminal work on leveraging microscopic random walks to compute macroscopic observables includes the introduction of Monte Carlo methods [15] and the derivation of the Feynman-Kac formula [16]. Subsequently, these ideas led to the formulation of quantum Monte Carlo methods [17], where sampling-based stochastic algorithms are applied to solve quantum-mechanical problems. In diffusion Monte Carlo, for instance, an ensemble of random walkers is simulated over configuration space with the aim of satisfying, at the macroscopic population level, the dynamics of the Schrödinger equation in imaginary time, whereby excited states are gradually filtered out by a combination of diffusion and a potential function-dependent source term [18]. This method has found significant success in computing the ground state of various quantum systems, from small molecules in quantum chemistry [19,20] to fluids [21] and solids [22], and is still today an active area of research. Recent developments include the use of real-space grids for representing spatially resolved densities [23] and for a better estimate of the wave function's nodal structure [24], investigations of population control bias [25], and neural network-based techniques [26,27].

Despite the technical success of this class of methods, it has been pointed out that, at the conceptual level, there is still an interpretability gap between the Schrödinger equa-

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tion and the diffusion equation [8,28–31], as the latter enjoys a clear microscopic interpretation based on stochastic dynamics [32]. While it is true that diffusion Monte Carlo offers a framework where branching random walks are simulated as a means to solve the imaginary-time Schrödinger equation, interpretability is clouded by the need to implement the fixed node approximation, to choose a trial wave function, and to adjust the reference energy for population control [33]. Here, we show unambiguously how the dynamics of a two-species random walk model can be mapped onto that of imaginary-time propagation (ITP) of the Schrödinger equation to yield the eigenstates of the corresponding Hamiltonian. The model consists of an ensemble of signed walkers evolving on a discrete spatial grid and in discrete time. At each time step, the configuration of the population evolves due to four influences (Sec. II A): a variable step probabilistic displacement, a survival test mediated by interaction with a potential function, cross-species annihilation, and the injection of new walkers to maintain a constant population size. Notably, we develop the propagator for the population density (Sec. II B) and equate it with that of ITP for small time steps (Sec. II C). As such, the model is implemented semianalytically, by direct propagation of the population density instead of the simulation of individual walkers. The explicit correspondence with ITP provides a unique constraint for key model parameters, namely, the absorption coefficient and the displacement distribution variance, which, in turn, enables the model to converge precisely toward the correct eigenstates for the chosen potential function (Sec. III B). In addition, a sparse orthogonalization step is proposed to enforce convergence toward excited states (Sec. III A). By introducing a simple and concise correspondence between the random walk model and ITP, this work solidifies the interpretative framework of ITP based on microscopic, stochastic dynamics. As such, it contributes a step toward uncovering the richness of random walk models in light of their emergent, macroscopic features, with a particular application to the imaginary-time Schrödinger equation.

II. MODEL AND THEORY

A. Numerical simulations

We present here the two-species random walk model in one dimension (1D) for clarity, but generalization to higher dimensions is possible (see Appendix A). Let $\{x_i \equiv id\}_{i=-L}^L$ be a discrete spatial grid of step d on which two populations of particles, *walkers* and *antiwalkers*, navigate. At each time step, $\{t_j \equiv j\Delta t\}_{j=0}^T$, the occupation number of walkers and antiwalkers at site i is $N^{(+)}(x_i, t_j)$ and $N^{(-)}(x_i, t_j)$, respectively. At every time step, particles undergo diffusion by taking a spatial step drawn from a symmetric displacement probability distribution, $P_{\Delta X}^{(\sigma)}$, with standard deviation $\sigma = \sigma(\Delta t)$. For self-consistency, i.e., to ensure statistical regularity when varying Δt , we require $\sigma \propto \sqrt{\Delta t}$, which is made explicit in Sec. II C. The distribution $P_{\Delta X}^{(\sigma)}$ is chosen uniform for the initial tests presented in the current section, and Gaussian for the main results of Sec. III. At every time step, this distribution is sampled for each particle, and their positions are updated accordingly. Particles are assumed independent during this diffusion process.

Next, influence of the environment on particles occurs by means of a potential function, $V > 0$: $\{V_i \equiv V(x_i)\}_{i=-L}^L$. This function defines a survival probability such that, at each time step, a particle located at site i survives with probability $P_{\text{surv}}^{(C)}(V_i) = \exp(-CV_i)$, where $C = C(\Delta t) > 0$ is called the absorption coefficient—absorption occurs with probability $1 - P_{\text{surv}}^{(C)}$. We assume here (and justify in Sec. II C) that C depends linearly on Δt and that $C(\Delta t = 0) = 0$, ensuring that $P_{\text{surv}}^{(C(\Delta t_1 + \Delta t_2))} = P_{\text{surv}}^{(C(\Delta t_1))} P_{\text{surv}}^{(C(\Delta t_2))}$. A standard uniform number is drawn for each particle and is compared to the corresponding $P_{\text{surv}}^{(C)}$, such as to determine whether survival or absorption occurs.

Particles of the same type do not interact with one another. Across species, however, walkers and antiwalkers interfere through a process of annihilation when located on the same site. More precisely, the occupation numbers after annihilation become

$$\begin{aligned} N^+(x_i, t_j) &\leftarrow \max(0, N^+(x_i, t_j) - N^-(x_i, t_j)), \\ N^-(x_i, t_j) &\leftarrow \max(0, N^-(x_i, t_j) - N^+(x_i, t_j)). \end{aligned} \quad (1)$$

Hence, at the end of this annihilation process, only one species survives at any given site. This motivates the definition of the net occupation number as $N(x_i, t_j) = N^{(+)}(x_i, t_j) - N^{(-)}(x_i, t_j)$.

Given the absorption and annihilation processes outlined above, the total population would monotonically decrease in size, as all particles would eventually be removed from the system. To compensate for this effect, we maintain the population size constant by normalizing the occupation numbers across the spatial grid at the end of each time step. Let α be the fraction of particles remaining after absorption and annihilation, relative to the initial population size. Then, at the end of each time step, the occupation numbers are scaled by $\frac{1}{\alpha}$ and rounded to the nearest integer.

When subjected to this sequence of processes (diffusion, absorption, annihilation, normalization), ensembles of random walkers and antiwalkers reach a steady-state configuration. Numerical simulations of this model are shown in Fig. 1 (blue crosses), for an ensemble of 20 000 particles evolving in a quadratic potential, with a random initial placement of walkers and antiwalkers. This type of simulation is akin to what is implemented in diffusion Monte Carlo methods, of which there are many variants. To better compare these simulation results with the theory to follow (Sec. II B), we compute occupation densities for walkers and antiwalkers as

$$\psi^{(\pm)}(x_i, t_j) = \frac{N^{(\pm)}(x_i, t_j)}{\sqrt{\sum_i N^2(x_i, t_j)d}}, \quad (2)$$

and the net population density as

$$\psi(x_i, t_j) = \psi^+(x_i, t_j) - \psi^-(x_i, t_j), \quad (3)$$

where we choose the normalization such that, in a continuum limit ($d \rightarrow 0$), the net density would satisfy $\int_{\mathbb{R}} \psi^2(x, t_j) dx = 1$, which will facilitate the connection to the wave function in Sec. II C.

