SUPPLEMENTAL MATERIAL: ULTRADILUTE LOW-DIMENSIONAL LIQUIDS

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The diffusion Monte Carlo (DMC) technique provides the exact ground-state energy when (*i*) the simulation time goes to infinity, (*ii*) time step goes to zero, and (*iii*) population size goes to infinity. Deviations from these limits introduce statistical and systematic errors which we control and minimize according to a given accuracy goal. The convergence towards limits (*i*)-(*iii*) depends on the choice of the guiding wave function which we discuss in Sec. I. The statistical error is reduced by making the simulation series large enough (the statistical error comes from a finite simulation time and is estimated by a standard block-averaging procedure). As for the systematic errors, to improve the convergence we use a quadratic time step algorithm with time step $\Delta t = 0.01$ in units where the mass m, mean interparticle separation $n^{-1/d}$, and $\hbar$ are equal to 1. We have verified that the diffusion algorithm without branching for this time step recovers the variational energy within the accuracy goal. All simulations have been performed with the population size of 1000 walkers which we find to be sufficient. The calculations are done in a box with periodic boundary conditions for various particle numbers and we extrapolate the result to the thermodynamic limit. This procedure is well controlled since we know the finite-size correction in the Bogoliubov approximation (see Sec. II). In the two-dimensional case we choose sufficiently short-range interaction potentials in order to claim that the results are valid in the zero-range limit (see Sec. III). In one dimension we work directly with zero-range potentials.

I. GUIDING WAVE FUNCTION

We chose the guiding wave function in the pair-product form

$$\Psi_T(\mathbf{r}_1^{\uparrow},\cdots,\mathbf{r}_{N_\uparrow}^{\uparrow},\mathbf{r}_1^{\downarrow},\cdots,\mathbf{r}_{N_\downarrow}^{\downarrow}) = \prod_{i<j}^{N_\uparrow} f_{\uparrow\uparrow}(|\mathbf{r}_i^{\uparrow}-\mathbf{r}_j^{\uparrow}|)\prod_{i<j}^{N_\downarrow} f_{\downarrow\downarrow}(|\mathbf{r}_i^{\downarrow}-\mathbf{r}_j^{\downarrow}|)\prod_{i=1}^{N_\uparrow}\prod_{j=1}^{N_\downarrow} f_{\uparrow\downarrow}(|\mathbf{r}_i^{\uparrow}-\mathbf{r}_j^{\downarrow}|) \tag{1}$$

and seek to incorporate as much physical information into the Jastrow terms $f_{\sigma\sigma'}(r)$ as possible. Reatto and Chester[1] showed by using hydrodynamic approach that the "phononic" long-range part of a single component many-body wave function $\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_N)$ can be written in a Jastrow pair-product form

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_N) = \exp\left[-\frac{1}{2}\sum_{i<j}\chi(|\mathbf{r}_i-\mathbf{r}_j|)\right], \tag{2}$$

where asymptotic long-range decay is $\chi(r) = mc/(\pi^2 n\hbar r^2) \propto 1/r^2$ in three dimensions and $\chi(r) \propto 1/r$ in two dimensions. Here n is the density and c is the speed of sound, corresponding to the long-wavelength phonons. We chose a form similar to that of Eq. (2) for describing the long-range part of $f_{\sigma\sigma'}(r)$ in (1).

When two particles come close to each other, the dominant physical process is the scattering between those two particles. We chose the short range part of $f_{\sigma\sigma'}(r)$ as a solution of the two-body scattering problem for the corresponding interaction potential $U_{\sigma\sigma'}(r)$.

A. Two dimensions

In the two-dimensional case, the intraspecies interactions are modelled by soft disks (SD)

$$U_{\uparrow\uparrow}(r) = U_{\downarrow\downarrow}(r) = \begin{cases} U_0^{SD}, & \text{if } r \le R_0 \\ 0, & \text{otherwise} \end{cases} \tag{3}$$

and the interspecies interactions by square wells (SW)

$$U_{\uparrow\downarrow}(r) = \begin{cases} -U_0^{SW}, & \text{if } r \le R_0 \\ 0, & \text{otherwise} \end{cases} \tag{4}$$

with the same range R_0. The height $U_0^{SD} > 0$ of the soft disk and the depth $U_0^{SW} > 0$ of the square well are adjusted in order to obtain the desired values of the s-wave scattering length $a_{\sigma\sigma'}$. We also considered hard disks

(HD), obtained from soft disks in the limit of an infinite height of the interaction potential $U_0^{SD} \to \infty$, in which the s-wave scattering length a corresponds to the diameter of the hard disk, $a = R_0$.

