

Quantum Information Perspective on Many-Body Dispersive Forces

Christopher Willby,^{1,2} Martin Kiffner³, Joseph Tindall⁴, Jason Crain,^{5,1} and Dieter Jaksch^{2,1}

¹Clarendon Laboratory, *University of Oxford*, Parks Road, Oxford OX1 3PU, United Kingdom

²Institut für Quantenphysik, *Universität Hamburg*, 22761 Hamburg, Germany

³PlanQC GmbH, Lichtenbergstraße 8, 85748 Garching, Germany

⁴Centre for Computational Quantum Physics, *Flatiron Research Institute*, New York, New York 10010 USA

⁵IBM Research Europe, The Hartree Centre STFC Laboratory, Sci-Tech Daresbury, Warrington WA4 4AD, United Kingdom



(Received 4 July 2024; revised 17 March 2025; accepted 11 August 2025; published 11 September 2025)

Despite its ubiquity, the quantum many-body properties of dispersion remain poorly understood. Here, we investigate the entanglement distribution in assemblies of quantum Drude oscillators, minimal models for dispersion-bound systems. We establish an analytic relationship between entanglement and correlation energy and show how entanglement monogamy determines whether many-body corrections to the pair potential are attractive, repulsive, or zero. These findings, demonstrated in trimers and extended lattices, apply in more general chemical environments where dispersion coexists with other cohesive forces.

DOI: [10.1103/PhysRevLett.135.110403](https://doi.org/10.1103/PhysRevLett.135.110403)

Introduction—Any pair of neutral atoms or molecules experiences an attraction due to the formation of transient electric dipoles. Though weaker than other forms of binding, this so-called dispersion force is the only intermolecular interaction present in all materials: It spans a wide range of length scales and its cumulative effects can exert decisive influence over physical, chemical, and biological processes [1–10]. These include stability of condensed phases in noble gases [11–13], hydrocarbons [14], molecular crystals [15,16] as well as noncovalent binding of drugs to proteins [17–19] and even the ability of geckos to climb up flat surfaces [20,21].

In many cases, dispersion is approximated in material simulations as a pairwise interaction attenuated by a $1/R^6$ distance dependence. However, failures of the pairwise approximation and the importance of many-body corrections are now widely acknowledged in numerous contexts including supramolecular chemistry [22], clusters [23], low dimensional systems including layers, chains and wires [24], nanomaterials [25–27], inorganic [27], and alkaline earth compounds [28], as well as polymorphism in molecular crystals [6,29–31]. In rare gas condensates, many-body effects can account for nearly 10% of the cohesive energy [32], and in layered systems, their contributions can be much larger [33].

The elementary picture of dispersion interactions between two particles is that of “flickering” dipole moments, arising from correlated zero-point fluctuations of the molecular or

atomic charge density. However, such a model has no immediate or systematic generalization to the many-body case. Consequently, it is not known *a priori*, when or why the pairwise approximation fails, when perturbative corrections will be sufficient, or whether or under what circumstances the net contributions from many-body effects will be attractive or repulsive. Ultimately, the residual interactions governing both pairwise and many-body dispersion are quantum phenomena with no classical analog.

Correlated vacuum fluctuations give rise to entangled ground states, where the state of each particle cannot be described independently of the others. Going from the pairwise to the many-body case, however, will incur certain restrictions on the allowed amount of entanglement two particles may share in a multipartite system [34–36]. These restrictions, known as the monogamy of entanglement [37–46], are expressed by inequalities that give upper bounds for the pairwise entanglement. Within the confines of the monogamy inequalities the amount of shareable entanglement increases with the dimensionality of the local Hilbert space of the particles [35,47,48]. For infinite dimensional Gaussian states, there is thus a rich interplay between the enhancement of pairwise entanglement in the multipartite setting and its limitations due to monogamy restrictions [46].

Despite being considered a key property of entanglement, the ramifications of the monogamy property on chemical binding, are still largely unexplored. Moreover, finding the relationship between binding energy and entanglement measures remains mostly uncharted, with some work relating correlation energy to entropy measures [49,50].