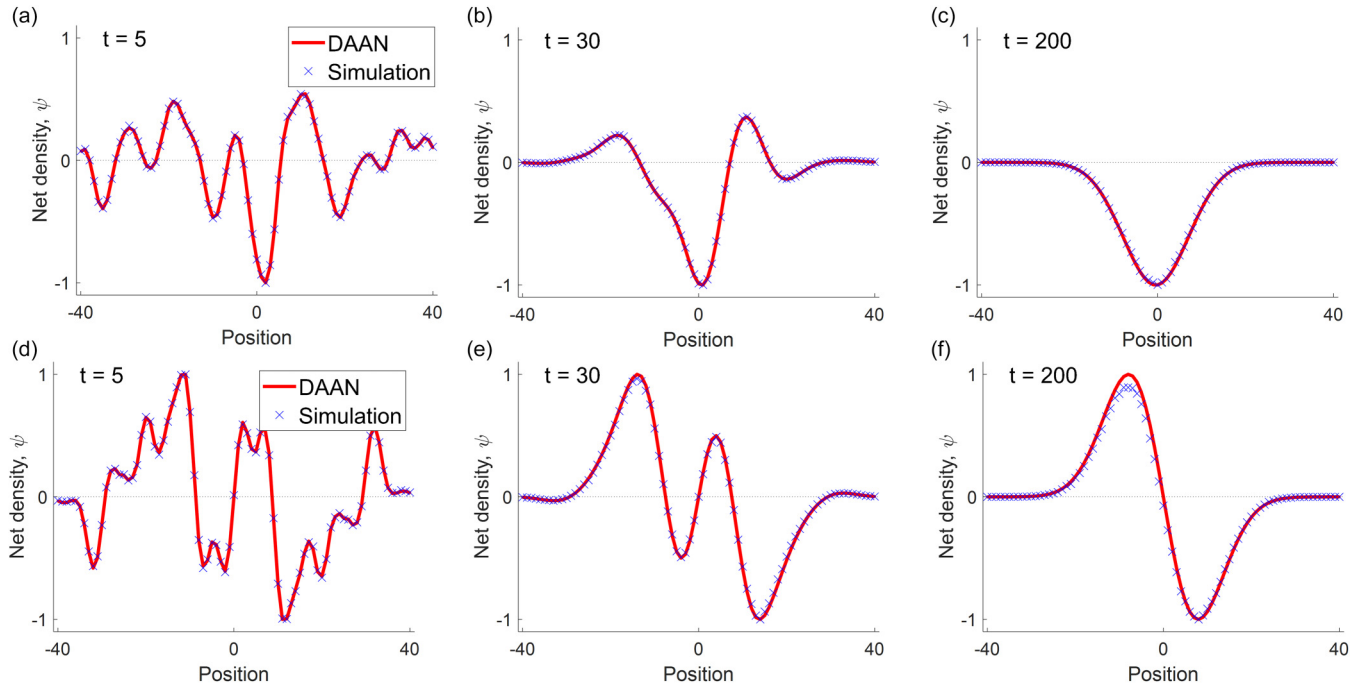


FIG. 1. Comparison of the net density, $\psi(x_i, t_j)$, between a particle-based simulation of 20 000 walkers and antiwalkers (blue crosses) and the DAAN procedure of Eq. (7) (red curve). In panels (a)–(c), the initial density, ψ_{ini} , is completely random (Gaussian noise), while in panels (d)–(f) it is antisymmetric by construction, but otherwise random (i.e., a random configuration of walkers is first sampled, and for each walker at position x , an antiwalker is placed at position $-x$). The displacement probability distribution, $P_{\Delta X}^{(\sigma)}$, is given by $[\frac{1}{3}, \frac{1}{3}, \frac{1}{3}]$, corresponding to equal probability of a step to the left, to the right, or to maintain the current position. The potential function is quadratic, and the survival probability $P_{\text{surv}}^{(C)}$ is given by $\exp(-1 \times 10^{-4} x^2)$. The annihilation and normalization processes are as described in the text. For the particle-based simulations, particles reaching $|x| > 40$ are automatically eliminated, which is equivalent to imposing an infinite potential barrier for $x = \pm 40$.

B. Asymptotic behavior

We now turn to a theoretical representation of the random walk model described above, in the limit of large number of particles. Asymptotically, we expect the net density, ψ , to behave deterministically and we seek a mathematical representation of its evolution over time—The four processes outlined in Sec. II A (diffusion, absorption, annihilation, normalization) should correspond to well-defined operations on ψ . Moreover, by the law of large numbers, the numerator in Eq. (2) will converge to its expectation value and thus be proportional to the probability, $P_X^{(\pm)}(x_i, t_j)$, of finding a given particle at site i at time t_j . Following the path of such a particle during the diffusion process, let $\xi(t_j)$ be its position at the j th time step, such that at the next time step, its position is given by the sum $\xi(t_j) + \delta x$, where δx is drawn from $P_{\Delta X}^{(\sigma)}$. The probability mass function $P_X^{(\pm)}(x_i, t_{j+1})$ is thus equal to the convolution of $P_{\Delta X}^{(\sigma)}$ with $P_X^{(\pm)}(x_i, t_j)$. Given that $\psi^{(\pm)} \propto P_X^{(\pm)}$, this reasoning extends to the occupation densities:

$$\psi^{(\pm)}(x_i, t_{j+1}) = (\psi^{(\pm)}(\cdot, t_j) * P_{\Delta X}^{(\sigma)})(x_i). \quad (4)$$

Equation (4) would hold if diffusion were the only process imposed on the population of particles. With the absorption process, however, particles survive with probability $P_{\text{surv}}^{(C)}(V_i)$, leading to a spatially dependent reduction of the population. This process is enforced by scaling the occupation densities of Eq. (4) by the survival probability:

$$\psi^{(\pm)}(x_i, t_{j+1}) \leftarrow P_{\text{surv}}^{(C)}(V_i) \psi^{(\pm)}(x_i, t_{j+1}). \quad (5)$$