The following Jastrow terms are used in two dimensions:

- for the soft-disk potential

$$f_{\uparrow\uparrow}^{SD}(r) = f_{\downarrow\downarrow}^{SD}(r) = \begin{cases} AI_0(\kappa r), & \text{if } r \le R_0 \\ B\ln(r/a), & \text{if } R_0 < r \le R_{par} \\ C\exp(-D/r + E/r^2), & \text{if } R_{par} < r \le L/2 \\ 1, & \text{if } r > L/2 \end{cases} \tag{5}$$

- for the hard-disk potential

$$f_{\uparrow\uparrow}^{HD}(r) = f_{\downarrow\downarrow}^{HD}(r) = \begin{cases} 0, & \text{if } r \le R_0 \\ A\ln(r/a), & \text{if } R_0 < r \le R_{par} \\ B\exp(-C/r + D/r^2), & \text{if } R_{par} < r \le L/2 \\ 1, & \text{if } r > L/2 \end{cases} \tag{6}$$

- for the square-well potential

$$f_{\uparrow\downarrow}^{SW}(r) = \begin{cases} AJ_0(\kappa^{\uparrow\downarrow} r), & \text{if } r \le R_0 \\ B\ln(r/a_{\uparrow\downarrow}), & \text{if } R_0 < r \le R_{par}^{\uparrow\downarrow} \\ C\exp(-D/r + E/r^2), & \text{if } R_{par}^{\uparrow\downarrow} < r \le L/2 \\ 1, & \text{if } r > L/2 \end{cases} \tag{7}$$

Here, $I_0(r)$ and $J_0(r)$ are modified Bessel function of the first kind. The characteristic momenta κ and $\kappa^{\uparrow\downarrow}$ are defined by the height (depth) of the interaction potential according to $\kappa = \sqrt{mU_0^{SD}}/\hbar$ and $\kappa^{\uparrow\downarrow} = \sqrt{mU_0^{SW}}/\hbar$. The short-range part, $r < R_{par}$ and $r < R_{par}^{\uparrow\downarrow}$, corresponds to the zero-energy scattering solution on interaction potentials (3) and (4). The long-range part, $r > R_{par}$ and $r > R_{par}^{\uparrow\downarrow}$, has the phononic asymptotic (2). Coefficients A, B, C, D, E are fixed by the conditions of the continuity of the function itself, $f(r)$, its first derivative, $f'(r)$, and by the periodic boundary conditions which are satisfied by imposing zero derivative at the half size of the box, $f'(L/2) = 0$. The variational parameters R_{par} and $R_{par}^{\uparrow\downarrow}$ are optimized by minimizing the variational energy. For the repulsive interactions (SD and HD), parameter R_{par} corresponds to the matching distance between the two-body scattering and the phononic regimes. For attractive SW interaction, parameter $R_{par}^{\uparrow\downarrow}$ effectively changes the value of $f(r = 0)$ and physically describes how strongly is localized a pair of two particles in the many-body system.

B. One dimension

In the one-dimensional case we perform simulations directly for the δ-pseudopotential [2] thus avoiding any finite-range bias. This can be done by imposing Bethe-Peierls boundary condition on the many-body wave function

$$\frac{d}{dr}[f^{\sigma\sigma'}(r)]_{r=0} = -\frac{1}{a_{\sigma\sigma'}}[f^{\sigma\sigma'}(r)]_{r=0}. \tag{8}$$

The δ-pseudopotential acts only at the contact point, $|r| = 0$, while for any finite separation between two particles a good choice for the short-range part of the Jastrow terms is a plane wave (repulsive interaction) or a decaying exponent (attractive interaction).

