

**Bose-Fermi mixtures of self-assembled filaments of fermionic polar molecules**

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Fermionic polar molecules in deep one-dimensional (1D) optical lattices may form self-assembled filaments when the electric dipoles are oriented along the lattice axis. These composites are bosons or fermions depending on the number of molecules per chain, leading to a peculiar and complex Bose-Fermi mixture, which we discuss in detail for the simplest case of a three-well potential. We show that the interplay among filament binding energy, transverse filament modes, and trimer Fermi energy leads to a rich variety of possible scenarios ranging from a degenerate Fermi gas of trimers to a binary mixture of two different types of bosonic dimers. We study the intriguing zero-temperature and finite-temperature physics of these composites for the particular case of an ideal filament gas loaded in 1D sites, and we discuss possible methods to probe these chain mixtures.

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**I. INTRODUCTION**

A new generation of experiments is starting to explore systems where the dipole-dipole interaction (DDI) plays a significant and possibly dominant role. Due to the long-range anisotropic character of the DDI, dipolar quantum gases offer a fascinating novel physics [1,2]. Exciting phenomena have been recently reported for experiments on Bose-Einstein condensates (BECs) of atomic magnetic dipoles, especially on chromium BEC [3], but also on spinor rubidium BECs [4], potassium [5], and lithium [6]. Magnetic atomic dipoles are however rather weak. In contrast, heteronuclear molecules, especially at their lowest rovibrational state, may present a very large electric dipole moment ( $\gtrsim 1$  Debye) [7–9]. Although quantum degeneracy has not been yet achieved, the rapid pace of development allows for expectation of degenerate gases of polar molecules in the near future. These gases are expected to be largely dominated by the DDI.

Deep one-dimensional (1D) optical lattices (formed by counterpropagating lasers) may slice a gas into nonoverlapping samples. For nondipolar (short-range interacting) particles, these nonoverlapping gases may be considered as independent parallel experiments. The situation is completely different in dipolar gases since the DDI leads to intersite interactions. For weak DDI (e.g., atomic magnetic dipoles), these intersite interactions lead to scattering between BECs at different sites [10], collective excitations shared by nonoverlapping sites [11], or damping of Bloch oscillations [5]. For bosonic polar molecules, the nonlocal dipolar effects may be much stronger, leading to fascinating effects such as pair-superfluidity for ladder-like lattices [12] and filament BEC [13].

Filamentation is indeed an interesting possibility introduced by the DDI. This phenomenon, first suggested in the context of ferrofluids by de Gennes and Pincus [14], has attracted a considerable theoretical interest for the case of classical dipoles [15]. Dipolar chains in classical ferrofluids were recently observed in superparamagnetic iron colloids [16] and single-domain magnetite colloids [17]. In Ref. [13], it was shown that a similar filamentation process may occur for bosonic polar molecules in deep lattices, which may organize into chains sustained by an attractive intersite DDI, forming a dipolar chains liquid (DCL) that may Bose-condense [13].

In this article, we consider DCLs of fermionic polar molecules. Far from being a trivial extension of the bosonic case, fermionic polar molecules lead to a very different and rich physics. Whereas for bosonic molecules the chains are obviously bosons, for fermionic molecules, the bosonic or fermionic character of the filaments depends on the number of molecules in the chain. This has particularly relevant consequences when the number of available lattice sites is odd. Here we focus on the simplest nontrivial case, namely a three-well potential (Fig. 1). For simplicity, we restrict our discussion to the ideal gas regime, where interfilament interactions are neglected. Although this approximation is of limited quantitative validity (and would demand mesoscopic samples in specific 1D arrangements as discussed in the following), it contains already many of the qualitatively new features that may be expected for more general scenarios of polar Fermi molecules in deep 1D and two-dimensional (2D) optical lattices. In particular, the competition between trimer or dimer binding and trimer Fermi energy results in a nontrivial dependence of the character of the DCL as a function of the number of molecules per site  $N$ . If  $N$  is smaller than a critical  $N_c$ , the DCL is a Fermi-degenerate gas of trimers. However, for  $N > N_c$ , the trimers coexist with a Bose mixture formed by pseudo-spin-1/2 dimers and spinless dimers, leading to a peculiar Bose-Fermi mixture. We show that these Bose-Fermi DCLs may be probed by monitoring the spatial distribution of the molecules.

