

Statistical theory of electronic degrees of freedom in wave packet molecular dynamics

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We derive statistical distributions for the degrees of freedom in wave packet molecular dynamics models. Specifically, a theory is developed for the width distributions of Gaussian wave packets in both isotropic and anisotropic formulations. The resulting distribution functions show good agreement with molecular dynamics data under warm dense matter conditions, providing practical guidance for constraining the confining potential, an empirical parameter in the model. We also discuss how these distributions influence the resulting effective Coulomb interactions.

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I. INTRODUCTION

The modeling of many-body quantum systems from first principles presents a formidable challenge. A particularly demanding regime is so-called warm dense matter [1], which has attracted significant interest because it occurs in planetary interiors, brown dwarfs, and white dwarf envelopes [2–4], as well as during the compression phase of inertial confinement fusion capsules [5]. While exact wave function propagation is computationally unfeasible for many-particle systems, finite-temperature quantum-statistical approaches such as path integral Monte Carlo (PIMC) can provide a range of static equilibrium properties [6–8]. Alternatively, density functional theory (DFT)-based methods can be employed, which provide access to many static and dynamic properties [1,5,7–10]. Additionally, simple pair potentials may be used in the semiclassical regime [11–13].

Wave packet molecular dynamics (WPMD) is an alternative approach based on restricting the electronic wave function to yield a computationally feasible method [14–18]. This scheme enables simulations involving many thousands of particles, significantly reducing finite-size effects compared to PIMC- and DFT-based methods. Such an approach could also be complementary to the more established methods for a variety of additional reasons. In equilibrium, WPMD captures the joint evolution of electrons and ions over long timescales, enabling direct study of interspecies coupling beyond the Born-Oppenheimer approximation. In addition to dynamic electron properties [19,20], this allows electron-ion collisional

transport to be directly modeled [21]. Furthermore, WPMD has been employed in an ongoing debate regarding the effect of electronic fluctuations on both diffusive and acoustic ion modes in dense plasma [22–24]. The method has also been extended to include bound-state wave functions [25,26], which allowed the latter reference to extract the self-consistent ionization states using the scheme in Ref. [27]. In the nonequilibrium context, the method was used to study the relaxation of a two-temperature electron-proton plasma and yielded slow relaxation rates when compared with semiclassical models [28].

However, care must be taken to ensure that the restricted functional form of the electronic wave function does not lead to unphysical behavior. A primary example is the confining potential, which controls the electron extent and hence regulates many properties of the model [20,26,29]. The purpose of this work is to highlight how the statistical distribution of the additional electron degrees of freedom in WPMD may be predicted from the Hamiltonian structure of the underlying equations. This provides a practical means to assess the effect of the confining potential. Here we focus on the statistical properties of WPMD using a Gaussian ansatz, which has been widely applied to the study of warm dense matter and partially ionized plasmas.

II. GAUSSIAN WAVE PACKET MODELS

We employ an anisotropic Gaussian wave packet ansatz developed in Ref. [30] and subsequently used in Refs. [19,26]. The key results are briefly recalled for the purposes of this work. We start with N classical protons and N quantum electrons and employ the mixed quantum-classical approach of Ehrenfest dynamics [31]. For the protons, the resulting evolution is dictated by the Ehrenfest Hamiltonian

$$\mathcal{H} = \sum_I \frac{\mathbf{P}_I^2}{2M_I} + \frac{e^2}{4\pi\epsilon_0} \sum_{I<J} \frac{1}{|\mathbf{R}_I - \mathbf{R}_J|} + \mathcal{H}^{\text{eff}}. \quad (1)$$

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Here M_I , $\mathbf{R}_I$, and $\mathbf{P}_I$ denote the mass, position, and momentum of the I th ion, respectively; additionally e is the electron charge and ϵ_0 is the permittivity of free space. The corresponding Hamiltonian equations of motion are

$$\frac{d\mathbf{R}_I}{dt} = \frac{\mathbf{P}_I}{M_I}, \quad \frac{d\mathbf{P}_I}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{R}_I}. \quad (2)$$

The effective Hamiltonian representing the quantum subsystem is the expectation value of the electron Hamiltonian with respect to the many-body wave function $|\Psi\rangle$,

$$\mathcal{H}^{\text{eff}} = \langle \Psi | \hat{H}_e(\{\mathbf{R}_I\}) | \Psi \rangle, \quad (3)$$

where $\hat{H}_e$ is the electronic Hamiltonian operator. This operator depends parametrically on the ionic coordinates $\{\mathbf{R}_I\}$ and includes the electron kinetic energy together with all electron interaction terms. In Ehrenfest dynamics, $|\Psi\rangle$ is allowed to evolve in the full electronic Hilbert space. Meanwhile, the ions evolve under forces obtained from the gradient of the expectation value of the electronic Hamiltonian with respect to the ionic coordinates. This corresponds to a mean-field treatment, in which the nuclei experience the averaged influence of the electronic state rather than evolving on a single potential energy surface. In WPMD, $|\Psi\rangle$ is parametrized by a finite set of continuous parameters $\{q_\mu\}$ which define a manifold in the full Hilbert space. To distinguish this case we perform the replacement

$$|\Psi\rangle \rightarrow |Q(\{q_\mu\})\rangle, \quad \mathcal{H}^{\text{eff}} \rightarrow \mathcal{H}^{\text{WP}} = \langle Q | \hat{H}_e(\{\mathbf{R}_I\}) | Q \rangle, \quad (4)$$

where $|Q\rangle$ is the parametrized wave function with the explicit parameter dependence suppressed and $\mathcal{H}^{\text{WP}}$ is the corresponding wave packet Hamiltonian. The two restricted Gaussian wave functions studied in this work will now be specified.

Anisotropic form. A Hartree product of single-particle Gaussian orbitals is chosen, each with the functional form

$$\langle \mathbf{x} | q_i \rangle = \mathcal{N} \exp \left(-(\mathbf{x} - \mathbf{r}_i)^T \mathbf{M}_i (\mathbf{x} - \mathbf{r}_i) + \frac{i}{\hbar} \mathbf{p}_i^T (\mathbf{x} - \mathbf{r}_i) \right), \quad (5)$$

where $\mathbf{r}_i$ and $\mathbf{p}_i$ correspond to the expected position and momenta, respectively. Additionally, $\mathcal{N}$ is a normalization factor [30] and $\hbar$ is the reduced Planck constant. The symmetric complex 3×3 shape matrix

$$\mathbf{M}_i = \frac{1}{4} \Sigma_i^{-1} - \frac{i}{\hbar} \Pi_i \quad (6)$$

is commonly decomposed into a real covariance part Σ_i , which is positive definite with units of length squared, and a conjugate shape-momentum variable Π_i . Explicitly, the electronic subsystem now depends on the real parameters $\{\mathbf{r}_i, \mathbf{p}_i, \Sigma_i, \Pi_i\}_{i=1}^N$, where i labels an electron in the system. The equations of motion are of Hamiltonian form

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial \mathcal{H}^{\text{WP}}}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial \mathcal{H}^{\text{WP}}}{\partial \mathbf{r}_i} \quad (7)$$

for the vector degrees of freedom, while the matrix degrees of freedom have the symmetrized Hamiltonian

structure

$$\begin{aligned} \frac{d}{dt} \Sigma_{i\beta\alpha} &= \frac{1}{2} \left(\frac{\partial \mathcal{H}^{\text{WP}}}{\partial \Pi_{i\alpha\beta}} + \frac{\partial \mathcal{H}^{\text{WP}}}{\partial \Pi_{i\beta\alpha}} \right), \\ \frac{d}{dt} \Pi_{i\alpha\beta} &= -\frac{1}{2} \left(\frac{\partial \mathcal{H}^{\text{WP}}}{\partial \Sigma_{i\alpha\beta}} + \frac{\partial \mathcal{H}^{\text{WP}}}{\partial \Sigma_{i\beta\alpha}} \right), \end{aligned} \quad (8)$$

where $\Sigma_{i\alpha\beta} = [\Sigma_i]_{\alpha\beta}$ is the α, β component of the symmetric width matrix and similarly $\Pi_{i\alpha\beta} = [\Pi_i]_{\alpha\beta}$ is a component of the conjugate width-momentum matrix, both corresponding to the i th electron.