We take the long-range part of Jastrow terms from the hydrodynamic expression, Eq. (2). The presence of phonons in 1D induce slowly-decaying quantum correlations[1] between particles, $\chi(r) = -(2/K_L)\ln[\sin|\pi r/L|]$, where $K_L = \pi\hbar n/(mc)$ is the Luttinger parameter. As a result, instead of exponential Jastrow terms in higher dimensions, here the decay is instead of a power-law type, $f(r) = |\sin|\pi r/L||^{1/K_L}$.

The following Jastrow terms are used in two dimensions:

- for the repulsive intraspecies δ-pseudopotenial

$$f_{\uparrow\uparrow}(r) = f_{\downarrow\downarrow}(r) = \begin{cases} A\cos(k|r - B|), & \text{if } |r| \le R_{par} \\ |\sin(|\pi r/L|)|^{1/K_{par}}, & \text{if } R_{par} < |r| \le L/2 \\ 1, & \text{if } |r| > L/2 \end{cases} \tag{9}$$

- for the attractive interspecies δ-pseudopotenial

$$f_{\uparrow\downarrow}(r) = \begin{cases} A\exp(-|r|/a_{\uparrow\downarrow}), & \text{if } |r| \le R_{par}^{\uparrow\downarrow} \\ |\sin(\pi|r|/L)|^{1/K_{par}^{\uparrow\downarrow}}, & \text{if } R_{par}^{\uparrow\downarrow} < |r| \le L/2 \\ 1, & \text{if } |r| > L/2 \end{cases} \tag{10}$$

where coefficient A is chosen according to the continuity condition at the matching point. Periodic boundary conditions are automatically satisfied by using hydrodynamic/Luttinger-liquid tails. Coefficients R_{par}, $R_{par}^{\uparrow\downarrow}$, K_{par} and , $K_{par}^{\uparrow\downarrow}$ are optimized by minimizing the variational energy. We note that the exponential short-range part in Eq. (10) reminds the exact wave function by McGuire for an attractive single-component Bose gas.

II. FINITE-SIZE EFFECTS

As stated in the main text, the ground-state energy in the Bogoliubov approximation is given by

$$E = \frac{1}{2}\sum_{\sigma\sigma'} g_{\sigma\sigma'} n_\sigma n_{\sigma'} + \frac{1}{2}\sum_{\pm}\sum_{|\mathbf{k}|<\kappa} [E_\pm(k) - k^2/2 - c_\pm^2] \, . \tag{11}$$

In a box of size L^d with periodic boundary conditions the summation is performed over momenta $\mathbf{k} = 2\pi\mathbf{n}/L$, where vector $\mathbf{n}$ is a list of d integers. In the thermodynamic limit we replace the summation over $\mathbf{k}$ by integration. The finite-size correction originates from the discrete character of the lowest Bogoliubov modes and scales as a power of the ratio ξ/L, where $\xi = 1/c_+$ is the healing length corresponding to the Bogoliubov + mode.

A. Two dimensions

The ground-state energy density of the two-dimensional mixture with $a_{\uparrow\uparrow} = a_{\downarrow\downarrow} = a$ and $n_\uparrow = n_\downarrow = n$ including the leading-order finite-size correction reads

$$E_{2\mathrm{D}} = \frac{8\pi n^2}{\ln^2(a_{\uparrow\downarrow}/a)}[\ln(n/n_0) - 1] + C\sqrt{\frac{2\pi}{\ln(a_{\uparrow\downarrow}/a)}}\frac{n^2}{N^{3/2}} \, , \tag{12}$$

where

$$C = 2\pi \lim_{\alpha\to 0}\left[\sum_{m,n}\sqrt{m^2+n^2}e^{-\alpha(m^2+n^2)} - \int |k| e^{-\alpha k^2} d^2k\right] \approx -1.438. \tag{13}$$

Figure 1 shows the energy per particle calculated for finite N by using the DMC method (symbols) and the analytical result Eq. (12) (solid lines) for $1/\ln(a_{\uparrow\downarrow}/a) = 0.01$. The relative deviation of finite-N curves from the thermodynamic limit (dashed line) scales as $[\ln(a_{\uparrow\downarrow}/a)/N]^{3/2} \propto (\xi/L)^3$ and, for larger $1/\ln(a_{\uparrow\downarrow}/a)$, we need less atoms to reach the thermodynamic limit (within a given accuracy goal). Results presented in the main text are the extrapolation to this limit.

