Comment on "Absence of Off-Diagonal Long-Range Order in hcp ^{4}He Dislocation Cores"

In a recent Letter [1], de Koning *et al.* report results of first-principle computer simulations of bulk solid (hcp) ^{4}He, in the presence of a single dislocation (various types thereof are considered). The calculation, carried out at zero temperature, shows that the one-body density matrix (OBDM), *averaged over the whole system*, decays in the same fashion as in a perfect crystal. This is interpreted as the absence of off-diagonal long-range order, and therefore of superfluidity inside the dislocation core. According to the authors, these results are inconsistent with the superfluid dislocation network scenario [2] and invalidate the superclimb mechanism [3], which was further expounded in Refs. [4,5] as the explanation for the unique features of the superflow through solid ^{4}He effect [6–8].

In this Comment, we contend that the results of de Koning *et al.* do not support this conclusion, nor are they inconsistent in any way with the results and predictions of Refs. [2–5]. We explain the origin of the apparent controversy and how to resolve it. Specifically, the OBDM, defined as

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \langle \hat{\Psi}^\dagger(\mathbf{r}_2)\hat{\Psi}(\mathbf{r}_1)\rangle, \tag{1}$$

where $\hat{\Psi}$, $\hat{\Psi}^\dagger$ are the Bose field operators and $\langle \ldots \rangle$ stands for (ground state) expectation value, is a function of both the relative distance $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ *and* the center-of-mass position $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$. Superfluidity (or absence thereof) in the dislocation core is revealed through the slow power-law decay of ρ as a function of $r = |\mathbf{r}|$ when *both* $\mathbf{r}_2$ and $\mathbf{r}_1$ are located *inside* the core.

If $\mathbf{r}_1$, $\mathbf{r}_2$ are allowed to be *anywhere*, not just inside the core, one is mainly probing the properties of the insulating crystal (i.e., outside the core), and the dislocation signal can easily remain undetectable within the error bars. But this is exactly what is done in the calculation of de Koning *et al.*, i.e., $\rho(\mathbf{r}_1, \mathbf{r}_2)$ is averaged over the entire system for a given r, ostensibly on the assumption that a superfluid response confined to the core of the dislocation should give rise to a finite bulk condensate fraction n_0.

Aside from the fact that Bose condensation and superfluidity are distinct concepts (the absence of the former not implying that of the latter), averaging over the whole crystal, i.e., ignoring the crucial fact that the dislocation contribution to $\rho(\mathbf{r}_1, \mathbf{r}_2)$ is highly nonuniform and anisotropic function of $\mathbf{R}$ and $\mathbf{r}$, leads to an enormous suppression of n_0, $\sim 1/L^4$, where L is the linear size of the simulated sample in units of the interparticle distance. Thus, not only does $n_0 \to 0$ in the thermodynamic limit, in a system whose linear size L exceeds ten times the interparticle distance the numerical estimate of n_0 is guaranteed to be smaller than that of liquid ^{4}He at the solidification pressure by a factor greater than 10^4; the data shown in Fig. 2(b) are *entirely* consistent with such behavior ($10^{-2} \times 10^{-4} = 10^{-6}$). Generally speaking, it is not possible to extract any information about the existence of a finite, quasi-one-dimensional superfluid response from the bulk condensate fraction, rendering the criticism of our Letter by de Koning *et al.* unfounded.

Furthermore, it needs to be emphasized that, in a finite sample, boundary effects, strain fields, and pressure gradients are unavoidable. All these shift the phase diagram of finite samples. As argued in Ref. [5], it is then important to count the local density from the shifted melting density in the simulation cell because both numerically and experimentally the window for superfluidity is very narrow [8]. An enhanced local pressure at the dislocation core in ^{4}He suppresses its superfluid response—dramatically or completely. Since dislocation contribution to bulk-averaged OBDM at interatomic distance is negligible, the data of de Koning *et al.* [Fig. 2(b)] clearly demonstrate that samples with CS and CE dislocations are at elevated bulk pressure—the corresponding OBDMs are suppressed in comparison with the one for the ideal crystal. This renders their ultimate conclusion about the state of dislocation cores—based on comparison with ideal crystals at a lower pressure—unjustified.

Even in the putative absence of local overpressure, the treatment of exchange cycles by de Koning *et al.* remains insufficient. They find, by visual inspection of snapshots, no long exchange cycles. Here it is important to emphasize that (i) one has to study statistics of exchange cycles in the dislocation cores (individual snapshots are not representative given that even in the liquid at freezing density the condensate fraction is only about 1%) and (ii) there is a fundamental difference between measuring exchange cycles and OBDM in the path-integral ground state. While the OBDM is a property of the ground-state wave function, the statistics of exchange cycles is a property of the imaginary-time evolution operator $e^{-\tau H}$ in the path-integral representation. Correspondingly, the projection time τ for the OBDM can be arbitrarily short—depending on the quality of the trial wave function. But to start seeing long exchange cycles, having an appropriately long τ is imperative, even when the trial wave function is the exact ground state. Furthermore, in *one-dimensional* superfluids, macroscopic exchange cycles appear only when the projection time is macroscopically large, $\tau \propto L$.

In principle, finite-T path integral schemes and $T = 0$ projection methods such as path-integral ground state are exact and should give consistent results for the same Hamiltonian. It is important to compute the one-dimensional dislocation OBDM and statistics of exchange cycles in the core for identically prepared samples by both methods. Only then one can establish whether the ground state properties starting from a (nonorthogonal) trial wave function have been reached.

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