Interspecies annihilation is implemented directly via the definition of the net density, whereby only the excess number of walkers or antiwalkers at a given site is relevant for subsequent calculations. By linearity of the convolution, Eq. (3) combines with Eqs. (4) and (5) to yield the net density:

$$\psi(x_i, t_{j+1}) = \exp[-CV(x_i)] [\psi(\cdot, t_j) * P_{\Delta X}^{(\sigma)}](x_i), \quad (6)$$

where the survival probability has been written out explicitly. Finally, to avoid the gradual collapse of ψ , we enforce at every time step a normalization operation similar to that of Eq. (2): $\hat{N}\{f_i\} = f_i / (\sum_i f_i^2 d)^{1/2}$, for an arbitrary square-integrable function, f . To summarize, the combined effect of diffusion, absorption, annihilation, and normalization (henceforth, DAAN) shapes the evolution of the net density over each time step according to

$$\psi(x_i, t_{j+1}) = \hat{N} \{ \exp[-CV(x_i)] [\psi(\cdot, t_j) * P_{\Delta X}^{(\sigma)}](x_i) \}. \quad (7)$$

Equation (7) encapsulates the DAAN procedure and provides a semianalytic iterative update rule for ψ , based on the specification of an initial density ψ_{ini} . To assess the validity of this iterative procedure, we compare it to the particle-based simulations of Sec. II A for a quadratic potential (Fig. 1), and for an infinite square potential (Fig. S1 of the Supplemental Material [34]). An equally satisfying match is achieved in both cases. As a first test, the initial density is chosen as purely Gaussian noise [Figs. 1(a)–1(c)]. After a sufficient number of iterations (see Sec. III B), Eq. (7) reaches a steady-state density, which we refer to as ψ_{DAAN} . The absorption coefficient, C , and the displacement standard deviation, σ , both have a

significant impact on the width of this steady-state density (e.g., too little absorption leads to wider distribution, and vice versa). So far, both of these parameters are unconstrained, but this is addressed in Sec. II C.

Some properties of Eq. (7) are readily apparent. First, due to the invariance of the normalization operation under multiplication by a positive scalar, the DAAN procedure is invariant under a constant shift of the potential function, $V \rightarrow V + \Delta V$. Second, for a purely random initial density, a symmetry breaking occurs whereby either walkers or antiwalkers will go extinct [e.g., Fig. 1(c)]. Third, if V and $P_{\Delta X}^{(\sigma)}$ are even functions, then DAAN should preserve the parity, if any, of the initial density—An initial density lying in the subspace of even (odd) functions should, theoretically, converge to an even (odd) steady-state density when propagated in time through Eq. (7). This is indeed what we observe in Figs. 1(d)–1(f), where the even component of ψ_{ini} has been removed. In this case, the net density converges to an odd steady state (for both DAAN and numerical simulations). Anecdotaly, the two (even and odd) steady-state densities are conspicuously similar to the ground-state and first excited-state wave functions within the corresponding potential function. In Sec. II C, we indeed establish a correspondence between the output of the DAAN procedure and the wave function associated with the potential function V . This correspondence relies on constraining the relationship between C and σ via the time step size, Δt . Furthermore, we show in Sec. III that DAAN can converge to several steady-state densities, as long as specific components from other orthogonal subspaces are removed, and that these correspond to higher-order excited-state wave functions.

C. Imaginary-time propagation

Here, we postulate an equivalence between the DAAN procedure and imaginary-time propagation of the Schrödinger equation, in the limit of small time steps. This leads to a constraint between C and σ that allows for a precise match between the steady-state DAAN density and the theoretical wave function associated with the potential function, V . ITP is achieved by performing a Wick rotation on the nonrelativistic time-dependent Schrödinger equation. Let $\tau = it$ denote imaginary time, then

$$-\hbar \frac{\partial}{\partial \tau} |\psi(\tau)\rangle = \hat{H} |\psi(\tau)\rangle \quad (8)$$

is the imaginary-time Schrödinger equation. For an initial wave function, $|\psi(0)\rangle$, the solution is

$$|\psi(\tau)\rangle = \exp\left(-\frac{\tau \hat{H}}{\hbar}\right) |\psi(0)\rangle. \quad (9)$$

Given an eigenstate $|\phi_n\rangle$ of $\hat{H}$, it is understood that $e^{\hat{H}} |\phi_n\rangle = e^{E_n} |\phi_n\rangle$, where E_n is the corresponding eigenvalue. Expanding the initial wave function in the energy eigenbasis, $|\psi(0)\rangle = \sum_n c_n |\phi_n\rangle$, it becomes apparent that ITP preserves the ground state ($n = 0$) as a dominant term, while more rapidly suppressing the excited states ($n \geq 1$):

$$|\psi(\tau)\rangle = \sum_n c_n \exp\left(-\frac{\tau E_n}{\hbar}\right) |\phi_n\rangle, \quad (10)$$

provided that $c_0 = \langle \psi(0) | \phi_0 \rangle \neq 0$. Given that this behavior is consistent with the results of Sec. III, and that the imaginary-time Schrödinger equation, when expressed in the position basis, is a generalized diffusion equation, the search for an explicit correspondence between DAAN and ITP is motivated.

For a small time step, $\Delta\tau$, the evolution from $|\psi(\tau)\rangle$ to $|\psi(\tau + \Delta\tau)\rangle$ can be approximated through Eq. (9):

$$|\psi(\tau + \Delta\tau)\rangle \approx \left(1 - \frac{\Delta\tau \hat{H}}{\hbar}\right) |\psi(\tau)\rangle. \quad (11)$$

In the position basis, let $\psi = \psi(x, \tau)$ be wave function and

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x). \quad (12)$$

Similarly, reinterpreting Eq. (7) in continuous space, and mapping t_j to τ , we write the small time step approximation for the DAAN procedure as

$$\psi(x, \tau + \Delta\tau) \approx [1 - CV(x)] [\psi(\cdot, \tau) * P_{\Delta X}^{(\sigma)}](x), \quad (13)$$

where the assumed proportionality between the time step and C justifies truncating the Taylor expansion of the exponential. Here, the normalization operation, $\hat{N}$ is omitted to keep the analysis coherent with the fact that ITP is not norm preserving. In practice, *ad hoc* normalization is imposed on ITP-based calculations, as is the case for the full DAAN procedure. At this stage, however, this normalization step is not required.