Isotropic form. The isotropic case is also studied. Constraining the matrices to

$$\Sigma_i = s_i \mathbf{I}, \quad \Pi_i = \pi_{s,i} \mathbf{I}, \quad (9)$$

where $\mathbf{I}$ is the identity matrix and s_i and $\pi_{s,i}$ are real scalars, gives the isotropic state

$$\langle \mathbf{x} | g_i \rangle = \mathcal{N} \exp \left(-m_i (\mathbf{x} - \mathbf{r}_i)^2 + \frac{i}{\hbar} \mathbf{p}_i^T (\mathbf{x} - \mathbf{r}_i) \right), \quad (10)$$

with the complex width variable

$$m_i = \frac{1}{4s_i} - \frac{i}{\hbar} \pi_{s,i}. \quad (11)$$

While the equations of motion for the expected position $\mathbf{r}_i$ and expected momentum $\mathbf{p}_i$ remain with the same form given in Eq. (7), the evolution equations for the internal degrees of freedom reduce to

$$\frac{ds_i}{dt} = \frac{1}{3} \frac{\partial \mathcal{H}^{\text{WP}}}{\partial \pi_{s,i}}, \quad \frac{d\pi_{s,i}}{dt} = -\frac{1}{3} \frac{\partial \mathcal{H}^{\text{WP}}}{\partial s_i}. \quad (12)$$

The factor of 3 is a direct result of transitioning from a 3×3 matrix to a single variable in Eq. (9). This form is closely related to the isotropic Gaussian first used to model dense plasmas [16] and subsequently studied by many authors.

Additional potentials

In WPMD models for dense plasma, additional effective potentials are typically included (see, e.g., Refs. [16,30,32]). First, so-called Pauli potentials are additional two-body potentials motivated by a pairwise truncation of the antisymmetrization operator [15,16], partially addressing the limitation of the Hartree product in the restricted wave function. We employ Pauli potentials in this work, although directly antisymmetrized wave functions have previously been considered [17]. Alternative schemes inspired by exchange-correlation energy approximations from DFT have also been investigated [18,33]. Second, a confining potential is used to enforce localized Gaussian wave packets, which is standard in high-temperature applications of WPMD. This is what we focus on in the present work. An additional potential energy operator is added to the electronic Hamiltonian [19,26],

$$\hat{V} = \frac{A}{2} \sum_i \hat{W}_i = \frac{A}{2} \sum_i (\hat{\mathbf{x}}_i - \langle \hat{\mathbf{x}}_i \rangle)^2, \quad (13)$$

where $\hat{\mathbf{x}}_i$ denotes the position operator of the i th electron and $\langle \hat{\mathbf{x}}_i \rangle$ denotes its expectation value. We have also defined the width-squared operator $\hat{W}_i$, which will be used to characterize

the extent of the electron wave function. As will be demonstrated, adjusting A modulates the distribution of the width variables (Σ_i or s_i) in the model. This changes the effective Coulomb interactions and resulting structural properties [26]. An alternative scheme based on a global confining potential to impose reflecting wall boundary conditions has also been studied in Refs. [18,34]. We outline how the statistical framework can be extended to such potentials in Appendix A.

III. STATISTICAL THEORY FOR THE WIDTH DISTRIBUTION

In this section we develop a statistical theory for the internal degrees of freedom based on the noninteracting limit. Specifically, we assume single-particle contributions to the total energy are dominant and that the presence of width-dependent Coulomb and Pauli interactions has a small effect on the internal degrees of freedom. This assumption is correct for sufficiently weakly coupled systems. More generally, its validity may be assessed by comparison to interacting molecular dynamics simulations, as performed in Sec. IV; results from these simulations are also used in Appendix B to quantify the effective coupling Γ^{eff} . Of course, at sufficiently strongly coupled conditions, when $\Gamma^{\text{eff}} > 1$, the presence of interactions will perturb the width distribution away from the ideal case. Finally, we note that width distributions have been discussed for isotropic wave packets in previous works (see, e.g., Refs. [28,33–36]), but not directly predicted.

A. Anisotropic case

In an ideal gas of anisotropic wave packets, the Hamiltonian is a sum over kinetic terms and confining potential terms:

$$\mathcal{H}^{\text{WP}} = \sum_i \left(\mathcal{T}_i + \frac{A}{2} \text{Tr}(\Sigma_i) \right). \quad (14)$$

As discussed in the preceding section, the final term represents the confining potential with empirical strength A . This term arises from evaluating the expectation value of Eq. (13) for an anisotropic Gaussian wave function, given in Eq. (5). Without this term, the partition function diverges due to infinite wave packet spread [29]. For anisotropic wave packets the kinetic energy is given by [30]

$$\mathcal{T}^{\text{ani}} = \frac{\mathbf{p}^2}{2m} + \frac{2}{m} \text{Tr}(\Pi \Sigma \Pi) + \frac{\hbar^2}{8m} \text{Tr}(\Sigma^{-1}), \quad (15)$$

where m is the electron mass and the particle index has been suppressed. In a noninteracting system with classical Hamiltonian equations, the many-body distribution function factorizes into a set of N single-particle distribution functions,

$$f_1(\mathbf{p}, \Sigma, \Pi) = \frac{1}{Z_1} \exp \left[-\beta \left(\mathcal{T} + \frac{A}{2} \text{Tr}(\Sigma) \right) \right], \quad (16)$$

where $\beta = 1/(k_B T)$ is the inverse temperature and Z_1 is the single-particle partition function associated with the extended phase space of the model. Note that no closed-form expression is readily available for Z_1 . Introducing two-body interactions into Eq. (14) would couple the particle degrees of freedom, meaning that the Hamiltonian would no longer be separable into independent single-particle contributions.

The full N -particle distribution function would therefore no longer factorize into single-particle terms, which is the central assumption underlying Eq. (16). A complete treatment of the interacting system would require sampling this high-dimensional distribution, for instance, using Monte Carlo methods.