The structure of the article is as follows. In Sec. II, we discuss the physics of individual filaments. Section III is devoted to the statistical properties of the chain gas. In Sec. IV, we discuss how the spatial distribution of molecules may provide important information concerning the nature of the filament gas. The finite-temperature physics is also significantly affected by the competition between bosonic and fermionic filaments, as shown in Sec. V. Finally, in Sec. VI, we comment on the validity of the ideal gas approximation and summarize our conclusions.

**II. SINGLE FILAMENTS OF FERMIONIC POLAR MOLECULES**

We consider fermionic polar molecules with mass  $m$  and electric dipole  $d$  in a deep three-well potential along

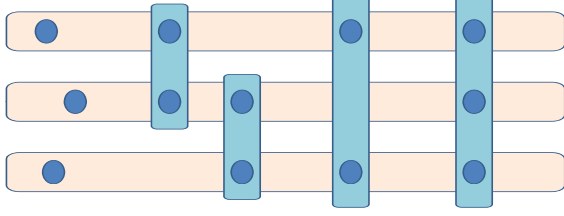


FIG. 1. (Color online) Polar fermionic molecules in a three-well potential may remain unpaired and form fermionic trimers or bosonic dimers between nearest neighbors or next-nearest neighbors.

the  $z$  direction, with intersite spacing  $\Delta$ . This arrangement may be created by, for example, selectively emptying all sites of a strong 1D optical lattice except three neighboring ones. The potential barriers are large enough to prevent any intersite hopping. Due to reasons discussed in the following, the analysis of the problem simplifies notably if the gas is considered as strongly confined along the  $y$  direction (e.g., in a single node of a lattice as that in the  $z$  direction). Along the remaining  $x$  direction, we consider a shallow harmonic confinement with frequency  $\omega$ . The molecules interact via the DDI  $V_d(\mathbf{r}) = d^2(1 - 3\cos^2\theta)/r^3$ , where  $\theta$  is the angle formed by  $\mathbf{r}$  with the dipole orientation. We assume that the dipoles form an angle  $\alpha$  with the  $z$  direction, such that  $\sin^2\alpha = 1/3$ . Although this particular orientation and the 1D character of the sites are not needed for the formation of the DCL gas, which may occur also in stacks of 2D sites [13], this particular scenario allows both for a strong attraction between dipoles placed on top of each other and for a vanishing DDI between molecules at the same site. This largely reduces the interfilament interaction, allowing for a simplified ideal gas scenario, as discussed in the following.

The attraction between polar molecules placed on top of each other may be strong enough to bind two or more polar molecules into self-assembled chains (Fig. 1). Whereas for bosonic molecules these chains are in any case bosons [13], for fermionic molecules, the fermionic or bosonic character of the filaments depends on the odd or even number of molecules in a given chain. In particular, the three-well configuration allows for fermionic trimers (and of course monomers), and two different kinds of bosonic dimers, namely those between two molecules at nearest neighbors (type I dimers), and those between two molecules at the highest and lowest site (type II dimers) (Fig. 1). Note that dimers I are actually pseudo-spin-1/2 bosons since dimers in sites 1 and 2 are not equivalent to dimers in sites 2 and 3.

The ground state of a single filament of  $M$  molecules is calculated as for bosonic molecules [13], and hence, we just sketch for completeness the basic ideas. Let  $\mathbf{r}_j$  ( $\hat{\mathbf{p}}_j$ ) be the position (momentum) operator of a molecule at site  $j$ . Introducing  $\hat{\mathbf{P}} = \sum_{j=1}^M \hat{\mathbf{p}}_j/M$ ,  $\mathbf{R} = \sum_{j=1}^M \mathbf{r}_j/M$ ,  $\mathbf{q}_j = \mathbf{p}_j - \mathbf{P}$ , and  $\mathbf{s}_j = \mathbf{r}_j - \mathbf{R} = \{x_j, y_j, z_j\}$ , the Hamiltonian splits into  $\hat{H} = \hat{H}_{\text{CM}} + \hat{H}_{\text{rel}}$ , where  $\hat{H}_{\text{CM}} = \hat{\mathbf{P}}^2/2Mm + Mm\omega^2 R_x^2/2$  describes the filament center-of-mass and

$$\hat{H}_{\text{rel}} = \sum_{j=1}^M \left\{ \frac{\hat{\mathbf{q}}_j^2}{2m} + \frac{m}{2} [\omega_{\perp}^2 (y^2 + z_j^2) + \omega^2 x^2] \right\} + \sum_{i,j>i} V_d[\mathbf{s}_i - \mathbf{s}_j] \quad (1)$$