Here, we derive a bound on the pairwise and many-body dispersive energy contributions in terms of the reduced tangle, defined via a monogamous entanglement metric for Gaussian states. The tightness of this bound is

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demonstrated in both a trimer and arbitrary lattice structures. For the trimer, we partition the parameter space into a monogamous regime, where monogamy constraints suppress pairwise entanglement and a promiscuous regime, where the multipartite interaction allows for enhanced pairwise entanglement. The boundary separating these regimes closely aligns with the transition between repulsive and attractive many-body energy contributions, along which pairwise additivity remains valid. We further show that the relationship between monogamy constraints and many-body energy contributions persists in larger systems. Since the trimer captures key features of many-body dispersion in lattices, our findings provide a quantum information perspective on many-body energetics.

Finally, we consider how our methods and conclusions extend to realistic chemical environments. Our findings apply both to scenarios where dispersion is the sole cohesive force and to more general cases where it coexists with other forms of bonding. This generality arises because we focus on quantum fluctuations around an equilibrium configuration. While other interactions may shift the equilibrium positions, the fluctuations around these points persist. As such, our entanglement-based characterization of dispersion remains applicable across a wide range of chemical systems, from dispersion-dominated noble-gas crystals to dispersion-influenced molecular complexes.

Model—We model many-body dispersion forces at long range in molecular systems as assemblies of dipole coupled quantum Drude oscillators (QDOs) [23,51–63]. The QDO model has been demonstrated to capture the dominant physics of non-reactive condensed matter systems, and outperforms competitor models in terms of accuracy and computational efficiency, in many instances [63–67]. In particular, the dipole-order QDO Hamiltonian is employed to amend many-body dispersive corrections into density functionals, via the so-called many-body dispersion (MBD) method [6,22,23,30,31,68], the accuracy of which is well established in the literature. See Supplemental Material (SM) [69] for a greater discussion of the applicability of the dipole QDO model, through MBD.

In the QDO model a particle, molecule or molecular fragment is treated as a three dimensional quantum harmonic oscillator (given by three quantum harmonic oscillators or modes per QDO), with mass m_μ , frequency ω_μ , nuclear charge $+q_\mu$ and Drude quasiparticle of charge $-q_\mu$. The instantaneous dipole moment $q_\mu \hat{\mathbf{r}}_\mu$ is proportional to the displacement, $\hat{\mathbf{r}}_\mu = (\hat{r}_\mu^x, \hat{r}_\mu^y, \hat{r}_\mu^z)$ of the QDO from its equilibrium, determined by the center position of the particle. The corresponding momentum vector is given by $\hat{\mathbf{p}}_\mu = (\hat{p}_\mu^x, \hat{p}_\mu^y, \hat{p}_\mu^z)$.

Dipolar interactions between the QDOs arise from the Coulomb potential and are described by a $3N \times 3N$ coupling matrix $\mathcal{T}$. Individual 3×3 blocks of $\mathcal{T}$ describe the interaction between QDO μ and ξ , given by

$$e_\mu^T \mathcal{T} e_\xi = \frac{1}{R_{\mu\xi}^3} \left(\mathbb{1}_3 - \frac{3\mathbf{R}_{\mu\xi} \otimes \mathbf{R}_{\mu\xi}}{R_{\mu\xi}^2} \right) \quad \text{for } \mu \neq \xi, \quad (1)$$

and $e_\mu^T \mathcal{T} e_\mu = 0_3$, where 0_3 is the 3×3 zero matrix. Here $\otimes$ denotes the outer product, e_μ^T is a $3 \times 3N$ matrix, e.g., $e_1^T = [\mathbb{1}_3, 0_3, \dots, 0_3]$, $e_2^T = [0_3, \mathbb{1}_3, \dots, 0_3]$ etc and $\mathbf{R}_{\mu\xi} = (x_\mu - x_\xi, y_\mu - y_\xi, z_\mu - z_\xi)$, where (x_μ, y_μ, z_μ) is the position of the QDO in Cartesian space.