To study the resulting distribution over widths, we proceed by integrating the single-particle distribution function over both the position and momentumlike degrees of freedom to find a marginal distribution in terms of the Σ matrix:

$$f_{\Sigma}^{\text{ani}}(\Sigma) = \int d^3 \mathbf{r} \int d^3 \mathbf{p} \int d^6 \Pi f_1(\mathbf{p}, \Sigma, \Pi). \quad (17)$$

The Σ matrix is symmetric and therefore admits an eigendecomposition $\Sigma = \Lambda D \Lambda^T$, where $\Lambda \in \mathbb{R}^{3 \times 3}$ is an orthogonal matrix of eigenvectors ($\Lambda^T \Lambda = I$) and $D = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ is a diagonal matrix of eigenvalues. Therefore, upon making the change of variables $\Pi' = \Lambda^T \Pi \Lambda$, the trace may be written as $\text{Tr}(\Pi \Sigma \Pi) = \text{Tr}(\Pi' D \Pi')$. Orthogonal transformations preserve volume and so the integration measure remains unchanged, i.e., $d^6 \Pi = d^6 \Pi'$, and the total distribution becomes

$$f_{\Sigma}^{\text{ani}}(\Sigma) = \mathcal{Z} \exp \left[-\beta \left(\frac{\hbar^2}{8m} \text{Tr}(\Sigma^{-1}) + \frac{A}{2} \text{Tr}(\Sigma) \right) \right] I_1, \quad (18)$$

where $\mathcal{Z}$ is used henceforth as a normalization constant that is redefined as necessary to absorb prefactors. The last term is the following integral:

$$I_1 = \int \exp \left(-\beta \frac{2}{m} \text{Tr}(\Pi' D \Pi') \right) d^6 \Pi'. \quad (19)$$

The matrix Π' is symmetric, so the trace can be expanded accordingly:

$$\text{Tr}(\Pi' D \Pi') = \sum_{p=1}^3 \lambda_p (\Pi'_{pp})^2 + \sum_{1 \leq p < q \leq 3} (\lambda_p + \lambda_q) (\Pi'_{pq})^2.$$

Therefore, the integral factorizes into six independent Gaussian integrals. Performing these integrals yields

$$f_{\Sigma}^{\text{ani}}(\Sigma) = \mathcal{Z} \left(\prod_{p=1}^3 \frac{1}{\sqrt{\lambda_p}} \right) \left(\prod_{1 \leq p < q \leq 3} \frac{1}{\sqrt{\lambda_p + \lambda_q}} \right) \times \exp \left[-\beta \left(\frac{\hbar^2}{8m} \text{Tr}(\Sigma^{-1}) + \frac{A}{2} \text{Tr}(\Sigma) \right) \right]. \quad (20)$$

Since the shape matrix Σ is symmetric, it has six degrees of freedom. We wish to study the distribution of widths, which depend on the three eigenvalues of Σ , denoted by λ_1, λ_2 , and λ_3 . To isolate these, we express the integral in terms of these three variables and integrate over the three rotation variables μ_1, μ_2 , and μ_3 which parametrize the possible orientation of the eigenbasis. It is possible to show that the Jacobian associated with this transformation is [37]

$$\begin{aligned} \mathcal{J}(\lambda_1, \lambda_2, \lambda_3, \mu_1, \mu_2, \mu_3) \\ = \prod_{1 \leq p < q \leq 3} |\lambda_p - \lambda_q| g(\mu_1, \mu_2, \mu_3), \end{aligned} \quad (21)$$

where g is the distribution function of the μ degrees of freedom. After integrating over the rotational degrees of freedom,

the marginal distribution function over the eigenvalues is

$$f_{\lambda}^{\text{ani}}(\lambda_1, \lambda_2, \lambda_3) = \mathcal{Z} \left(\prod_{p=1}^3 \frac{1}{\sqrt{\lambda_p}} \right) \left(\prod_{1 \leq p < q \leq 3} \frac{|\lambda_p - \lambda_q|}{\sqrt{\lambda_p + \lambda_q}} \right) \times \exp \left[-\beta \left(\frac{\hbar^2}{8m} \sum_{p=1}^3 \frac{1}{\lambda_p} + \frac{A}{2} \sum_{p=1}^3 \lambda_p \right) \right]. \quad (22)$$

To characterize the resulting distribution we sample directly from the joint distribution of the eigenvalues $\lambda = (\lambda_1, \lambda_2, \lambda_3)$ defined in Eq. (22). From each set of sampled eigenvalues we calculate the widths

$$\sigma_p = \sqrt{\lambda_p} \quad \text{for } p = 1, 2, 3, \quad (23)$$

which provide a more natural physical interpretation. In order to characterize the statistics of these widths we consider the distribution of an individual width, denoted by P_{σ}^{ani} , obtained by pooling all σ_p values across samples. Additionally, to measure the total wave packet extent, we define the root-mean-square (rms) width as

$$\bar{\sigma} = \sqrt{\frac{1}{3} \langle \hat{W} \rangle} = \sqrt{\frac{1}{3} (\sigma_1^2 + \sigma_2^2 + \sigma_3^2)}, \quad (24)$$

where the first equality is the general definition in terms of the width-squared operator defined in Eq. (13). Evaluating the state average for the specific case of anisotropic wave packets yields the second equality. The marginal probability distribution of the rms width $\bar{\sigma}$ is denoted by $P_{\bar{\sigma}}^{\text{ani}}$. These two marginal distributions capture the typical fluctuations of a single component and the collective behavior of the total width, respectively.

B. Isotropic case

The equivalent Hamiltonian for an ideal gas of isotropic wave packets is

$$\mathcal{H}^{\text{WP}} = \sum_i \left(\mathcal{T}_i + \frac{3A}{2} s_i \right), \quad (25)$$

which includes the state average of the confining potential using the isotropic wave packet form given in Eq. (10). Here s_i is the isotropic covariance parameter of the i th wave packet. For isotropic wave packets, the kinetic energy is

$$\mathcal{T}^{\text{iso}} = \frac{p^2}{2m} + \frac{6}{m} \pi_s^2 s + \frac{3\hbar^2}{8ms}, \quad (26)$$

where the particle index is suppressed. Following the same procedure as the preceding section and integrating over all momentumlike degrees of freedom gives the following distribution function over s :

$$f_s^{\text{iso}}(s) = \sqrt{\frac{3A\beta}{2\pi s}} \exp \left[-\beta \left(\frac{3\hbar^2}{8ms} + \frac{3}{2} As - \frac{3}{2} \hbar \sqrt{\frac{A}{m}} \right) \right]. \quad (27)$$

Here the normalization factor has been explicitly calculated. The width metric employed for the anisotropic case can also be applied to the isotropic case. Specifically, we define the

isotropic width variable

$$\sigma = \sqrt{\frac{1}{3} \langle \hat{W} \rangle} = \sqrt{s}, \quad (28)$$

where the second equality is evaluated for the isotropic Gaussian [Eq. (10)] in contrast to the anisotropic wave function used to evaluate the state average appearing in the second equality of Eq. (24). The width variable σ has the marginal distribution function

$$f_{\sigma}^{\text{iso}}(\sigma) = 2\sigma f_s^{\text{iso}}(\sigma^2), \quad (29)$$

which is the isotropic equivalent to the marginal probability of the averaged width $P_{\bar{\sigma}}^{\text{ani}}$. It is also possible to find a closed-form expression for the mean width of the distribution,

$$\langle \sigma \rangle^{\text{iso}} = \int \sigma f_{\sigma}^{\text{iso}}(\sigma) d\sigma = \sqrt{\frac{3\hbar^2\beta}{2\pi m}} \exp \left(\frac{3}{2} \beta \hbar \sqrt{\frac{A}{m}} \right) K_1 \left(\frac{3}{2} \hbar \beta \sqrt{\frac{A}{m}} \right), \quad (30)$$

where $\langle \cdot \rangle^{\text{iso}}$ denotes the statistical average with respect to the isotropic width distribution function and $K_{\alpha}(\cdot)$ denotes the modified Bessel function of the second kind of order α . Additionally, the maximum of the distribution, calculated with

$$\frac{\partial f_{\sigma}^{\text{iso}}}{\partial \sigma} = 0, \quad (31)$$

gives the isotropic modal width

$$\text{mode}(\sigma) = \left(\frac{\hbar^2}{4mA} \right)^{1/4}, \quad (32)$$

which is equivalent to equating shape kinetic energy and confining potential terms and has previously been used to ascribe an approximate electronic length scale to the confining strength in WPMD [26,38].