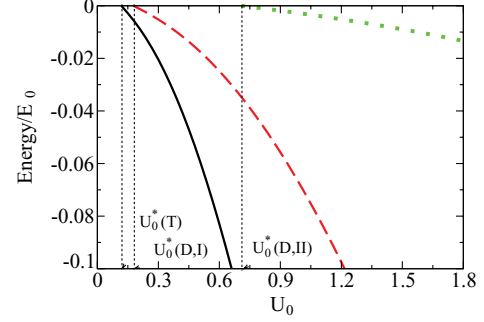


FIG. 2. (Color online) Binding energy (in units of  $E_0 = \hbar^2/m\Delta^2$ ) of the different composites of Fig. 1 as a function of  $U_0 = md^2/\hbar^2\Delta$ .

the relative motion. The on-site  $yz$  confinement is approximated by a strong isotropic harmonic oscillator of frequency  $\omega_{\perp}$ . The wave function of the  $j$ -th molecule is chosen as  $\psi_j(x_j - x_{j0})\varphi_j(y_j)\varphi_j(z_j - z_{j0})$ , where  $\varphi_j(\eta) = \exp(-\eta^2/2l_{\perp}^2)/\sqrt{l_{\perp}\sqrt{\pi}}$  and  $\psi_j(\eta) = \exp(-\eta^2/2R_0^2)/\sqrt{\sqrt{\pi}R_0}$ , with  $l_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$  and  $R_0$  is the variational width of the  $x$  wave packets. For deep lattices, one may approximate  $l_{\perp} \rightarrow 0$  (energy corrections are  $\lesssim 1\%$  for depths  $> 14$  recoil energies  $\hbar^2\pi^2/2m\Delta^2$ ).

Minimizing the energy of straight filaments ( $x_{j0} = 0$ ) with respect to  $R_0$ , we obtain the filament binding energy.<sup>1</sup> We denote as  $-E_T$ ,  $-E_{D,I}$ , and  $-E_{D,II}$  the binding energies for, respectively, trimers, dimers I, and dimers II. These energies grow with the dipole strength  $U_0 = md^2/\hbar^2\Delta$ . There exists a critical  $U_0^*$  such that for  $U_0 < U_0^*$  the composites unbind ( $R_0 \gtrsim l_{\text{HO}} = \sqrt{\hbar/m\omega}$ ). Note that  $U_0^*(T) < U_0^*(D, I) \ll U_0^*(D, II)$  (Fig. 2) due to the different strengths of the DDI in each composite. In the following, we consider the regime  $U_0 > U_0^*(D, II)$ , where  $R_0 \ll l_{\text{HO}}$  for all of the possible composites of Fig. 1.

Transverse filament excitations contribute to the gas entropy, which is relevant at finite temperature  $T$ . In addition, and in contrast to the case of bosonic molecules [13], transverse modes are important for fermionic molecules also at very low  $T$  since they may significantly reduce the trimer Fermi energy. For a chain of  $M$  molecules, we obtain the low-lying modes  $\xi_{v=1,\dots,M}$  after expanding the chain energy  $E$  around its minimum and diagonalizing  $\partial^2 E/\partial x_j \partial x_{j'}$ , where  $j, j' = 1, \dots, M$ .

### III. QUANTUM STATISTICS OF FILAMENTS

In the following, we consider the filament statistics, assuming an ideal filament gas. This largely simplifies the analysis of the problem, while allowing for the discussion of key qualitative features of these systems, in particular the competition between different Bose and Fermi composites. This approximation is just quantitatively valid for mesoscopic samples in the arrangement discussed earlier, as we discuss at the end of this article.

<sup>1</sup>For simplicity, we neglect that the minimal-energy configuration is slightly tilted from the vertical with an angle  $\sim \pi/10$ .