For simplicity we here consider the case where the QDO parameters are all identical given by (q, m, ω) , for the general case see the SM [69]. We define operators $\hat{\chi}_\mu = \hat{\mathbf{r}}_\mu \sqrt{\omega m / \hbar}$, $\hat{\mathbf{P}}_\mu = \hat{\mathbf{p}}_\mu / \sqrt{\hbar m \omega}$. Then by introducing the polarizability $\alpha = q^2 / (m \omega^2 4\pi \epsilon_0)$, the dipole order QDO Hamiltonian in units of $\hbar \omega$ is

$$\hat{H} = \frac{1}{2} \left(\sum_{i=1}^{3N} \hat{\mathbf{P}}_i^2 + \sum_{i=1}^{3N} \hat{\chi}_i^2 \right) + \alpha \sum_{i>j} \hat{\chi}_i \mathcal{T}_{ij} \hat{\chi}_j. \quad (2)$$

We use the indices i, j to label the individual harmonic oscillators or modes.

Dispersive binding—The dispersive binding energy is the difference between the ground state energy of the noninteracting and interacting QDOs. The dispersive binding energy, inclusive of the many-body contributions, is written as $E = 3N/2 - (\sum_{i=1}^{3N} \sqrt{\lambda_i})/2$, where λ_i are the normal eigenvalues of the $3N \times 3N$ potential matrix V , with $V_{ii} = 1$ and $V_{ij} = \alpha \mathcal{T}_{ij}$, $\forall i \neq j$. The expression for the dispersive binding energy E follows from the adiabatic connection fluctuation dissipation theorem and can be found in [79,80]. The binding energy E is always positive (see SM [69] for details). In order for the energy to be real, the matrix V must be positive definite. This enforces the constraint $\alpha t_i > -1 \forall i$, where t_i are the eigenvalues of the real symmetric matrix dipole coupling $\mathcal{T}$.

The dispersive binding energy is often treated as a perturbative correction to the non-interacting groundstate [3,81–83], leading to the familiar pair potential. This is derived by a second order Taylor expansion of $\sqrt{\lambda_i}$ in small parameters αt_i . This is possible when $\alpha \|\mathcal{T}\|_2 < 1$, equivalent to $\max(\alpha |t_1|, \dots, \alpha |t_{3N}|) < 1$. We will assume $\alpha \|\mathcal{T}\|_2 < 1$ holds throughout, explicitly stating instances when this is not the case. As $\sum_{i=1}^{3N} t_i^k = \text{tr}(\mathcal{T}^k)$ and $\mathcal{T}$ is traceless, the full power series expansion of E in terms of αt_i can be written as follows:

$$E = \sum_{k=2}^{\infty} \delta_k, \quad \delta_k = \frac{(-1)^k (2k-3)!!}{2^{k+1} k!} \alpha^k \text{tr}(\mathcal{T}^k). \quad (3)$$

The pairwise potential δ_2 , aptly named as it can be written additively over all pairs in the system, gives the leading order correction to the noninteracting energy [57,84],

$$\delta_2 = \frac{\alpha^2}{16} \text{tr}(\mathcal{T}^2) = \frac{3\alpha^2}{4} \sum_{\mu>\xi} R_{\mu\xi}^{-6} > 0. \quad (4)$$

The many-body (MB) correction to the binding energy is thus given by $\delta_{\text{MB}} = E - \delta_2$ and can be repulsive or attractive. The so called Axilrod-Teller (AT) triple dipole approximation is given by δ_3 [62,85]. The MB effect can thus be written in terms of the higher order corrections to the pairwise potential, $\delta_{\text{MB}} = \sum_{k=3}^{\infty} \delta_k$.

Gaussian states—The perturbative approach, can be readily compared to the exact solution of the quadratic QDO Hamiltonian, which has a Gaussian ground state, that can be calculated efficiently [86–98]. Gaussian ground states are completely characterized by a vector of single element correlation functions and a correlation matrix (CM) of two point correlation functions [87,99,100]. As the equilibrium displacement of the QDOs is set to zero, we can describe the properties of the ground state, solely by the CM. The ground state CM can be written in terms of the potential matrix V [87,95,101],

$$\gamma_0 = V^{-1/2} \oplus V^{1/2}, \quad (5)$$

where the matrix square root is given by $V^{1/2} = \text{Odiag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_{3N}})O^T$, and O is the orthogonal matrix that diagonalizes V , where $(V^{-1/2})_{ij} = \langle \hat{x}_i \hat{x}_j \rangle$ and $(V^{1/2})_{ij} = \langle \hat{p}_i \hat{p}_j \rangle$.