IV. COMPARISON AGAINST INTERACTING MOLECULAR DYNAMICS DATA

A. Numerical details

1. Molecular dynamics

We now compare the noninteracting theory developed in the preceding section with fully interacting molecular dynamics data for warm dense hydrogen. The full model being employed, including confining and Pauli potentials, corresponds to the fully ionized model specified in Ref. [26]. The long-range Coulombic interactions are computed in reciprocal space according to the Ewald treatment in Ref. [30]. A time step of 5×10^{-5} fs and real-space cutoff for Pauli interactions of $12a_0$ ensures stable energy conservation. Results are presented for a Brueckner density parameter of $r_s = 2$ and a quantum degeneracy parameter of $\theta = k_B T / E_F = 1$, where E_F is the Fermi energy. Width distribution data are time averaged over snapshots that encompass a 25-fs period.

2. Markov chain Monte Carlo

To compute the width distributions in the noninteracting statistical theory of anisotropic wave packets, we sample $\lambda =$

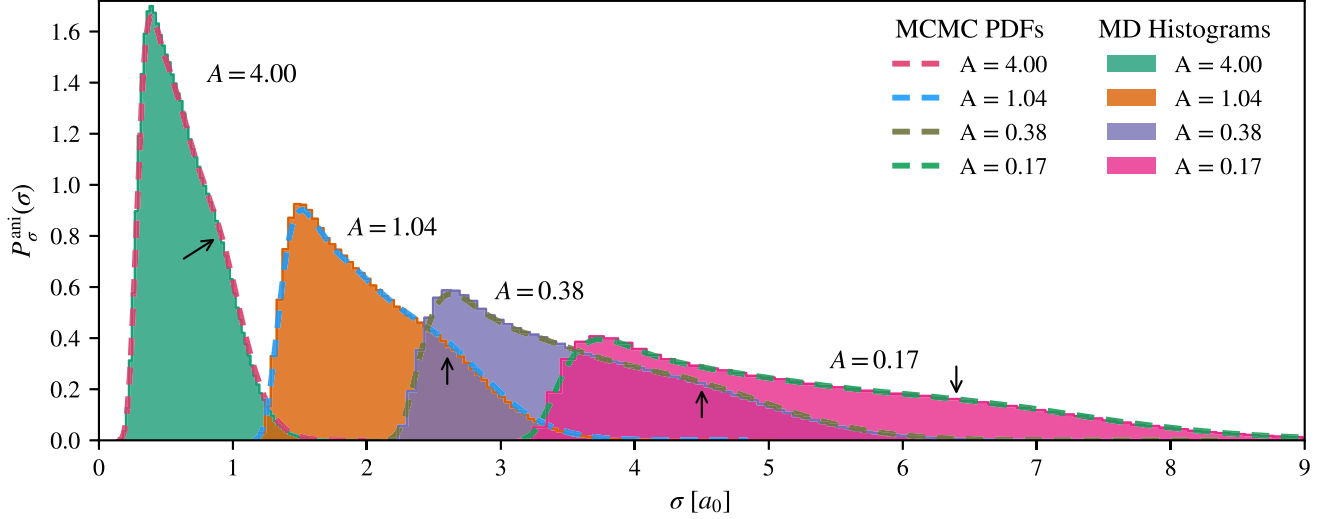


FIG. 1. Marginal width probability distribution functions (PDFs) for an anisotropic wave packet plasma at $r_s = 2$ and $\theta = 1$ for different confining potentials. Excluding the $A = 4.00$ Ha/ a_0^2 case, each curve is shifted by $1a_0$ relative to the curve to its left for clarity. The histograms correspond to molecular dynamics results in the microcanonical ensemble, while the dashed lines correspond to Markov chain Monte Carlo sampling of Eq. (22). Arrows indicate the shoulder feature discussed in the text. The simulations are performed within a cubic box of side length $L = 52.5a_0$. Hartree atomic units are used in the legend.

$(\lambda_1, \lambda_2, \lambda_3)$ from Eq. (22) using a Markov chain Monte Carlo (MCMC) sampling routine. Specifically, to generate samples from the target density we employ the random-walk Metropolis algorithm [39–41]. At each step the algorithm proposes a move in parameter space and then accepts or rejects it according to the Metropolis rule. Concretely, starting from an initial state $\lambda^{(0)}$, the algorithm iterates the following steps.

(i) Propose a new point $\lambda^{\text{prop}} = \lambda^{(t)} + \eta$, where $\eta \sim \mathcal{N}(\mathbf{0}, \sigma_{\text{prop}}^2 I)$.

(ii) Compute the logarithm of the unnormalized target density at the proposal and the current state and form the acceptance probability

$$\alpha = \min \{1, \exp [\log f_{\lambda}^{\text{ani}}(\lambda^{\text{prop}}) - \log f_{\lambda}^{\text{ani}}(\lambda^{(t)})]\}.$$

(iii) With probability α , accept the proposal and set $\lambda^{(t+1)} = \lambda^{\text{prop}}$; otherwise, keep the current state $\lambda^{(t+1)} = \lambda^{(t)}$.

Evaluating the density in logarithmic space prevents numerical underflow and converts products into sums, which is more numerically stable.

The Gaussian proposal width σ_{prop} is varied to yield a reasonable acceptance rate of around 0.3. Each independent chain consists of 2×10^6 iterations, with the first 10^5 discarded as burn-in and every 20th sample retained for analysis. For each parameter set, the retained samples from ten independent chains are combined to estimate the reported distributions. The retained states are transformed to $\sigma_p = \sqrt{\lambda_p}$, from which we construct the single-particle distribution P_{σ}^{ani} and the averaged-width distribution $P_{\bar{\sigma}}^{\text{ani}}$. Convergence was assessed using integrated autocorrelation times and Gelman-Rubin statistics across the ten chains. In the worst case across all sampled and derived quantities, the mean autocorrelation time was $\tau \simeq 398$ MCMC steps [42], corresponding to a minimum effective sample size of $N_{\text{eff}} \simeq 4.8 \times 10^4$. The maximum Gelman-Rubin statistic was $\hat{R} = 1.000144$ [42,43], close to the limiting value of unity expected for well-mixed

chains. These diagnostics, combined with the good agreement shown in the following section, indicate robust convergence.