In order to establish an explicit correspondence between DAAN and ITP, we equate Eqs. (11) and (13) (omitting the arguments x and τ for notational clarity):

$$\begin{aligned} [(1 - CV)P_{\Delta X}^{(\sigma)}] * \psi &= \left(1 + \frac{\hbar \Delta\tau}{2m} \frac{d^2}{dx^2} - \frac{\Delta\tau}{\hbar} V\right) \psi \\ &= \left[\frac{\hbar \Delta\tau}{2m} \delta'' + \left(1 - \frac{\Delta\tau}{\hbar} V\right) \delta\right] * \psi, \end{aligned} \quad (14)$$

where $\delta = \delta(x)$ is the Dirac delta and δ'' its second derivative, with the property that $\frac{d^2 \psi}{dx^2} = \delta'' * \psi$. Equation (14) should hold for the two limiting cases of no absorption ($V = 0$) and of no diffusion ($\hat{T} = 0$). From the former case, we get

$$P_{\Delta X}^{(\sigma)} * \psi = \left(\delta + \frac{\hbar \Delta\tau}{2m} \delta''\right) * \psi. \quad (15)$$

Hence, in the other limiting case—without the kinetic term—this displacement distribution assumes the expected form $P_{\Delta X}^{(\sigma)}(x) = \delta(x)$, and Eq. (14) becomes

$$(1 - CV)\psi = \left(1 - \frac{\Delta\tau}{\hbar} V\right) \psi, \quad (16)$$

leading to the conclusion $C = \frac{\Delta\tau}{\hbar}$. We validate *a posteriori* that this value of C holds also for the general case.

An equally simple expression can be obtained for σ^2 , the variance of the displacement distribution. Assuming a Gaussian representation of $\delta(x)$, we have

$$\delta''(x) = \lim_{s \rightarrow 0} \delta_s(x) \left(\frac{x^2 - s^2}{s^4}\right), \quad (17)$$

where $\delta_s(x) = \frac{1}{s\sqrt{2\pi}} e^{-\frac{x^2}{2s^2}}$ is a zero-mean Gaussian distribution of standard deviation s , serving as a delta sequence in the limit $s \rightarrow 0$. From Eq. (15), it thus follows that

$$\begin{aligned}\sigma^2 &= \int_{\mathbb{R}} P_{\Delta X}^{(\sigma)}(x) x^2 dx \\ &= \lim_{s \rightarrow 0} \int_{\mathbb{R}} \delta_s(x) \left[1 + \frac{\hbar \Delta \tau}{2m} \left(\frac{x^2 - s^2}{s^4} \right) \right] x^2 dx \\ &= \lim_{s \rightarrow 0} \left[\left(1 - \frac{\hbar \Delta \tau}{2ms^2} \right) \int_{\mathbb{R}} x^2 \delta_s(x) dx + \frac{\hbar \Delta \tau}{2ms^4} \int_{\mathbb{R}} x^4 \delta_s(x) dx \right],\end{aligned}$$

where we recognize the second and fourth moments of the Gaussian distribution, s^2 and $3s^4$, respectively, yielding $\sigma^2 = \frac{\hbar \Delta \tau}{m}$. In Sec. III, we show that by adopting the values of C and σ^2 obtained here, the DAAN procedure indeed converges to the exact eigenstates of the Hamiltonian with potential function V . First, however, we introduce an orthogonalization scheme that enables DAAN to extract excited eigenstates.

III. RESULTS

A. Orthogonalization

As seen from Eq. (10), an arbitrary initial wave function, ψ_{ini} , will eventually converge to the ground state, ϕ_0 , under the influence of ITP, provided that $c_0 = \langle \psi_{\text{ini}} | \phi_0 \rangle \neq 0$. If, however, ψ_{ini} is chosen orthogonal to ϕ_0 , then it is the first excited state that dominates the ITP, and so forth. Assuming a correspondence between DAAN and ITP, we expect to find a similar behavior for an initial density propagated through DAAN, that is, a convergence to ϕ_n when $c_k = 0$, $\forall k \in \{0, 1, \dots, n-1\}$.

What we observe, instead, is that the excited states are metastable. After some time of apparent stability, excited states collapse to the ground state. This is exemplified in Fig. 2(a), where DAAN is applied in a two-dimensional (2D) asymmetric quadratic potential, and where ψ_{ini} is constructed such that it is orthogonal to the first (red) or to the first eight eigenstates (yellow), but is otherwise random. The targeted excited state is indeed approached and maintained transiently (as seen by a brief narrowing of the uncertainty), but eventually decays toward the ground-state energy. This decay is associated with a nonmonotonic energy uncertainty as a function of time. We next investigate whether this behavior is affected by the temporal discretization. As shown in Fig. 2(b), doubling or quadrupling the value of Δt does not qualitatively affect the observed metastability, as taking longer time steps results in a proportionally shortened period of metastability. In other words, if Fig. 2(b) were expressed in seconds rather than time steps, all three curves would be confounded. From this test, we conclude that approximation errors accumulate and contaminate $\psi(x, t)$ with orthogonal components along the eigenstates of energy lower than the one being targeted. Additional orthogonalization is thus required to maintain the density free of components from that subspace (i.e., in addition to the one applied to ψ_{ini}). We find that performing an orthogonalization once every $T = 200$ time steps is sufficient to counter the accumulation of error. In fact, we show in Fig. S2 of the Supplemental Material [34] that DAAN is robust to

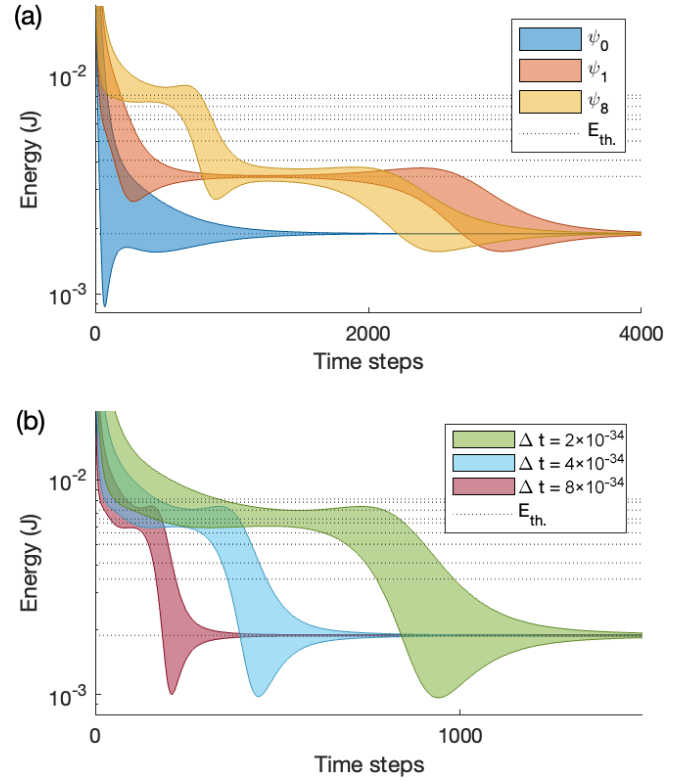


FIG. 2. Application of DAAN in the 2D quadratic potential well $V(x, y) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2)$, $\omega_x = 1.4817 \times 10^{31} \text{ rad s}^{-1}$, and $\omega_y = 2.0955 \times 10^{31} \text{ rad s}^{-1}$. Shaded areas show the energy spread $\langle E \rangle(t) \pm \Delta E(t)$ as the density evolves through DAAN, and dashed lines show the theoretical energy eigenvalues. (a) A random initial density converges to the correct ground-state energy, with a monotonically decreasing uncertainty (blue). If, however, the initial density is constructed orthogonal to the span of lower eigenstates (red and yellow), DAAN converges only transiently to the targeted eigenstate, with an eventual collapse to the ground-state energy. (b) Doubling or quadrupling the time step Δt does not qualitatively affect the metastability of excited states, as shown here for the transient stability of ψ_5 , with three different values of Δt . This test shows that additional orthogonalization is required in order for DAAN to converge to excited states.

changes in T up to $T \approx 2000$. Beyond that value, the energy uncertainty of the final iteration starts to grow as T increases.