The tangle—We quantify the entanglement present in the ground state by the Gaussian tangle which is an entanglement measure, i.e., vanishing for separable states and nonincreasing under local operations and classical communication (LOCC), with a verifiable monogamy property [39,48,102]. The tangle quantifies the entanglement in a bipartition between mode i and the other $3N - 1$ modes in the system,

$$\tau_G(i) = \frac{1}{4} (\|\hat{\rho}^{T_i}\|_1 - 1)^2, \quad (6)$$

where $\hat{\rho}$ is a *pure* density matrix of a Gaussian state and $\hat{\rho}^{T_i}$ is the partial transpose with respect to the i th mode. From the CM framework, $\|\hat{\rho}^{T_i}\|_1 = \sqrt{\langle \hat{x}_i^2 \rangle \langle \hat{p}_i^2 \rangle} + \sqrt{\langle \hat{x}_i^2 \rangle \langle \hat{p}_i^2 \rangle} - 1$ [39,103].

The pairwise tangle, shared between modes i and j is denoted by $\tau_G(i:j)$. This is computable for a mixed state in terms of the convex roof construction. See SM [69] for a definition of $\tau_G(i:j)$ and Refs. [104,105] for further details. The monogamy inequality imposes a constraint on the sum of pairwise tangles, $\tau_G(i) \geq \sum_{j=1}^{3N} \tau_G(i:j)$, $\forall j \neq i$. The monogamy constraint arises from upper bounds on each pairwise tangle, $f(-\langle \hat{x}_i \hat{x}_j \rangle \langle \hat{p}_i \hat{p}_j \rangle) \geq \tau_G(i:j) \forall i \neq j$, where $f(x) = (\sqrt{x} + \sqrt{x+1} - 1)^2/4$ for $x > 0$ and $f(x) = 0$, given $x < 0$, [39]. If $\langle \hat{x}_i \hat{x}_j \rangle \langle \hat{p}_i \hat{p}_j \rangle > 0$, then $\tau_G(i:j) = 0$, due to the positive partial transpose (PPT) criterion [106,107].

Results—We study the entanglement and energy in terms of a dimensionless parameter $\rho = R/\alpha^{1/3}$, with

$R = \min_{\mu, \xi} R_{\mu\xi} \forall \mu \neq \xi$. In addition to ρ , the entanglement and energy depend on the geometry of the fixed equilibrium positions of the N QDOs. By using the simple cubic lattice as a reference frame, the authors in [57], estimated the region $2.3 \leq \rho \leq 3$, to be an interval of primary importance, for solids and liquids.

In the ground state of the two-mode Hamiltonian, $\hat{H}_{ij} = (1/2)(\hat{x}_i + \hat{x}_j + \hat{p}_i + \hat{p}_j) + \alpha \mathcal{T}_{ij} \hat{x}_i \hat{x}_j$, the inequalities on the pairwise tangle, described in the previous section, saturate. We shall label the pairwise tangle computed from the ground state of the *bipartite* Hamiltonian $\hat{H}_{ij}$ as $\tau_G^{\text{ref}}(i:j) = (\sqrt{\epsilon_+/\epsilon_-} - 1)^2/4$, with $\epsilon_{\pm} = \sqrt{1 \pm \alpha |\mathcal{T}_{ij}|}$ (see SM [69] for derivation). The reference tangle $\tau_G^{\text{ref}}(i:j)$ captures the entanglement shared between modes i and j , due to the dimensionless dipole bond $\alpha \mathcal{T}_{ij}$, as if all other modes were screened away. Conversely, in the ground state of the *multipartite* QDO Hamiltonian in Eq. (2), the upper bound on the pairwise tangle is written as $\tau_G^{\text{sys}}(i:j) = f(-\langle \hat{x}_i \hat{x}_j \rangle \langle \hat{p}_i \hat{p}_j \rangle)$, accounting for the indirect contributions and collective correlations present in the full ground state system, involving all $3N$ modes.