B. Model comparison

Figure 1 shows the sampled distributions compared to the interacting molecular dynamics (MD) simulations specified in the preceding section for different values of the confining strength A . The agreement between the classical statistical theory and interacting width distributions is remarkable. Additionally, a shoulder feature is observed in the tail of each distribution, as indicated by the arrows in Fig. 1. This feature arises due to the eigenvalue difference term $\prod_{1 \leq p < q \leq 3} |\lambda_q - \lambda_p|$ present in the marginal distribution over eigenvalues, which appears in the second product of Eq. (22). This eigenvalue repulsion suppresses configurations with a similar spatial extent in each diagonalized spatial dimension, because fewer distinct covariance matrices Σ correspond to such points. This term directly originates from the rotational degrees of freedom in the model, which provide additional relaxation pathways. Further evidence for the link between the rotational degrees of freedom and the shoulder feature is provided in Appendix C, where a wave packet model with three independent widths but no rotational degrees of freedom is considered. The equivalence between the width distribution from the statistical theory and from the interacting system provides direct evidence that the effective interactions of the model are mediated by the classical statistics of the wave packet Hamiltonian $\mathcal{H}^{\text{WP}}$. To demonstrate this point we plot effective interparticle interactions in Fig. 2. These interactions are computed from the Coulomb interactions of an isotropic Gaussian with a width given by the mean of the corresponding distributions in Fig. 1. For narrow wave packets, the interparticle Coulomb interaction is greater at smaller separations given that the charge distribution is more localized, while for larger separations with respect to the wave

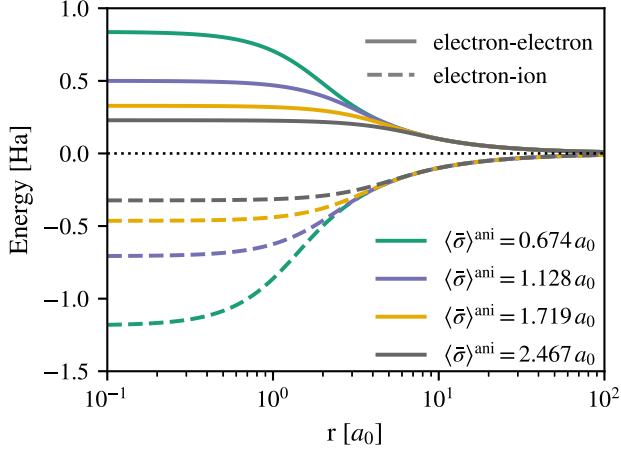


FIG. 2. Effective interparticle Coulomb interactions corresponding to the distributions plotted in Fig. 1. Calculation details for effective interactions are explained in Appendix B.

packet width, the pair potentials asymptote to the Coulomb potential. At this condition, full ionization is expected, and the effect of interactions has little impact on the width PDFs. A comparison between the isotropic and anisotropic restricted wave functions is presented in Fig. 3. Figure 3(a) shows the isotropic distribution $f_{\sigma}(\sigma)$ computed with both MD and MCMC techniques, alongside the probability distribution for the average width of an anisotropic wave packet $P_{\bar{\sigma}}^{\text{ani}}$. For

an equivalent confining potential, the average extent of the anisotropic wave packet is significantly larger. Additionally, the isotropic wave packet distribution is slightly more localized than its corresponding ideal distribution, which can be attributed to the larger effective coupling for isotropic wave packets, as quantified in Appendix B. Figure 3(b) depicts the corresponding marginal distribution over individual width variables, which exhibits a prominent tail in the width distribution extending beyond $6a_0$ and a shoulder feature. Figure 3 also demonstrates that the width of each anisotropic wave packet is underestimated by the mode of the isotropic distribution. While emphasizing the role of the underlying classical statistics, this comparison elucidates the difference in the two restricted wave functions. The isotropic wave functions are considerably more localized for a given confining potential. This is likely explained by additional rotational degrees of freedom present in the anisotropic wave packet ansatz that provide additional relaxation pathways in the dynamics, which manifest as eigenvalue repulsion. The stronger localization in the isotropic ansatz for a given confining strength means it will have stronger electron-electron and electron-ion interactions, explaining weaker correlations observed for the anisotropic ansatz in a previous comparison [30], albeit for a different form of the confining potential.

V. DISCUSSION

WPMD-based simulations can capture the concurrent time evolution of thousands of coupled ions and electrons. However, applications in plasma physics require the use of a confining potential to appropriately constrain the electron widths. In this work we have presented a method by which the effect of the confining potential can be predicted *a priori* for both isotropic and anisotropic variants of WPMD. From a practical perspective, this may allow confinement strength heuristics, such as those discussed in Refs. [29,38], to be developed and then applied, without the need to explicitly scan the parameter using molecular dynamics simulations to find a suitable choice, as was required in Ref. [27]. Additionally, we have investigated the distribution of electronic widths within a classical statistical theory. The comparison of two wave packet models reveals that, even under equivalent confining potentials, they exhibit different mean widths and therefore different effective Coulomb interactions. This finding accounts for the structural differences previously reported between these models in the warm dense matter regime [30]. The results presented here could also be extended to the case of a global external confining potential and therefore used to predict its impact on the equilibrium density profile [18].

From a theoretical perspective, we have demonstrated that the distribution of variables in wave packet models is closely connected to the statistical properties of the underlying classical Hamiltonian $\mathcal{H}^{\text{WP}}$. For the model to yield correct effective pairwise interactions, which are known from quantum statistical considerations to be Coulomb-like at large separations and finite at small separations in weakly coupled, fully ionized plasmas [11], it should relax to a nondivergent width distribution. As $A \rightarrow 0$ in either the anisotropic or isotropic case, the average width diverges and the distribution functions themselves [Eqs. (22) and (27)] become unnormalizable. This

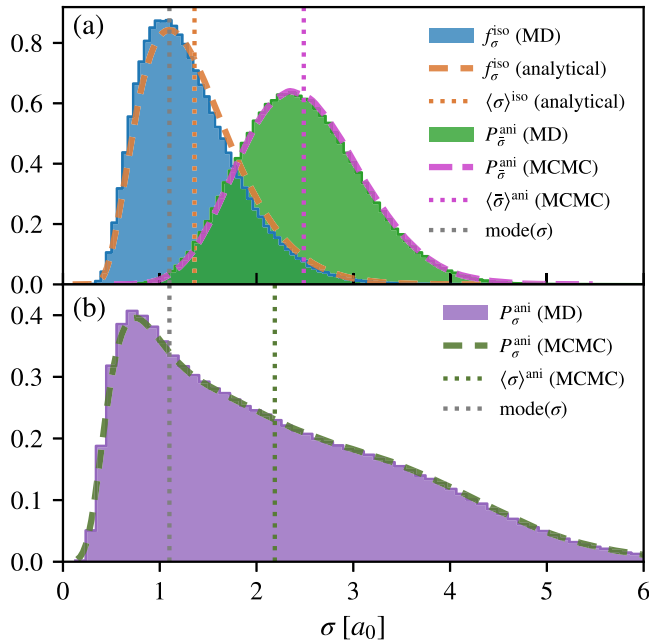


FIG. 3. Comparison between isotropic and anisotropic width distribution functions at $r_s = 2$ and $\theta = 1$ for a confining potential of $A = 0.17 \text{ Ha}/a_0^2$. (a) Average width distribution functions for the isotropic and anisotropic models. (b) Distribution of individual width variables in the anisotropic model. The gray dashed line indicates the modal width of the isotropic model given by Eq. (32). The mean values of each distribution are also plotted, with the isotropic case given by Eq. (30) and the anisotropic case calculated numerically.

observation establishes the confining potential as an essential ingredient for enforcing the correct behavior in weakly coupled regimes. Similar models, such as those used for nuclear collisions, often address this feature by fixing the wave packet width directly [44].