The fermionic or bosonic character of the chains is reflected by the average occupations for trimers, dimers I, dimers II, and monomers:

$$N_T(n, \nu_T) = \{e^{\beta[-E_T + \xi_{\nu_T} + \epsilon_n - (2\mu_1 + \mu_2)]} + 1\}^{-1}, \quad (2)$$

$$N_{D,I}(n, \nu_{D,I}) = \{e^{\beta[-E_{D,I} + \xi_{\nu_{D,I}} + \epsilon_n - (\mu_1 + \mu_2)]} - 1\}^{-1}, \quad (3)$$

$$N_{D,II}(n, \nu_{D,II}) = [e^{\beta(-E_{D,II} + \xi_{\nu_{D,II}} + \epsilon_n - 2\mu_1)} - 1]^{-1}, \quad (4)$$

$$N_{S,j}(n) = [e^{\beta(\epsilon_n - \mu_j)} + 1]^{-1}, \quad (5)$$

where  $N_{S,j}$  denotes the average occupation of individual molecules at site  $j$ ,  $\xi_{\nu_{T,D,I,D,II}}$  the transverse filaments modes of the different composites,  $\epsilon_n = \hbar\omega(n + 1/2)$  the harmonic oscillator levels, and  $\beta = 1/k_B T$  the inverse temperature. In the previous expressions, we have assumed symmetric configurations such that the number of dimers I in sites 1 and 2 is the same as the number of dimers I in sites 2 and 3 and is equal to  $N_{D,I}(n, \nu_{D,I})$ . Note that  $\mu_1 = \mu_3$  is the chemical potential for molecules at the highest and lowest sites, whereas  $\mu_2$  denotes the chemical potential for molecules in the middle site. These different chemical potentials are necessary to fulfill the normalization conditions, in which we assume  $N$  molecules per lattice site. By imposing symmetry between the highest and the lowest sites, these conditions acquire the form:

$$N = N_T + N_{D,I} + N_{D,II} + N_{S,1}, \quad (6)$$

$$N = N_T + 2N_{D,I} + N_{S,2}, \quad (7)$$

where  $N_T$ ,  $N_{D,I}$ ,  $N_{D,II}$ ,  $N_{S,1}$ , and  $N_{S,2}$  denote, respectively, the total number of trios, dimers I in sites 1 and 2 (or 2 and 3), dimers II, monomers in site 1 (or 3), and monomers in site 2. From (6) and (7), we obtain  $\mu_1(N, T)$  and  $\mu_2(N, T)$ , and from (2)–(5), we obtain the occupation numbers.

Due to the attractive DDI between molecules in the filament, the most bound chain is the trimer. The difference in binding between dimers and trimers induces that for sufficiently small  $N$ , and at low enough  $T$ , the DCL becomes a degenerate Fermi gas of trimers. The trimers fill up oscillator levels (and also transverse trimer modes) up to the corresponding Fermi energy  $E_F(N)$ , which equals  $N\hbar\omega$  for rigid filaments, but it is actually smaller due to the transverse trimer modes. However, if the number of molecules per site is sufficiently large, the growth

in Fermi energy overcomes the binding energy difference. This transition may be easily estimated by comparing the average energy per molecule for the case of two trimers and that for the case of two dimers I and one dimer II. This leads to a condition for the critical number of molecules per site  $N_c(U_0, \omega)$ ,  $E_F(N_c) = 2E_T - 3(E_{D,I} + E_{D,II})/2$  (which we have confirmed numerically). Note that  $N_c$  grows with growing  $U_0$  and decreasing  $\omega$ . For  $N < N_c$ , the DCL is a degenerate trimer gas, whereas for  $N > N_c$ , the trimer gas coexists with a mixture of pseudo-spin-1/2 bosons (dimers I) and spinless bosons (dimers II).