In order to numerically demonstrate the geometric and ρ dependence of the monogamy constraints on the pairwise tangle, contained within a given two QDO subsystem, we define the two QDO entanglement distribution index (EDI),

$$\delta_{\tau_G}^{\mu, \xi} = \frac{\sum_{i,j} \tau_G^{\text{sys}}(i:j)}{\sum_{i,j} \tau_G^{\text{ref}}(i:j)} \quad \forall i \in \mu, j \in \xi. \quad (7)$$

The EDI quantifies how monogamy constraints shape the entanglement distribution in a two QDO subsystem. For sufficiently weak interactions only the lowest two levels of each QDO can be occupied. The monogamy constraint can then limit the pairwise tangle leading to $\delta_{\tau_G}^{\mu, \xi} < 1$, reflecting the *monogamous* behavior of entanglement in qubit systems. For stronger interactions higher lying QDO levels may be occupied thus increasing the size of the accessible local Hilbert space and the overall amount of shareable entanglement. In this *promiscuous* regime $\delta_{\tau_G}^{\mu, \xi} > 1$ (for details see the simple three mode examples in SM [69]).

We consider three QDOs (trimer); see Fig. 1(a) for a depiction of the setup. We focus on the EDI between QDOs 1 and 2 in the trimer. By symmetry, this is identical to the subsystem of QDOs 2 and 3, highlighted by the two QDOs encircled by the dashed line within the three-QDO trimer in Fig. 1(a). Figure 1(b) shows that for the most acute trimer geometries, the monogamy constraint restricts nearest-neighbor pairwise entanglement sharing at weak interactions, but this restriction is lifted as the interaction strength increases.

Figure 1(c) shows that both the geometric and ρ dependence of the entanglement distribution directly correlates with the MB potential in the trimer. The parameter space of the trimer is partitioned into its promiscuous and