In fully ionized warm dense systems, as studied here, a significant fraction of the electrons are expected to be in spatially extended states. However, a fully delocalized Gaussian wave packet will effectively cease to interact with the system and has no mechanism to relocalize. Therefore, by regulating the model by choosing an appropriate confining potential, physically meaningful results can be obtained [18,19,26].

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DATA AVAILABILITY

The data used to generate the figures in the main text are openly available [45].

APPENDIX A: GLOBAL CONFINING POTENTIALS

In the main text, a width-dependent confining potential that penalizes the spatial extent of each wave packet is considered. Some authors have considered a global external potential acting directly on the electronic coordinates [18,34]:

$$\hat{V}_g = \sum_i V_g(\hat{\mathbf{x}}_i). \quad (\text{A1})$$

For a Gaussian wave packet, this contributes to the wave packet Hamiltonian through the state average

$$U_g(\mathbf{r}_i, \Sigma_i) = \langle V_g(\hat{\mathbf{x}}_i) \rangle = \int d^3x \rho_i(\mathbf{x}; \mathbf{r}_i, \Sigma_i) V_g(\mathbf{x}), \quad (\text{A2})$$

where ρ_i is the single-particle probability density associated with the Gaussian wave packet. For example, in the case of anisotropic Gaussians, $\rho_i = |\langle \mathbf{x} | q_i \rangle|^2$. Continuing with the example of anisotropic wave packets, the ideal single-particle distribution considered in Sec. III A would then be replaced

by

$$f_1(\mathbf{r}, \mathbf{p}, \Sigma, \Pi) = \frac{1}{Z_1} \exp\{-\beta[\mathcal{T}^{\text{ani}} + U_g(\mathbf{r}, \Sigma)]\}. \quad (\text{A3})$$

The momentum degrees of freedom can still be integrated out, giving a configurational distribution

$$f^{\text{conf}}(\mathbf{r}, \Sigma) = \int d^3\mathbf{p} \int d^6\Pi f_1(\mathbf{r}, \mathbf{p}, \Sigma, \Pi). \quad (\text{A4})$$

This object is the natural analog of the configurational distribution used in the main text. However, in contrast to the local width potential, a global potential generally couples the expected position $\mathbf{r}$ to the shape variable Σ through $U_g(\mathbf{r}, \Sigma)$.

The statistical distribution over widths is obtained by marginalizing Eq. (A4) over the expected position coordinate. For example, the marginal distribution over the covariance matrix is

$$f_\Sigma(\Sigma) = \int d^3\mathbf{r} f^{\text{conf}}(\mathbf{r}, \Sigma). \quad (\text{A5})$$

Although the momentum integration can be performed, a closed-form statistical distribution over widths is not guaranteed. This is automatic for the local width potential considered in the main text, because the expected position and width variables separate, but it is generally not true for a global potential. For special choices of V_g , such as a global harmonic potential, the dependence on $\mathbf{r}$ and Σ may separate. For more general global confinement schemes, including harmonic cubic box potentials, the coupling between the position and shape variables may prevent further analytical progress.

For models with external confining potentials, MCMC sampling of $f^{\text{conf}}(\mathbf{r}, \Sigma)$ provides a direct route to both the statistical width distribution and the corresponding spatially varying ideal equilibrium number density

$$n(\mathbf{x}) = N_e \int d^3\mathbf{r} \int_{\Sigma>0} d^6\Sigma f^{\text{conf}}(\mathbf{r}, \Sigma) \rho_i(\mathbf{x}; \mathbf{r}, \Sigma), \quad (\text{A6})$$

where the Σ integral is restricted to positive-definite symmetric matrices. This method may therefore be used to compare with published work on density distributions in global-confinement schemes [18].

APPENDIX B: EFFECTIVE COUPLING PARAMETER

In this Appendix, we define an effective Coulomb coupling parameter that estimates the role of interactions on the wave packet width distribution. We first present the Coulomb interaction generated by Gaussian charge distributions and then specialize the result to effective interactions for isotropic and anisotropic wave packets. Consider two anisotropic Gaussian wave packets with centers $\mathbf{r}_i$ and $\mathbf{r}_j$ and shape matrices Σ_i and Σ_j . The probability density of the i th wave packet is

$$|\langle \mathbf{x} | q_i \rangle|^2 = \mathcal{N}^2 \exp\left[-\frac{1}{2}(\mathbf{x} - \mathbf{r}_i)^T \Sigma_i^{-1}(\mathbf{x} - \mathbf{r}_i)\right], \quad (\text{B1})$$

with a similar expression for the j th wave packet. The Coulomb interaction between wave packets is

$$u_{ij}(\mathbf{R}_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0} \int d^3x \int d^3y \frac{|\langle \mathbf{x} | q_i \rangle|^2 |\langle \mathbf{y} | q_j \rangle|^2}{|\mathbf{x} - \mathbf{y}|}, \quad (\text{B2})$$

where $\mathbf{R}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the separation vector between the expected positions of the two wave packets.

For isotropic wave packets, $\Sigma_i = \sigma_i^2 I$ and Eq. (B2) reduces to the standard result

$$u_{ij}^{\text{iso}}(R) = \frac{q_i q_j}{4\pi\epsilon_0} \frac{\text{erf}(\zeta_{ij}R)}{R}, \quad \zeta_{ij} = \frac{1}{\sqrt{2(\sigma_i^2 + \sigma_j^2)}}. \quad (\text{B3})$$

For an electron-ion interaction with a point ion, one sets $\sigma_j = 0$, giving

$$\zeta_{iJ}^{\text{iso}} = \frac{1}{\sqrt{2}\sigma_i}. \quad (\text{B4})$$

For an anisotropic electron interacting with a point-charge ion, the exact interaction is obtained from Eq. (B2) with $|\mathbf{y}|q_j|^2 \rightarrow \delta(\mathbf{y} - \mathbf{r}_j)$. While the anisotropic interaction does not generally reduce to a simple error-function form, numerical schemes have been developed based on a decomposition of the Coulomb interaction kernel [30]. To obtain a scalar estimate that can be inserted into an effective coupling parameter, the instantaneous width may be replaced by the statistical rms width obtained from the width distribution, which for the electron-ion case yields

$$\zeta_{i,J}^{\text{ani}} = \frac{1}{\sqrt{2}\langle\bar{\sigma}\rangle^{\text{ani}}}, \quad \zeta_{i,J}^{\text{iso}} = \frac{1}{\sqrt{2}\langle\sigma\rangle^{\text{iso}}} \quad (\text{B5})$$

for anisotropic and isotropic wave packets, respectively. Note that this replacement is not intended to reproduce the exact orientationally averaged anisotropic Coulomb interaction; it provides a scalar estimate based on the typical rms width of the wave packet. For an electron-electron estimate with two comparable wave packet widths, σ_i and σ_j are both replaced by the corresponding statistical width. This gives an additional factor of $\sqrt{2}$ in the denominator of Eq. (B5). To quantify the effective coupling, we use the electron-ion case because the interaction with a point ion has the shortest smoothing length and therefore gives the largest short-range Coulomb magnitude among interactions involving an electron wave packet. We then define the following heuristic effective coupling parameter:

$$\Gamma^{\text{eff}}(N_d, \zeta) = \frac{e^2}{4\pi\epsilon_0} \frac{\text{erf}(\zeta a)}{a} \frac{1}{(N_d/3)k_B T}. \quad (\text{B6})$$