B. One dimension

In one dimension the ground-state energy density for the symmetric mixture ($g = g_{\uparrow\uparrow} = g_{\downarrow\downarrow}$ and $n = n_\uparrow = n_\downarrow$) including the leading finite-size correction reads

$$E_{1\mathrm{D}} = \delta g n^2 - \frac{4\sqrt{2}}{3\pi}(gn)^{3/2} - \frac{\pi}{3\sqrt{2}}\frac{\sqrt{g}n^{5/2}}{N^2} \, , \tag{14}$$

where the finite-size correction term is obtained by applying the Euler-Maclaurin formula to the one-dimensional sum over momenta in Eq. (11). Figure 2 shows the dependence of the energy per particle for various N calculated by the DMC method (symbols) and by the Bogoliubov theory Eq. (14) (solid lines) in the case $\delta g/g = 0.05$. The relative deviation from the thermodynamic result (dashed line) scales as $(N\delta g/g)^{-2} \propto (\xi/L)^2$. Our DMC results reported in the main text are the extrapolation to $N \to \infty$.

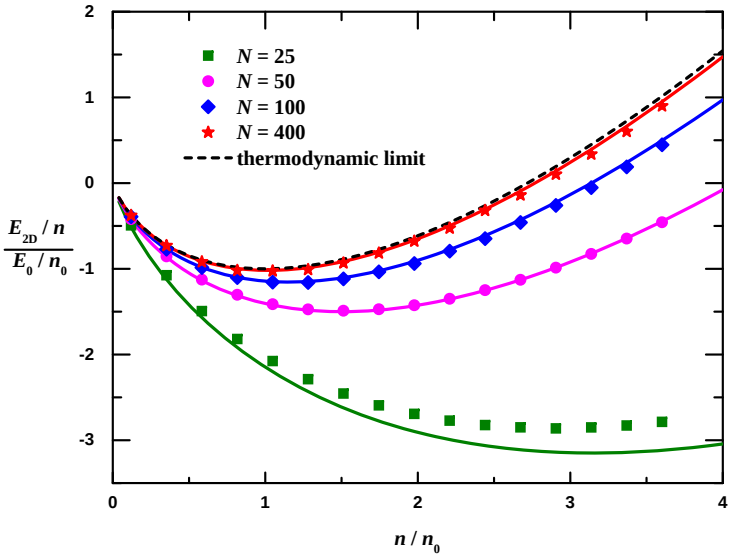

Figure 1: The energy per particle $E_{2D}/2n$ versus n for the two-dimensional mixture with $a_{\uparrow\uparrow} = a_{\downarrow\downarrow} = a$ and $n_\uparrow = n_\downarrow = n$ with $1/\ln(a_{\uparrow\downarrow}/a) = 0.01$ in a box with periodic boundary conditions for particle numbers in each component equal to $N = 25$ (green squares), 50 (pink circles), 100 (blue diamonds), and 400 (red stars). Solid curves are predictions of the Bogoliubov theory with the leading-order finite-size correction, Eq. (12). Dashed line is the Bogoliubov result in the thermodynamic limit.

III. FINITE-RANGE EFFECTS

In order to study the dependence of the energy on the interaction range we perform calculations of the symmetric two-dimensional mixture with soft-disk repulsive intraspecies and square-well attractive interspecies interaction potentials of variable range R_0 but for fixed scattering lengths. Figure 3 shows the energy per particle at the density $n = n_0$ as a function of R_0 for $1/\ln(a_{\uparrow\downarrow}/a) = 0.2$ (red circles), 0.1 (blue squares), and 0.05 (green diamonds). Solid lines in Fig. 3 are obtained by fitting the data with the empirical expression $E(R_0) = E[1 + AnR_0^2 \ln(Bn^{1/2}R_0)]$, where A and B are fitting parameters. Note that the Bogoliubov zero-range theory prediction is recovered for $1/\ln(a_{\uparrow\downarrow}/a) \to 0$ even for fixed $n^{1/2}R_0$. Results presented in the main text are obtained for $nR_0^2 = 5 \times 10^{-3}$, their difference from the zero-range asymptotic value is comparable to the symbol size. In one dimension both analytical and numerical approaches use contact δ-function potential.