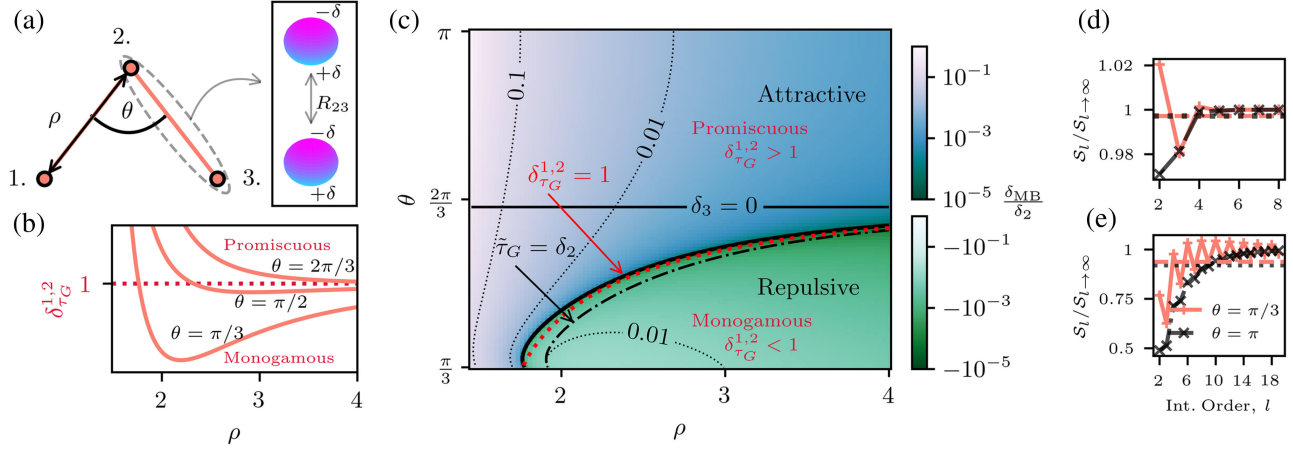


FIG. 1. (a) Depiction of the dipole interacting trimer setup. The correlated charge density fluctuations are shown by the instantaneous dipoles, denoted as $\pm\delta$. The coordinates of the three QDOs 1, 2, and 3 are $(0,0,0)$, $(R_{12} \sin[\theta/2], R_{12} \cos[\theta/2], 0)$ and $(2R_{12} \sin[\theta/2], 0, 0)$, where $\theta \in \{\pi/3, \pi\}$. The trimer depends on a dimensionless nearest neighbor separation ρ and geometry, θ . (b) Behavior of the nearest neighbor EDI, $\delta_{\tau_G}^{1,2}$, at different angles, with the dotted red line separating promiscuous and monogamous regions. (c) Above the red dotted line the sum of the pairwise tangle shared between the nearest neighbor QDOs behaves promiscuously, whereas below it behaves monogamously. The monogamy/promiscuity boundary overlaps the black line where MB energy corrections vanish and the pairwise additive approximation holds; above which MB corrections are attractive and below which they are repulsive; both shown as heat-maps, plotted on a log scale. In (d),(e), where $\rho = 2.60$ and $\rho = 1.55$ respectively, the crosses show S_l , where $S_l = \sum_{k=1}^l (k-1)\delta_k$, normalized by $S_{l \rightarrow \infty} = \sum_{k=1}^{\infty} (k-1)\delta_k$. The latter is computable from the CM matrix elements, (see SM [69] for calculation details). The dashed and dotted horizontal lines show the normalized value of the reduced tangle, i.e., $\tilde{\tau}_G/S_{l \rightarrow \infty}$ for the respective ρ and θ values (dashed line for $\pi/3$ and dotted line for π).

monogamous regions, separated by the dotted red line. The boundary between these two regions approximates the locus of points that separate the attractive and repulsive MB energies. For any $\rho \geq 2.3$, the deviation in θ between the two boundaries is less than 1.2% of the θ value where $\delta_{\text{MB}} = 0$. This correspondence becomes exact in the limit $\rho \rightarrow \infty$, where the boundary between the promiscuous and monogamous regimes asymptotically overlaps with the parameter space where the AT potential vanishes, i.e., $\delta_3 = 0$, indicated by the horizontal black line.

Next we substantiate our numerical findings by analytically relating measures of the ground state entanglement to the binding energy. We use the definition of the tangle to introduce the entanglement measure $\tilde{\tau}_G(i) = g(\tau_G(i))$, defined here as the reduced tangle, where $g(x) = x(1 + \sqrt{x})^2 / (1 + 2\sqrt{x})^2$. The function $g(x)$ is monotonically increasing for all positive x , ensuring the reduced tangle is an entanglement monotone under LOCC. We derive an inequality capturing the relation and dependence of pairwise and many-body contributions to the binding energy and the distribution of the reduced tangle as follows (see SM [69] for proofs),

$$\tilde{\tau}_G = \sum_{i=1}^{3N} \tilde{\tau}_G(i) \leq \sum_{k=2}^{\infty} (k-1)\delta_k. \quad (8)$$

Figures 1(d) and 1(e) show the convergence to the bound in Eq. (8) for different couplings strengths. Taking δ_2 away from both sides of Eq. (8), shows that $\tilde{\tau}_G - \delta_2 \leq$

$\sum_{k=3}^{\infty} (k-1)\delta_k$. Comparing this bound with the definition of the MB energy and the form of E in Eq. (3) explains the qualitative correspondence between the dashed-dotted black line in Fig. 1(c) and the sign of δ_{MB} , where the former divides the parameter space, into the regions where $\tilde{\tau}_G < \delta_2$ (below) and the regions where $\tilde{\tau}_G > \delta_2$.