Here $a = a_0 r_s$ is the characteristic interparticle separation. The quantity N_d is the number of momentum degrees of freedom per particle, a factor that can be motivated from the equipartition theorem (see Appendix D in Ref. [30]). For point particles, $N_d = 3$ and $\zeta \rightarrow \infty$ such that Eq. (B6) reduces to the usual classical Coulomb coupling parameter. For isotropic wave packets $N_d = 4$, reflecting the inclusion of the additional momentum variable π_s . For anisotropic wave packets $N_d = 9$, due to the presence of six degrees of freedom in the symmetric matrix Π . For Gaussian wave packets, finite ζ accounts for the regularization of the Coulomb interaction at short range by the spatial extent of the electronic charge density.

In Table I we present calculations of the effective coupling, finding that it lies below unity for the studied conditions. The isotropic wave packet coupling is greater, which can be observed in Fig. 3(a), where isotropic wave packets are more localized than the noninteracting theory predicts.

TABLE I. Computed effective Coulomb coupling parameters for isotropic and anisotropic wave packets. Width uncertainties are given in parentheses and denote one standard deviation in the final quoted digits.

A	$\langle\sigma\rangle^{\text{iso}}$	$\langle\bar{\sigma}\rangle^{\text{ani}}$	$\Gamma^{\text{eff}}(4, \zeta^{\text{iso}})$	$\Gamma^{\text{eff}}(9, \zeta^{\text{ani}})$
4.000	0.5183(4)	0.6736(7)	0.8166	0.3619
1.041	0.7525(15)	1.1282(17)	0.8102	0.3353
0.381	1.0126(27)	1.7190(22)	0.7772	0.2742
0.171	1.3051(36)	2.4671(33)	0.7142	0.2114

APPENDIX C: STATISTICS OF A DIAGONAL-ANISOTROPIC WAVE PACKET

To isolate the role of independent width directions from the role of rotational degrees of freedom, we consider an intermediate model with the parametrization

$$\langle \mathbf{x} | h_i \rangle = \mathcal{N} \exp \left(- \sum_{\alpha=1}^3 m_i^{(\alpha)} (x^{(\alpha)} - r_i^{(\alpha)})^2 + \frac{i}{\hbar} \mathbf{p}_i^T (\mathbf{x} - \mathbf{r}_i) \right), \quad (\text{C1})$$

where the (α) superscript denotes a vector component. As performed in Sec. II, the complex width variable may be decomposed into real and imaginary parts,

$$m_i^{(\alpha)} = \frac{1}{4s_i^{(\alpha)}} - \frac{i}{\hbar} \pi_i^{(\alpha)}. \quad (\text{C2})$$

This wave packet can expand independently along the three Cartesian directions, but its principal axes are fixed in the laboratory frame and therefore it cannot rotate. We refer to this intermediate model as the diagonal-anisotropic wave packet. This model has not been considered in the main text, nor implemented in the MD code, because it unphysically constrains the wave packet expansion along the three fixed axes and therefore imposes preferential expansion directions.

Dropping the particle index, the rms width of an arbitrary diagonal-anisotropic wave packet is

$$\bar{\sigma} = \sqrt{\frac{S}{3}} = \sqrt{\frac{1}{3}(s^{(1)} + s^{(2)} + s^{(3)})}, \quad (\text{C3})$$

where the intermediate variable S has been defined. Using the framework in Sec. III A, we find the combined PDF of the three covariance variables $\mathbf{s} = (s^{(1)}, s^{(2)}, s^{(3)})$ as

$$f_{\mathbf{s}}(s^{(1)}, s^{(2)}, s^{(3)}) = \prod_{\alpha=1}^3 f_s^{\text{diag}}(s^{(\alpha)}), \quad (\text{C4})$$

where

$$f_s^{\text{diag}}(s^{(\alpha)}) = \sqrt{\frac{A\beta}{2\pi s^{(\alpha)}}} \times \exp \left[-\beta \left(\frac{\hbar^2}{8ms^{(\alpha)}} + \frac{A}{2}s^{(\alpha)} - \frac{\hbar}{2}\sqrt{\frac{A}{m}} \right) \right]. \quad (\text{C5})$$

After changing variables from s to $\sigma = \sqrt{s}$, one obtains the single-direction width distribution $f_{\sigma}^{\text{diag}}(\sigma)$, which is directly comparable to the marginal eigenvalue width distribution of the fully anisotropic model. These distributions are plotted

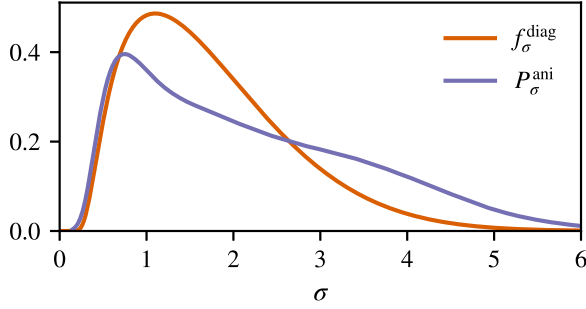


FIG. 4. Comparison between PDFs of diagonalized width variables for the diagonal-anisotropic wave packet introduced in Appendix C and the fully anisotropic wave packet discussed in the main text. The conditions are the same as those in Fig. 3.

in Fig. 4 for the condition studied in Fig. 3. The shoulder feature, present in the anisotropic model, no longer appears in the diagonal-anisotropic model. This feature, together with the extended distribution tail, can therefore be attributed to the additional rotational degrees of freedom present in the full anisotropic model.

To obtain a statistical distribution over rms widths, the PDF of S is first considered. This may be obtained by marginalizing the joint density over all configurations of s with the same value of S :

$$f_S(S) = \int_0^\infty ds^{(1)} \int_0^\infty ds^{(2)} \int_0^\infty ds^{(3)} f_s(s^{(1)}, s^{(2)}, s^{(3)}) \times \delta(S - s^{(1)} - s^{(2)} - s^{(3)}). \quad (\text{C6})$$

This PDF of S may be written as a convolution. Explicitly, after substituting the product form (C4), the inner integral in Eq. (C6) becomes

$$\int_0^\infty ds^{(3)} f_s^{\text{diag}}(s^{(3)}) \delta(S - s^{(1)} - s^{(2)} - s^{(3)}) = f_s^{\text{diag}}(S - s^{(1)} - s^{(2)}) \Theta(S - s^{(1)} - s^{(2)}), \quad (\text{C7})$$

where $\Theta(\cdot)$ is the Heaviside step function, which arises from the restriction that $s^{(3)} \geq 0$. For $S > 0$, the domain of Eq. (C7) is therefore restricted to

$$0 \leq s^{(1)} \leq S, \quad 0 \leq s^{(2)} \leq S - s^{(1)}. \quad (\text{C8})$$