More precisely, let ϕ_k be the target state, and $\psi(x, t)$ be an arbitrary density, either at the beginning or during the application of DAAN. Let $\{\phi_0, \dots, \phi_{k-1}\}$ be the set of components that we wish to remove from it—In practice, these are steady-state densities obtained from previous application of DAAN where lower-energy states were targeted. We implement the orthogonalization (akin to a Gram-Schmidt process) as

$$\psi_k(x, t) = \hat{N} \left[\psi(x, t) - \sum_{n=0}^{k-1} \phi_n(x) \langle \psi(x, t) | \phi_n(x) \rangle \right], \quad (18)$$

where ψ_k is then propagated through Eq. (7) until the next application of Eq. (18). Equation (18) is first applied at $t = 0$, and then at every T time steps after that. We find, as expected, that supplementing DAAN with such periodic (but sparse) orthogonalization leads to the targeted eigenstate, ϕ_k .

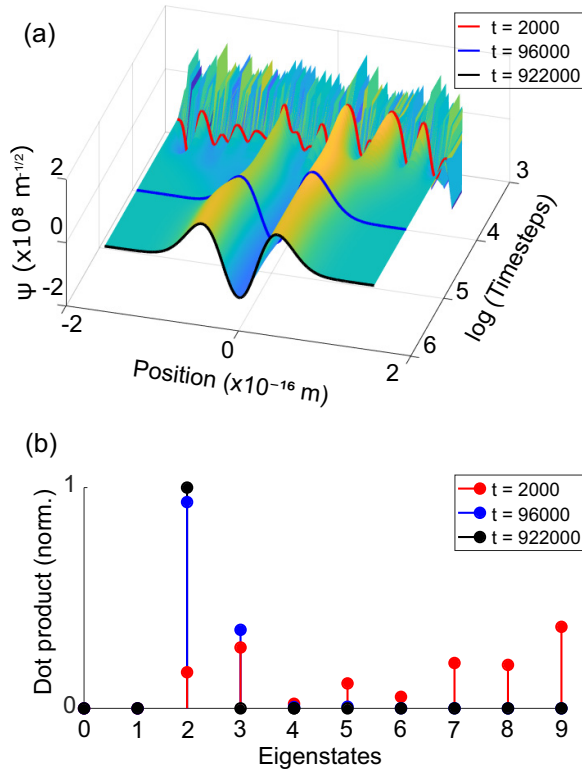


FIG. 3. Application of DAAN in a 1D quadratic potential, $V(x) = \frac{m\omega^2}{2}x^2$ with $\omega = 1.5 \times 10^{29} \text{ rad s}^{-1}$. Here, ϕ_2 is the target state, and Eq. (18) is applied at every $T = 200$ time steps (including at time $t = 0$) such as to remove from ψ the components along ϕ_0 and ϕ_1 . Aside from being orthogonal to the first two eigenstates, the initial density is random. In panel (a), three curves, representative of the early (red), middle (blue), and steady-state density (black), are shown over the full spatiotemporal density, $\psi(x, t)$. The corresponding energy decomposition is depicted in panel (b), and shows that DAAN indeed converges to a state lying solely along ϕ_2 .

As a first test, we show in Fig. 3 that this is indeed the case when DAAN is applied to a 1D quadratic well. Here, ϕ_2 is the target state, and components along ϕ_0 and ϕ_1 are removed as described above. Initially, the density is irregular [red curve, Fig. 3(a)], and is populated by components from all over the energy spectrum [red stems, Fig. 3(b)], except along E_0 and E_1 , by construction. With a periodic application of Eq. (18), DAAN converges toward the correct excited steady state [black curve, Fig. 3(a)], whose energy is exclusively E_2 [black stems, Fig. 3(b)].

Next, we revisit the 2D quadratic potential well and show in Fig. 4(a) that, contrary to Fig. 2 where no orthogonalization was applied, DAAN can successfully extract the targeted eigenstate when Eq. (18) is periodically enforced. Indeed, DAAN converges to densities whose energy corresponds to the theoretical value, with a monotonically decreasing energy uncertainty, ΔE . In Sec. III B, we offer a more systematic comparison to theory. Finally, as an additional validation test [Fig. 4(b)], we confirm that scaling down the time step, Δt , leads to a proportionally smaller relative energy uncertainty of the DAAN density. This scaling holds over at least 2 orders of magnitude.

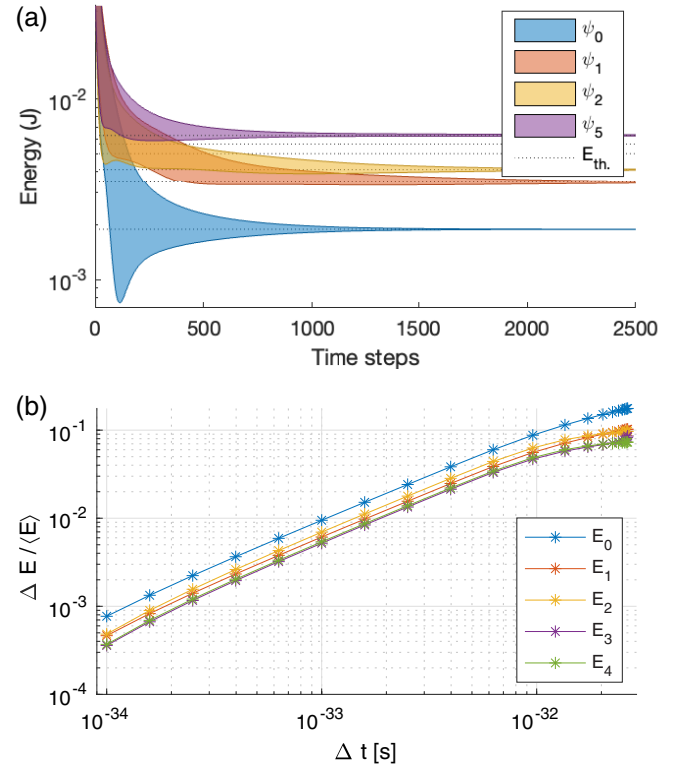


FIG. 4. (a) Dynamics of the energy spread, $\langle E \rangle(t) \pm \Delta E(t)$ (shaded areas), calculated from time-dependent DAAN densities, $\psi(x, t)$, for the same quadratic potential as in Fig. 2. Here, however, periodic orthogonalization is applied, as per Eq. (18), at every $T = 200$ time steps. In this case, the energy spread converges monotonically to the correct theoretical energy (dashed lines). (b) The relative energy uncertainty, calculated at the last DAAN iteration, scales with the size of the time step, Δt , over at least 2 orders of magnitude. Smaller time steps are associated with increasing precision, as expected.