The Gaussian state framework can be directly extended to arbitrary assemblies such as layered systems and 3D lattices, which we consider next. The features of the trimer, shown in Fig. 1(c), can be used to explain the sign of the MB contributions in the more complex lattices, shown in Fig. 2. At weak coupling, the sign of the MB effects are determined by the AT potential in the lattices. The AT potential can be written as a sum over triplets (trimers) of QDOs, (see SM [69]). The honeycomb lattice has a positive and negligible AT potential, following from where $\delta_3 = 0$ in Fig. 1(c), where the primitive translation vectors of the honeycomb lattice form an angle of $2\pi/3$. As the honeycomb lattice has a negligible AT potential, the MB effects in this lattice geometry only become visible through higher order terms. In Figs. 2(b)–2(d) and 2(h), where the AT potential is repulsive, a sign change occurs at strong coupling and the MB effects become attractive. The sign change also occurs in Fig. 1(c), as a function of ρ , for all geometries with repulsive AT corrections. Figures 2(a)–2(d) and 2(h) further show that $(\tilde{\tau}_G - \delta_2)/2 \approx \delta_{\text{MB}}$, on all the lattices at $\rho = 4$, indicated by the overlap of the solid and dashed dotted lines.

Figures 2(e)–2(g) display the EDI for nearest- and next-nearest-neighbor QDO pairs near the center of honeycomb,