#### IV. SPATIAL DENSITY DISTRIBUTIONS

The peculiar properties of the DCL translate into the spatial molecular distribution integrated over the three sites. For  $N < N_c$  and  $N < \xi_{1T}/\omega$ , only trimers in their internal ground state are formed, and hence, the gas behaves as a spinless Fermi gas of particles of mass  $3m$ , presenting a Thomas-Fermi density profile  $[1 - (x/R)^2]^{1/2}$  with  $R/l_{HO} = \sqrt{2N/3}$ . For  $\xi_{1T}/\omega < N < N_c$ , the DCL is still a trimer gas, but transversal modes may be populated. In that case, the density profile departs from the Thomas-Fermi profile (Fig. 3, left), due to the appearance of internally excited trimers in low harmonic oscillator levels. For  $N > N_c$ , the density profile changes dramatically. Note that since we consider 1D gases, dimer BEC is, strictly speaking, precluded. However, due to the finite size, the dimers quasicondense (at low enough  $T$ ) occupying the few lowest levels of the harmonic oscillator. Hence, when  $N$  surpasses  $N_c$ , a Bose cloud nucleates at the trap center. As a result, the distribution of the polar molecules shows a Gaussian-like peak at the trap center (Fig. 3, right).

For  $N \gg N_c$  and  $U_0 > U_0^*(D, II)$ , the DCL is at low  $T$  a basically pure Bose gas of dimers I and II (except for a small trimer fraction). Since both dimers have mass  $2m$ , the difference between them cannot be discerned from the analysis of the integrated density profile of the molecules. However, the different binding energy and excited dimer modes for both types of dimers may be studied spectroscopically to reveal the dual nature of the mixture. If  $N \gg N_c$  but  $U_0^*(D, I) \ll U_0 < U_0^*(D, II)$ , dimers II are precluded, and hence, the DCL will become at low  $T$  a Bose-Fermi mixture of dimers I bosons

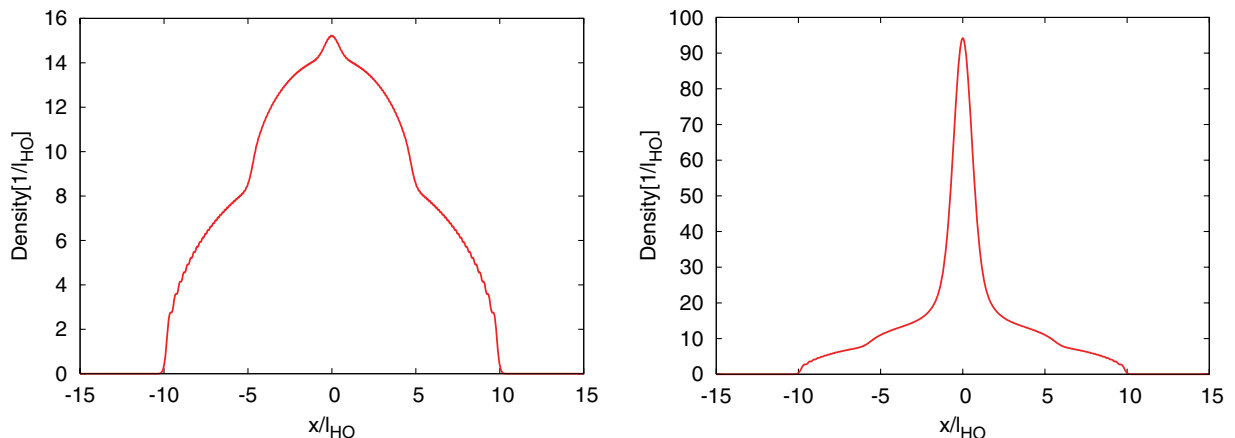


FIG. 3. (Color online) Integrated density profiles of the molecules, for units of  $\xi_{1T}/\omega < N < N_c$  (left) and  $N > N_c$  (right). We consider  $U_0 = 2$ ,  $\omega/2\pi = 1$  Hz, and  $m = 100$  amu, which lead to  $N_c = 230$ .

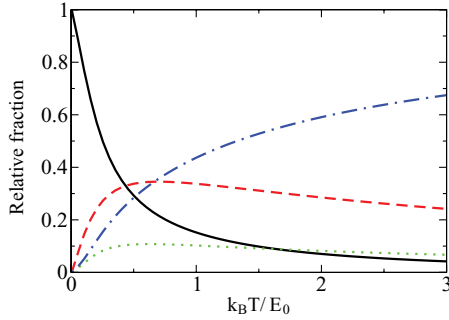


FIG. 4. (Color online) Temperature dependence of the fraction of molecules in trimers (solid), dimers I (dashed), dimers II (dotted), and monomers (dashed-dotted). We consider the parameters of Fig. 3 with  $N < N_c$ .

and degenerate monomers at sites 1 and 3 (which act as pseudo-spin-1/2 fermions). Again, this exotic mixture could be revealed from the corresponding dual-density profile.

