The superfluid density in continuous and discrete spaces:
Avoiding misconceptions

V.G. Rousseau

1Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA

We review the concept of superfluidity and, based on real and thought experiments, we use the formalism of second quantization to derive expressions that allow the calculation of the superfluid density for general Hamiltonians with path-integral methods. It is well known that the superfluid density can be related to the response of the free energy to a boundary phase-twist, or to the fluctuations of the winding number. However, we show that this is true only for a particular class of Hamiltonians. In order to treat all other classes, we derive a general expression of the superfluid density that is valid for any Hamiltonian, including Hamiltonians that do not conserve the number of particles and multi-species Hamiltonians. While the winding number is undefined when the number of particles is not conserved, our general expression allows us to calculate the superfluid density in all cases, as well as the superfluid densities associated to the individual components of multi-species Hamiltonians. The cases of continuous space and discrete space are considered, and we emphasize common mistakes that occur when considering lattices with non-orthonormal primitive vectors.

PACS numbers: 02.70.Uu, 05.30.Fk, 05.30.Jp, 47.37.+q, 67.25.D-, 67.25.dm

I. INTRODUCTION

Superfluidity is a manifestation of quantum mechanics at the macroscopic level, and its discovery is usually attributed to Kapitza, and Allen and Misener. While superfluidity is widely discussed in the literature, many references quantify this phenomenon by postulating formulae, or by making semi-empirical derivations. This induces some misconceptions about superfluidity that can lead to mistakes.

The aim of the present paper is first to give a definition of the superfluid density that is based on known experiments. Then, some expressions of the normal and the superfluid densities that can be used with path-integral methods are rigorously derived from a thought experiment by using the formalism of second quantization. We show that, for a particular class of Hamiltonians, the superfluid density is directly related to the response of the free energy to a boundary phase-twist. While many references improperly use this relation as a general definition of the superfluid density, we clearly state the condition that the Hamiltonian must meet for such a definition to be meaningful. We also derive how the free energy is related to the winding number, and recover the expression that was obtained earlier in the context of first quantization. A drawback associated to the winding number is that it is undefined for Hamiltonians that do not conserve the number of particles. This problem is common when considering systems with several species of particles where conversions between the different species occur, and results in the impossibility to calculate the superfluid densities of the individual species. However, our general expression of the superfluid density does not rely on the concept of the winding number, and can be used to determine the superfluid densities of all the species, whether their populations are conserved or not (see paragraph C for a concrete example).

The case of lattice Hamiltonians is considered by making a careful discretization of space. We point to some common mistakes that occur when considering lattices with non-orthonormal primitive vectors. In particular, we show that using the expression of the Laplacian in the natural coordinates of the lattice requires a change of the energy scale that must be reflected in the expression of the superfluid density. Also, the metric tensor associated to the natural basis of the lattice must be taken into account when calculating quantities that involve dot-products, such as the fluctuations of the winding number.

As an illustration, in addition to the usual expression of the superfluid density for the d-dimensional cubic lattice, we provide the correct expressions for the triangular, face-centered cubic, honeycomb, kagome, and pyrochlore lattices. Finally, we give two examples of Hamiltonians for which the well-known expressions of the superfluid density are not applicable. We determine the correct superfluid density by using our general expression, and we show that our results are consistent.

II. EXPERIMENTAL EVIDENCES OF SUPERFLUIDITY

As suggested by Legget, it is useful to consider two experiments that demonstrate fundamental defining properties of a superfluid (Fig. 1):

- A torus containing liquid Helium He at temperature $T > T_c$ is spun around its axis at low angular frequency, and left in freewheel. Eventually, because of friction, the liquid comes to equilibrium with the moving walls, resulting in a constant angular frequency $\omega$ of the torus. Reducing $T$ below $T_c$, an increased angular frequency $\omega' > \omega$ of the torus is observed. The conservation of angular momentum implies that a fraction of the liquid, the...
The expectation value of the superfluid circulation can be expressed as:

\[ \langle \hat{C} \rangle_s = -i\hbar \sum_{s=0}^{2} \langle \Psi | \int_{\Gamma} \nabla \cdot d\vec{r} | \Psi \rangle \]

\[ = -i\hbar \sum_{s=0}^{2} \langle \Psi | \vec{r} \nabla \langle \vec{r} | \Psi \rangle \cdot d\vec{r} d\Omega \]

\[ = -i\hbar \sum_{s=0}^{2} \langle \Psi | \vec{r} \nabla \langle \vec{r} | \Psi \rangle \rangle \cdot d\vec{r} d\Omega \]

\[ + \hbar \sum_{s=0}^{2} \langle \Psi | \vec{r} \nabla \phi \rangle \langle \vec{r} | \Psi \rangle \cdot d\vec{r} d\Omega \]

\[ = \int_{\Omega} \int_{\Gamma} \langle \Psi | \vec{r} \nabla \phi \rangle \langle \vec{r} | \Psi \rangle \cdot d\vec{r} d\Omega \]

(2)

Because \( \hat{P} \) is Hermitian, only the real part in (2) can be non-zero. Thus, the circulation depends only on the phase gradient of the wave function and takes the form:

\[ \langle \hat{C} \rangle_s = \hbar \sum_{s=0}^{2} \langle \vec{r} | \nabla \phi \cdot d\vec{r} \rangle_s \]

(3)