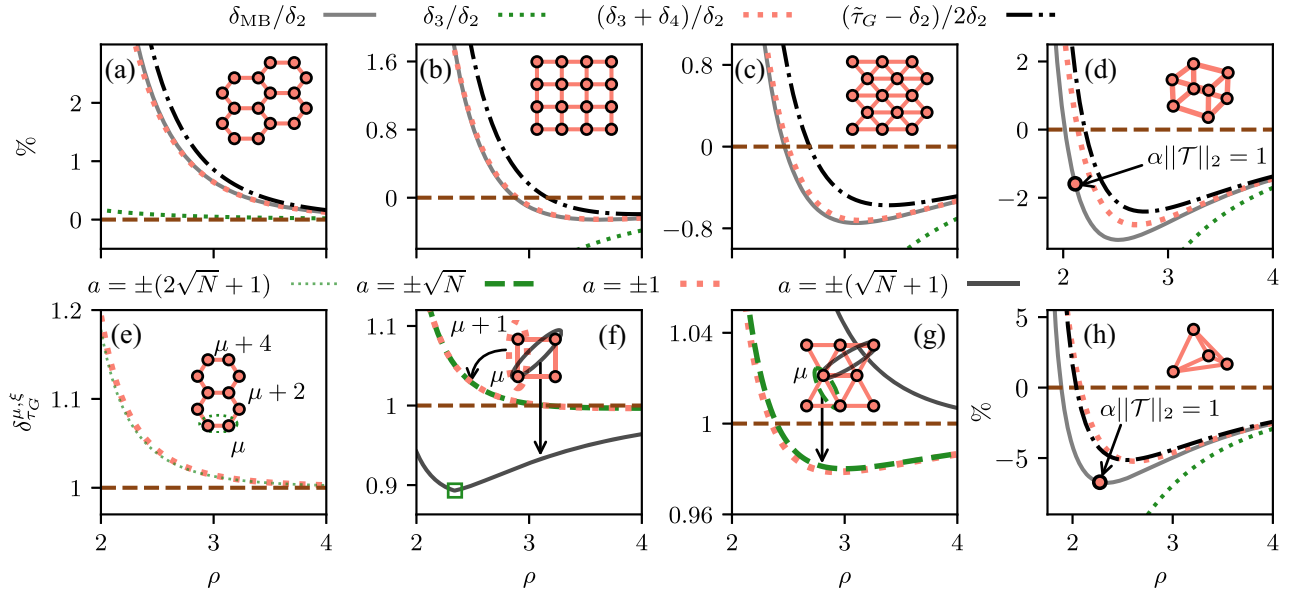


FIG. 2. Behavior of the MB effects and entanglement on various 2D and 3D lattices. In (a)–(d) and (h) the solid line shows the MB effects, the small green dotted line the AT correction, the large orange dotted line shows four-body corrections added to the AT potential, the dashed dotted line shows the deviation between the sum of the reduced tangle of each of the $3N$ modes and the pairwise bonding energy, $(\bar{\tau}_G - \delta_2)/2$, with the factor of $1/2$ included as $(\bar{\tau}_G - \delta_2)/2 \rightarrow \delta_3$ for $\rho \rightarrow \infty$. All the curves have been normalized by the pairwise bond energy and have been plotted as a function of the dimensionless nearest neighbor separation ρ . The following 2D lattices are shown: (a) $N = 47 \times 47 \times 2$ honeycomb lattice, (b) $N = 71 \times 71$ square lattice, (c) $N = 71 \times 71$ triangular lattice. The 3D lattices are (d) $N = 19 \times 19 \times 19$ cubic lattice and (h) $N = 4 \times 12 \times 12 \times 12$ pyrochlore lattice. All lattices calculations have been preformed with open boundary conditions. The EDI between μ and $\xi = \mu + a$ on the 2D lattices is shown in (e)–(g). The dashed horizontal line shows the monogamy/promiscuity boundary for the respective lattices, with the monogamous region lying below and the promiscuous region above. The ordering of the QDOs on the 2D lattices is shown in the insets in (e)–(g), where $\mu = 2256$ in (e), and $\mu = 2520$ in (f)–(g). The open green square in (f) shows where the PPT criterion ensures $\tau_G(3\mu:3\xi) = 0$.

square, and triangular lattices. In the honeycomb lattice, promiscuous entanglement sharing persists among its three nearest neighbors across all ρ values, reflecting its exclusively attractive MB potential. In contrast, the square and triangular lattices exhibit a transition from monogamous to promiscuous entanglement sharing as ρ decreases and the interaction strength increases. The deviation between the ρ value with average nearest neighbor EDI value equal to 1 and the ρ value at which the MB potential vanishes is 2.98% for the triangular lattice and 9.01% for the square lattice, relative to the ρ value where $\delta_{\text{MB}} = 0$. This suggests that the boundary between monogamous and promiscuous regions provides a good approximation for the ρ value at which the pairwise additive approximation holds on 2D lattices (see SM [69] for further evidence of EDI tracking the sign of the MB potential in the linear and zigzag chains).

Conclusion—We show that the many-body (MB) dispersive interaction energy is controlled, via an inequality, by an entanglement monotone defined in terms of a monogamous entanglement measure for Gaussian states. This constitutes, to the best of our knowledge, the first analytically rigorous relation between an entanglement measure and the significant contribution to the chemical correlation energy, due to dispersion.

We characterize the MB energetics through the monogamous or promiscuous behavior of entanglement distributions. Across a physically motivated parameter range, this classification accurately predicts the sign of many-body effects in the trimer. Our findings go beyond the Axilrod-Teller (AT) approximation, showing how AT predicts the wrong sign for the MB potential in the trimer. This may explain the failure of the AT potential to predict the attractive sign of the three-body effect in the parahydrogen trimer at short range, compared to high level quantum chemistry methods [108–111].

Arbitrary arrangements of N QDOs can be studied efficiently using our method, as extracting entanglement information only requires diagonalizing $3N \times 3N$ matrices, which scales as $\mathcal{O}(N^3)$. As this scaling is identical to that required for computing bond energies, existing approaches can be readily augmented with the entanglement metrics introduced here. Hence, while we have here focused on model systems, the same prescription, upon appropriate parameterization of the QDOs, can be extended to realistic materials. This would provide a direct link between their physical and chemical properties and the amount of entanglement shared by their constituents. Concepts from quantum information theory thus provide a novel path for shedding light on important chemical problems [112–119].

Acknowledgments—C. W. acknowledges helpful discussion with Lewis W. Anderson. Simulations were run on the University of Oxford Advanced Research Computing (ARC) facility. J. T. is grateful for ongoing support through the Flatiron Institute, a division of the Simons Foundation. D. J. acknowledges support by the European Unions Horizon Programme (HORIZON-CL42021-DIGITALEMERGING-02-10) Grant Agreement 101080085 QCFD, the Cluster of Excellence Advanced Imaging of Matter of the Deutsche Forschungsgemeinschaft (DFG)—EXC 2056—Project ID 390715994, and the Hamburg Quantum Computing Initiative (HQIC) project EFRE. The project is cofinanced by ERDF of the European Union and by Fonds of the Hamburg Ministry of Science, Research, Equalities and Districts (BWFG). C. W. acknowledges support from the Engineering and Physical Sciences Research Council and IBM.

Data availability—Code and data is freely available from the authors upon reasonable request.

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