[1] L. Reatto and G. V. Chester, "Phonons and the Properties of a Bose System", Phys. Rev. **155**, 88 (1967).
[2] G. E. Astrakharchik and S. Giorgini, "Correlation functions and momentum distribution of one-dimensional Bose systems", Phys. Rev. A **68**, 031602 (2003).

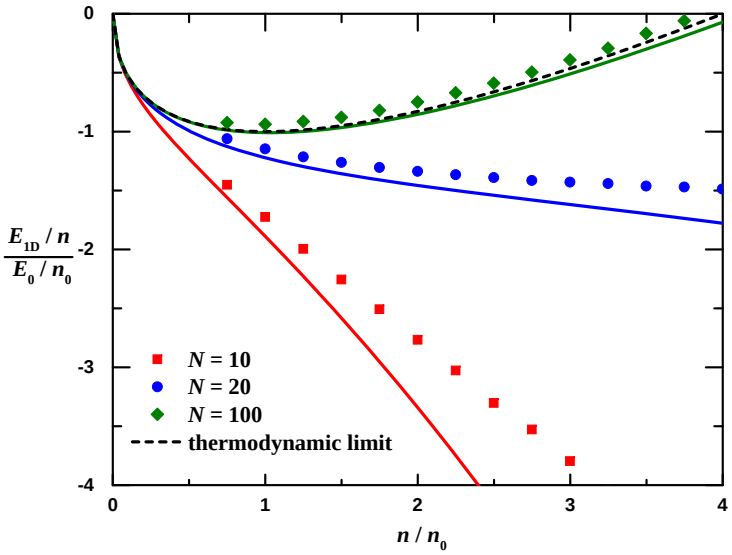

Figure 2: The energy per particle $E_{1D}/2n$ versus density n for the symmetric one-dimensional mixture with delta-function interactions and $\delta g/g = 0.05$ in a box with periodic boundary conditions with particle numbers in each component equal to $N = 10$ (red squares), 20 (blue circles), and 100 (green diamonds). Solid lines correspond to the Bogoliubov theory prediction with the leading-order finite-size correction, Eq. (14), which can be rewritten as $(E/n)/(E_0/n_0) = n/n_0 - 2\sqrt{n/n_0} - (2/9)(n/n_0)^{3/2}(g/N\delta g)^2$. Dashed curve is the Bogoliubov theory prediction in the thermodynamic limit.

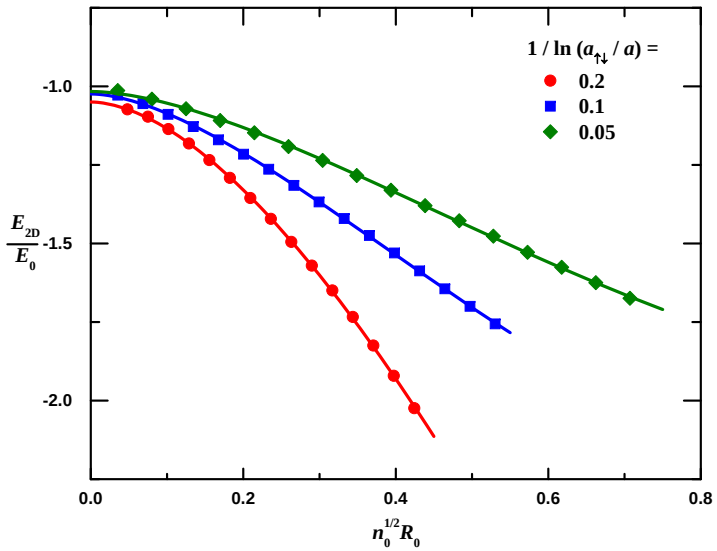

Figure 3: The energy per particle $E_{2D}/2n$ versus potential range R_0 for the symmetric two-dimensional mixture at $n = n_0$.