B. Comparison with theoretical eigenstates

The results of the preceding section suggest that by using values of C and σ obtained in Sec. II C and by applying periodic orthogonalization as described in Sec. III A, DAAN does indeed converge to steady-state densities, ψ_{DAAN} , that correspond to the theoretical eigenstates for a given potential function. Here, we evaluate this correspondence quantitatively by comparing steady-state DAAN densities with theoretical eigenfunctions for different potential functions (1D and 2D), and for different energy levels. Quantitative comparison is achieved by first calculating the energy expectation value, $\langle E \rangle$, and uncertainty, ΔE , from the DAAN density, ψ_{DAAN} :

$$\langle E \rangle = \int_{\mathbb{R}} \psi_{\text{DAAN}}(x) (\hat{H} \psi_{\text{DAAN}})(x) dx, \quad (19a)$$

$$\Delta E = \sqrt{\int_{\mathbb{R}} [(\hat{H} \psi_{\text{DAAN}})(x)]^2 dx - \langle E \rangle^2}, \quad (19b)$$

where the integrals are evaluated numerically, and where $(\hat{H} \psi_{\text{DAAN}})(x)$ is evaluated from Eq. (12), with the second derivative approximated by central difference. Then, three metrics are calculated to assess the precision of the DAAN

TABLE I. Quantitative assessment of DAAN performance in four different potential functions, and for various energy levels. All metrics are calculated from steady-state DAAN densities. The relative uncertainty (Rel. unc.), $\Delta E / \langle E \rangle$, quantifies how close ΔE is from vanishing. The relative energy error (Rel. err.), $|\langle E \rangle - E_{\text{th}}|/E_{\text{th}}$, and the error norm (Err. norm), $\|\psi_{\text{DAAN}} - \phi_{\text{th}}\|$, serve to compare the steady-state DAAN densities to the corresponding theoretical eigenvalue and eigenfunctions [35], respectively. Convergence time (Conv. time) is reported in number of time steps.

State	Rel. unc.	Rel. err.	Err. norm	Conv. time
1DSP				
0	4.30×10^{-2}	2.30×10^{-3}	1.59×10^{-6}	9.60×10^5
1	2.15×10^{-2}	2.30×10^{-3}	4.98×10^{-6}	1.30×10^6
2	1.43×10^{-2}	2.29×10^{-3}	1.02×10^{-5}	8.60×10^5
3	1.08×10^{-2}	2.30×10^{-3}	1.77×10^{-5}	5.60×10^5
4	8.63×10^{-3}	2.31×10^{-3}	2.72×10^{-5}	3.60×10^5
5	7.22×10^{-3}	2.31×10^{-3}	3.90×10^{-5}	5.00×10^5
1DHO				
0	1.65×10^{-5}	2.53×10^{-6}	2.97×10^{-11}	1.02×10^6
1	7.62×10^{-6}	4.21×10^{-6}	9.00×10^{-11}	8.60×10^5
2	5.97×10^{-6}	5.06×10^{-6}	2.14×10^{-10}	1.02×10^6
3	4.83×10^{-6}	7.22×10^{-6}	4.66×10^{-10}	9.80×10^5
4	4.74×10^{-6}	9.83×10^{-6}	1.74×10^{-9}	9.60×10^5
5	8.00×10^{-6}	1.03×10^{-5}	1.38×10^{-8}	7.40×10^5
2DSP				
0 0	3.90×10^{-2}	2.71×10^{-2}	3.77×10^{-4}	3.21×10^5
1 0	3.17×10^{-2}	2.58×10^{-2}	7.30×10^{-4}	5.31×10^5
0 1	3.35×10^{-2}	2.89×10^{-2}	8.89×10^{-4}	3.13×10^5
1 1	3.46×10^{-2}	2.78×10^{-2}	1.24×10^{-3}	9.95×10^5
2 0	3.36×10^{-2}	2.57×10^{-2}	1.32×10^{-3}	2.67×10^5
0 2	3.94×10^{-2}	3.00×10^{-2}	1.74×10^{-3}	8.54×10^5
2 1	3.84×10^{-2}	2.73×10^{-2}	1.83×10^{-3}	4.38×10^5
1 2	4.18×10^{-2}	2.94×10^{-2}	2.10×10^{-3}	1.46×10^6
3 0	3.96×10^{-2}	2.61×10^{-2}	2.15×10^{-3}	1.78×10^5
3 1	4.42×10^{-2}	2.73×10^{-2}	2.66×10^{-3}	3.00×10^6
2DHO				
0 0	7.03×10^{-4}	9.38×10^{-5}	1.62×10^{-7}	7.74×10^4
1 0	4.02×10^{-4}	1.20×10^{-4}	2.19×10^{-7}	1.55×10^5
0 1	3.79×10^{-4}	1.59×10^{-4}	2.76×10^{-7}	8.91×10^4
2 0	3.09×10^{-4}	1.77×10^{-4}	3.01×10^{-7}	1.87×10^5
1 1	2.84×10^{-4}	1.57×10^{-4}	3.33×10^{-7}	1.83×10^5
0 2	3.29×10^{-4}	2.53×10^{-4}	4.64×10^{-7}	3.00×10^5
3 0	2.83×10^{-4}	2.43×10^{-4}	5.12×10^{-7}	1.54×10^5
2 1	2.42×10^{-4}	1.88×10^{-4}	4.16×10^{-7}	1.80×10^5
1 2	2.68×10^{-4}	2.33×10^{-4}	6.58×10^{-7}	3.00×10^5
4 0	3.21×10^{-4}	3.12×10^{-4}	3.55×10^{-7}	2.24×10^5

density relative to theory: the relative energy uncertainty, $\Delta E / \langle E \rangle$, the relative energy error, $|\langle E \rangle - E_{\text{th}}|/E_{\text{th}}$, where E_{th} are the theoretical eigenvalues, and the error norm, $\sqrt{\int_{\mathbb{R}} [\psi_{\text{DAAN}} - \phi_{\text{th}}]^2 dx}$, where ϕ_{th} are the theoretical eigenfunctions. The theoretical eigenvalues and eigenfunctions relevant for these calculations can be found in Ref. [35].