### V. FINITE-TEMPERATURE ANALYSIS

The DCL presents as well an intriguing finite-temperature physics due to the role of filament modes and the different binding energy of dimers and trimers. This is particularly clear from a finite  $T$  analysis of a DCL with  $N < N_c$  (Fig. 4). Note that whereas at very low  $T$  the DCL is purely a trimer Fermi gas, at finite  $T$ , it becomes more favorable to populate dimers than to populate higher excited trimer states. As a consequence, the system presents a striking thermal enhancement of the bosonic modes. Interestingly, contrary to the standard situation, this leads to a maximal central peak density for a given finite  $T$ . For even larger  $T$ , the central density decreases again due to the occupation of dimers at higher oscillator modes and the breaking of the filaments into individual molecules.

### VI. CONCLUSIONS

The discussed ideal gas analysis allows for a relatively easy understanding of key qualitative features characterizing fermionic polar molecules in deep optical lattices under more general conditions, as the competition between filament-binding energy and Fermi energy of fermionic chains, the relevant role of the filament modes at zero and finite  $T$ , or the formation of peculiar mixtures of different types of composite bosons and fermions. However, the quantitative validity of the ideal gas approximation is rather limited (also

for bosonic molecules [13]), even for the previously discussed 1D arrangement with the particular choice for the dipole orientation. We may estimate the importance of the interfilament interactions by comparing the intertrimer interactions with the Fermi energy of rigid trimers ( $\epsilon_F = N\hbar\omega$ ). For deeply bound chains ( $R_0 \sim \Delta/2$ ) and at interfilament distances  $x > \Delta$ , we may approximate the interaction between molecules at different chains as that between two point dipoles. By adding up these interactions, we may estimate the mean intertrimer DDI  $V_{ff}(\bar{x})$ , where  $\bar{x}$  is the mean intertrimer distance. For the case of  $d = 0.8$  Debye,  $m = 100$  amu,  $\Delta = 0.5 \mu\text{m}$ , and  $\omega/2\pi = 1$  Hz, we obtain  $U_0 \simeq 2$  and  $N_c \simeq 230$ . For this value,  $\bar{x} \simeq 1.7\Delta$  and  $V_{ff} \simeq 0.33\epsilon_F$ . The ideal gas approximation is hence quantitatively valid only for dilute mesoscopic samples (as those considered in our numerical calculations). Once the dimer Bose gas nucleates at the trap center, the ideal gas condition is quickly violated, due to the larger bosonic densities, although the formation of the dual-density profile (similar to that in Fig. 3) still holds. For stacks of 2D sites, the ideal gas approximation fails even for extremely low 2D densities. However, the formation of dimer mixtures beyond a given critical density should also occur for 2D arrangements. These mixtures may be considered weakly interacting for 2D densities  $n$  such that  $nr_*^2 < 1$  with  $r_* = md^2/\hbar^2$ . For the previous values, this demands  $n \lesssim 1.1 \times 10^8 \text{ cm}^{-2}$ . For  $N \gg N_c$  [and  $U_0 > U_0^*(D, II)$ ], weakly interacting dimers will form a BEC of three different bosons (dimers I in sites 1 and 2, I in sites 2 and 3, and II), whose properties (e.g., miscibility versus phase separation) will largely depend on the precise determination of the different interdimer interactions, which will be the subject of a future work.

In conclusion, fermionic polar molecules in three-well potentials are expected to form a rather peculiar filament gas. Depending on the filling per site and the interaction strength, we expect that the character of the chain gas ranges from a pure trimer gas at low fillings to a bosonic mixture of pseudo-spin-1/2 and spinless dimers for large enough fillings and dipole strengths. Note, finally, that molecules in an even larger number of sites may form a quantum gas mixture of increasing complexity. Dipolar chain liquids are, hence, an exciting perspective for ongoing experiments with polar fermionic molecules.

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