Using these results, Eq. (C6) may be written

$$f_S(S) = \int_0^S ds^{(1)} \int_0^{S-s^{(1)}} ds^{(2)} \times f_s^{\text{diag}}(s^{(1)}) f_s^{\text{diag}}(s^{(2)}) f_s^{\text{diag}}(S - s^{(1)} - s^{(2)}), \quad (\text{C9})$$

where the limits arise due to the restriction to positive random variables. This form is equivalent to the triple convolution (see [46], Sec. 17.12, entry 5)

$$f_S(S) = (f_s^{\text{diag}} \star f_s^{\text{diag}} \star f_s^{\text{diag}})(S), \quad (\text{C10})$$

where $\star$ denotes a convolution. Given that $s > 0$ and we are considering a convolution, it is natural to use a Laplace transform approach to solve for f_S . Applying the transform to Eq. (C10) yields

$$\mathcal{L}\{f_S\}(\gamma) = [\mathcal{L}\{f_s^{\text{diag}}\}(\gamma)]^3, \quad (\text{C11})$$

where

$$\mathcal{L}\{f_s^{\text{diag}}\}(\gamma) = \int_0^\infty \exp(-\gamma s) f_s^{\text{diag}}(s) ds. \quad (\text{C12})$$

Using a known transformation (see [46], Sec. 3.471, entry 15), we perform the Laplace transform of f_s to find

$$\begin{aligned} \mathcal{L}\{f_s^{\text{diag}}\}(\gamma) &= \sqrt{\frac{\beta A}{\beta A + 2\gamma}} \exp\left[-\frac{\hbar\sqrt{\beta}}{\sqrt{2m}}\left(\sqrt{\gamma + \frac{\beta A}{2}} - \sqrt{\frac{\beta A}{2}}\right)\right]. \end{aligned} \quad (\text{C13})$$

By cubing this result, it directly follows from Eq. (C11) that

$$\begin{aligned} \mathcal{L}\{f_S\}(\gamma) &= \left(\frac{\beta A}{2}\right)^{3/2} \exp\left(\frac{3\beta\hbar}{2}\sqrt{\frac{A}{m}}\right) \left(\gamma + \frac{\beta A}{2}\right)^{-3/2} \\ &\times \exp\left(-\frac{3\hbar\sqrt{\beta}}{\sqrt{2m}}\sqrt{\gamma + \frac{\beta A}{2}}\right). \end{aligned} \quad (\text{C14})$$

Applying the inverse Laplace transform then yields the required distribution. The required inverse transform identity can be derived from the standard Laplace transform (see [46], Sec. 17.13, entry 30)

$$\mathcal{L}\left\{S^{-1/2} \exp\left(-\frac{a^2}{4S}\right)\right\}(\gamma) = \sqrt{\pi} \gamma^{-1/2} \exp(-a\sqrt{\gamma}), \quad (\text{C15})$$

where the Laplace transform is taken with respect to S . After dividing both sides by $\sqrt{\pi}\gamma$ and rearranging, we now apply an inverse Laplace transform and use the transform-of-an-integral rule (see [46], Sec. 17.12, entry 3). This yields

$$\begin{aligned} \mathcal{L}^{-1}\{\gamma^{-3/2} \exp(-a\sqrt{\gamma})\}(S) &= \frac{1}{\sqrt{\pi}} \int_0^S u^{-1/2} \exp\left(-\frac{a^2}{4u}\right) du \\ &= \frac{2\sqrt{S}}{\sqrt{\pi}} \exp\left(-\frac{a^2}{4S}\right) - a \operatorname{erfc}\left(\frac{a}{2\sqrt{S}}\right), \end{aligned} \quad (\text{C16})$$

where the final equality follows from an integration by parts.

We now use the derived identity, Eq. (C16), to take the inverse Laplace transform of Eq. (C14). In this case,

$$a = \frac{3\hbar\sqrt{\beta}}{\sqrt{2m}}, \quad (\text{C17})$$

and the argument of the transform is shifted according to

$$\gamma \mapsto \gamma + \frac{\beta A}{2}.$$

Using the shift theorem for Laplace transforms (see [46], Sec. 17.12, entry 4), we therefore obtain

$$\begin{aligned} f_S(S) &= \left(\frac{\beta A}{2}\right)^{3/2} \exp\left(\frac{3\beta\hbar}{2}\sqrt{\frac{A}{m}} - \frac{\beta A}{2}S\right) \\ &\times \left[\frac{2\sqrt{S}}{\sqrt{\pi}} \exp\left(-\frac{9\beta\hbar^2}{8mS}\right) - 6\sqrt{\frac{\beta\hbar^2}{8m}} \operatorname{erfc}\left(3\sqrt{\frac{\beta\hbar^2}{8mS}}\right)\right]. \end{aligned} \quad (\text{C18})$$

Finally, to transform the PDF in S to the PDF in $\bar{\sigma}$, we use $S = 3\bar{\sigma}^2$ and its derivative to write the rms-width distribution for diagonal-anisotropic wave packets,

$$f_{\bar{\sigma}}^{\text{diag}}(\bar{\sigma}) = 6\bar{\sigma} \left(\frac{\beta A}{2} \right)^{3/2} \exp \left(\frac{3\beta\hbar}{2} \sqrt{\frac{A}{m}} - \frac{3\beta A}{2} \bar{\sigma}^2 \right) \times \left[\frac{2\sqrt{3}\bar{\sigma}}{\sqrt{\pi}} \exp \left(-\frac{3\beta\hbar^2}{8m\bar{\sigma}^2} \right) - 6\sqrt{\frac{\beta\hbar^2}{8m}} \operatorname{erfc} \left(\sqrt{\frac{3\beta\hbar^2}{8m\bar{\sigma}^2}} \right) \right]. \quad (\text{C19})$$

This PDF for the rms width is directly comparable to the isotropic and anisotropic equivalents, namely, f_{σ}^{iso} and $P_{\bar{\sigma}}^{\text{ani}}$. Comparing these distributions in Fig. 5 shows that, as the number of degrees of freedom increases, from the isotropic model to the diagonal-anisotropic and finally to the anisotropic model, the rms-width distribution

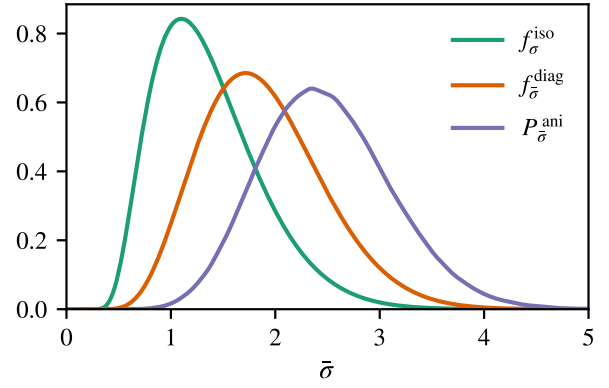


FIG. 5. Comparison between rms width PDFs for isotropic, diagonal-anisotropic, and anisotropic wave packets. The conditions are the same as those in Fig. 3.

shifts toward larger widths, corresponding to a reduction in localization.

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