These metrics are reported in Table I for a total of 32 eigenstates, across four different cases: 1D and 2D infinite square potentials (1DSP, 2DSP), and 1D and 2D harmonic oscillators (1DHO, 2DHO). For all cases, an initial random density evolves according to Eq. (7), first without orthogo-

nalization. The resulting density is stored as ϕ_0 . Then, a new random initial density is generated, but its component along ϕ_0 is removed by means of Eq. (18). Evolution through DAAN with periodic orthogonalization leads to a new density that we store as ϕ_1 . The process is repeated for all other excited states, which are maintained orthogonal to all previously obtained steady-state densities. Simulations are stopped when the relative difference of the energy expectation value over a period of 300 time steps is less than $1.5 \times 10^{-5}\%$, for 1D potentials, or $1 \times 10^{-11}\%$, for 2D potentials. Convergence time (in number of time steps) is also reported in Table I. In all cases, $m = m_e$ is the electron mass, $d = 2 \times 10^{-20}$ m, and $\Delta t = 1.05 \times 10^{-34}$ s, which gives $C = 1$ J and $\sigma = 7.81 \times 10^{-20}$ m.

Further validation of the DAAN procedure is shown in Figs. 5(a)–5(f), where ψ_{DAAN} (red curve) is plotted directly against the corresponding ϕ_{th} (dashed blue curve) for six of the 1D cases reported in Table I. Additional cases are shown in Figs. 5(g)–5(l) for 2D potentials, but without explicit comparison to the theoretical eigenfunctions. The 2D potential wells are chosen asymmetric such as to avoid any degeneracy, as discussed in Sec. IV.

IV. DISCUSSION

In this work, we show how DAAN—a two-species random walk model that includes diffusion, probabilistic absorption via a potential function, cross-species annihilation, and normalization of the population density—can be implemented semianalytically (i.e., by propagating the population density instead of simulating individual walkers) to yield the correct Hamiltonian eigenstates associated with the potential function. As a first test, in Fig. 1, we validate our approach for propagating the population density [Eq. (7)] against explicit random walk simulations of the model presented in Sec. II A. For population size on the order of 10^5 particles, a precise match between theory and simulation is reached within a few hundred time steps. An important aspect of this work is to show that key parameters of the DAAN procedure, namely, the absorption coefficient, C , and the diffusion displacement variance, σ^2 , are uniquely constrained by establishing an explicit correspondence between DAAN and imaginary-time propagation of the Schrödinger equation for small time steps (Sec. II C). Only for those particular values of $C = \frac{\Delta t}{\hbar}$ and $\sigma^2 = \frac{\hbar \Delta t}{m}$ does DAAN converge precisely to the theoretical eigenstates. Of course, we require Δt to be small, such as to justify the approximations employed in Sec. II C, and such that σ is maintained 2 or 3 orders of magnitude smaller than the spatial spread of the wave function.

A quantitative comparison between steady-state densities reached by DAAN propagation and the corresponding theoretical eigenfunctions is offered in Table I for cases in 1D and 2D, for square and harmonic potential wells, and for several energy levels. In some cases, in particular for the 1DHO and 2DHO, the error norm ranges from $\sim 10^{-7}$ to $\sim 10^{-11}$. Correspondingly, the relative uncertainty and relative energy error are $\sim 10^{-4}$ to $\sim 10^{-6}$. Notably, the energy uncertainty is merely 2 orders of magnitude larger than that calculated from theory, indicating numerical integration error as a significant factor in calculating ΔE [controlled by d ,

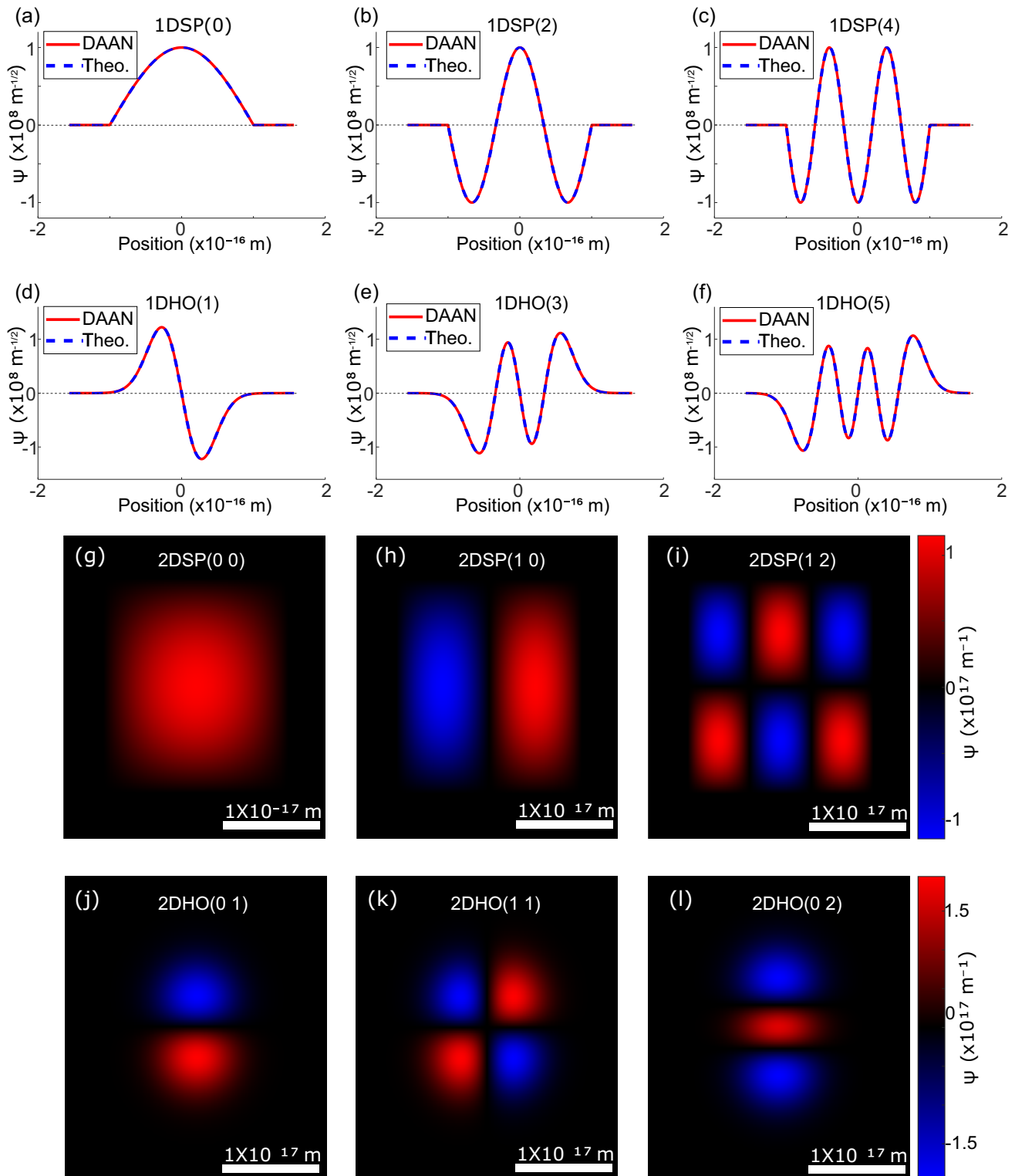


FIG. 5. Representative steady-states DAAN densities for different cases of Table I. (a)–(c) 1D infinite square potential of width $L = 2 \times 10^{-16}$ m. (d)–(f) 1D harmonic oscillator where $V(x) = \frac{m\omega^2}{2}x^2$ and $\omega = 1.5 \times 10^{29}$ rad s $^{-1}$. For the 1D cases, ψ_{DAAN} (red curve) is compared with the corresponding theoretical eigenfunction, ϕ_{th} (dashed blue curves). (g)–(i) 2D infinite square potential of width $L_x = 1.89 \times 10^{-17}$ m and $L_y = 1.57 \times 10^{-17}$ m. (j)–(l) 2D harmonic oscillator where $V(x, y) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2)$, $\omega_x = 1.568 \times 10^{31}$ rad s $^{-1}$, and $\omega_y = 2.217 \times 10^{31}$ rad s $^{-1}$. For the 2D cases, the displacement probability distribution is an isotropic bivariate Gaussian. Quantum numbers are shown in parentheses, e.g., 2DHO(0 1) represents the 2D harmonic oscillator with $n_x = 0$ and $n_y = 1$.

in Eq. (19)]. Moreover, additional tests (not shown) confirm that DAAN converges to steady states whose energy uncertainty extrapolates to zero in the limit of vanishing Δt —all of which indicate that DAAN succeeds in extracting the correct excited states, as seen visually in Fig. 5. For the case of the square potential well (1DSP and 2DSP), however, the comparison metrics are 2–6 orders of magnitude larger than for the harmonic well, likely due to errors associated with the discontinuity of the potential function. We posit that more iterations and a better spatial resolution near the barrier would correct this imprecision, and that by implementing a stricter convergence criterion, a similar precision to the harmonic well could be reached. Indeed, we see from Fig. 4 that the approach to the steady state can vary even for states within the same potential function, at least in terms of the dynamics of the energy spread (Fig. 4).

To enforce convergence toward a targeted excited state—rather than merely the ground state—we implement a sparse and periodic orthogonalization step where components of the DAAN density lying along lower-energy eigenstates are removed. This adjustment is sufficient to ensure that DAAN propagates the density within the subspace orthogonal to the span of the lower-energy states, while still converging toward the target state. Of course, in higher dimensions, eigenvalues tend to be degenerate. In those cases, neither DAAN nor ITP can discriminate between same-energy states lying in a common subspace. Instead, a linear combination of states within that subspace could be reached, and would still manifest itself as a density with vanishing ΔE under DAAN propagation. For the 2D cases of Sec. III B, we deliberately circumvent this issue by choosing an anisotropic potential function, such as to facilitate the comparison to theory. Nevertheless, as seen from Fig. 3, an energy spectrum initially spread over many excited states eventually preserves only that component along the target excited state. Without this orthogonalization step, excited states are unstable under DAAN propagation, and exhibit a transient stabilization (i.e., reduction in energy uncertainty) before decaying to the ground state (Fig. 2). We have not systematically tested whether orthogonalization could be made sparser. Future investigation could quantify the rate of decay toward the ground state as a function of the potential function, the energy level, and the value of Δt . The orthogonalization schedule could then be tailored based on these findings, such as to make it as sparse as possible for optimal convergence time. We also leave for future work the question of the shape of the displacement probability distribution, $P_{\Delta X}^{(\sigma)}$. Random walk models are known to exhibit many sloppy directions in their parameter spaces, while only a few are stiff [4]—Only variations of parameters along the stiff directions cause significant changes to the model’s output at the macroscopic level. It is therefore likely that many functional forms of $P_{\Delta X}^{(\sigma)}$ map onto the same macroscopic, steady-state density. The extent to which this is the case remains to be elucidated.

Overall, this work contributes toward clarifying the microscopic, probabilistic interpretation of ITP and, more generally,

adds to a body of knowledge where emergent features of collective stochastic dynamics serve as a basis for understanding the solutions of macroscopic partial differential equations.

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P.H.G., N.B., and A.M. conceptualized the research. P.H.G. wrote the code, developed the theory, performed the analyses, and drafted the manuscript. A.M. wrote, revised, and proof-read the manuscript. A.M. and P.H.G. interpreted the results.

DATA AVAILABILITY

The codes and simulation data that support the findings of this article are not publicly available. They are, however, available from the authors upon reasonable request.

APPENDIX: GENERALIZATION TO HIGHER DIMENSIONS

Implementation of DAAN in dimension higher than one is direct and requires only few adjustments. The population density, potential function, and displacement probability distribution become functions of the D -dimensional vector $\mathbf{x}$: $\psi(\mathbf{x}, t)$, $V(\mathbf{x})$, and $P_{\Delta X}^{(\sigma)}(\mathbf{x})$. The latter takes the form of a multivariate, isotropic, and zero-mean Gaussian distribution and is evaluated on the D -dimensional regular lattice of step d along each dimension. The main equation for DAAN propagation [Eq. (7)] is essentially unchanged, with the 1D convolution generalizing directly to D dimensions, while the Hamiltonian reads

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}). \quad (\text{A1})$$

On the other hand, Eq. (14) generalizes to

$$[(1 - CV)P_{\Delta X}^{(\sigma)}] * \psi = \left[\frac{\hbar\Delta\tau}{2m} \sum_{j=1}^D \delta_j'' + \left(1 - \frac{\Delta\tau}{\hbar}V\right)\delta \right] * \psi, \quad (\text{A2})$$

where $(\delta_j'' * \psi)(\mathbf{x}) = \frac{\partial^2 \psi(\mathbf{x})}{\partial x_j^2}$. In this case, one still finds $C = \frac{\Delta t}{\hbar}$ and $\sigma^2 = \frac{\hbar\Delta\tau}{m}$ (the variance of each marginal of the multivariate $P_{\Delta X}^{(\sigma)}$). Finally, generalization of Eq. (19) is trivial and is implemented numerically with standard numerical analysis techniques (i.e., central differences and trapezoidal rule).

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