Since the circulation of the phase gradient is along a closed loop, the total variation of the phase must vanish, unless the phase runs over \( n \) entire periods of \( 2\pi \). As a result, the circulation of the superfluid is quantized and can take only the values \( \langle \hat{C} \rangle_s = 2\pi n \hbar \). We note that, from Eq. (3), the existence of a non-zero circulation must be associated with a phase coherence. Expressing the circulation in terms of the velocity \( \vec{v} = \vec{P}/m \), with \( m \) the mass of one atom, we find the velocity quantization condition that was first proposed by Onsager:

\[ \int_{\Gamma} \vec{v}_s \cdot d\vec{r} = n\kappa_\alpha, \]

(4)

where \( \vec{v}_s = \langle \vec{v} \rangle_s \) and \( \kappa_\alpha = \frac{2\pi \hbar}{m} \) is the flux quantum. If the integration loop does not enclose a “hole” (a physical hole like in the torus under consideration, or a vortex), then the path can be shrunk continuously to a point where the circulation vanishes, corresponding to \( n = 0 \). Thus, the only possibility for the circulation to be non-zero is that the loop encloses at least one hole. For a loop that does not include any holes, the application of Stokes’ theorem implies that the superflow is irrotational:

\[ \nabla \times \vec{v}_s = 0 \]

(5)

We can now make precise what we meant by low and high velocities. When the initial velocity corresponds to less than half a flux quantum (low velocity), the superfluid seeks the nearest velocity satisfying (4) and comes to rest, thus excluding all flux (Meissner effect). When the initial velocity corresponds to more than half a flux quantum (high velocity), the superfluid seeks the nearest velocity satisfying (4) and settles in a persistent dissipationless flow.

The discussion above suggests that transitions between states with different quantum numbers \( n \) can be suspected to be associated with vortex formations. The details behind those transitions have been studied numerically for the case of the two-dimensional XY model.
III. DEFINITION AND CALCULATION OF THE NORMAL AND THE SUPERFLUID DENSITIES IN CONTINUOUS SPACE

A. Thought experiment and definitions

We consider here a thought experiment that idealizes the above real experiment made at low angular frequency. In this experiment, a fluid is enclosed between two infinite cylinders of radii \( R \) and \( R + \epsilon \) rotating at angular frequency \( \omega \) (Fig. 2, left). We denote by \( F \) the frame attached to the lab, and by \( F' \) the frame attached to the moving walls. In the limit \( R \gg \epsilon \), the system becomes equivalent to a fluid enclosed between two hyperplanes of infinite mass separated by a distance \( \epsilon \) and moving at constant velocity \( v = \mathbf{R} \omega \) with respect to \( F \), with a periodicity of \( 2\pi R \) in the direction of \( \mathbf{v} \) (Fig. 2, right). The outcome of this thought experiment is that, at temperature below \( T_c \), the superfluid comes to rest with respect to the lab frame, while the normal fluid remains at rest in the frame of the moving walls. Because of the infinite mass of the walls, their velocity with respect to \( F \) does not increase.

This “thought outcome” does not contradict Galileo’s principle of Relativity. It could be argued that there is no reason for the superfluid to choose to come to rest with respect to \( F \) instead of any other inertial frame. This apparent paradox is resolved by realizing that our description of the system enclosed between two moving hyperplanes is just a limit of the system enclosed between two hypercylinders. Therefore, the frames \( F \) and \( F' \) are not equivalent, \( F' \) is actually rotating and thus accelerated, and coming to rest with respect to \( F \) is the only way for the superfluid to avoid being accelerated.

This conclusion can be directly generalized to systems with periodicity in all directions: We consider an orthonormal basis \( B = \{ \mathbf{f}_1, \ldots, \mathbf{f}_d \} \) and a system with periodicity \( L_j \) along each direction \( \hat{r}_j \) with walls moving at velocity \( \mathbf{v} = (v_1, \ldots, v_d) \) with respect to the lab frame \( F \). As the temperature is lowered below \( T_c \), the superfluid is observed to come to rest with respect to \( F \), while the normal fluid remains at rest with respect to \( F' \). As a result, we define the superfluid density \( \rho_s \) as the mass \( M_s \) of the fluid that comes to rest with respect to the lab frame \( F \), divided by the volume \( \Omega \) of the system. In a similar way, we define the normal density \( \rho_n \) as the mass \( M_n \) of the fluid that comes to rest with respect to the frame of the moving walls \( F' \), divided by \( \Omega \). In the following, we also consider the total mass of the fluid, \( M = M_s + M_n \), and the total density, \( \rho = \rho_s + \rho_n \).

B. Second quantization preliminaries and notations

We give here a brief reminder of second quantization that is mainly meant to introduce the notation that we use all along this paper. In second quantization, any operator can be expressed as a functional of the creation and annihilation field operators \( \hat{\psi}^\dagger(\mathbf{r}) \) and \( \hat{\psi}(\mathbf{r}) \), with \( \mathbf{r} = (r_1, \ldots, r_d) \), which satisfy the relations

\[
[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')]_{\zeta} = [\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}(\mathbf{r}')]_{\zeta} = 0,
\]

\[
[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')]_{\zeta} = \delta(\mathbf{r}' - \mathbf{r}),
\]

where \([A, B]_{\zeta} \defeq AB - \zeta BA\) with \( \zeta = 1 \) for bosons and \( \zeta = -1 \) for fermions, and \( \delta(\mathbf{r}' - \mathbf{r}) \) is the \( d \)-dimensional Dirac distribution. The number operator \( \hat{N} \), the position operator \( \mathbf{R} \), and the momentum operator \( \mathbf{P} \) take the forms

\[
\hat{N} = \int_{\Omega} \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})d\Omega,
\]

\[
\mathbf{R} = \int_{\Omega} \hat{\psi}^\dagger(\mathbf{r})\mathbf{r}\hat{\psi}(\mathbf{r})d\Omega,
\]

\[
\mathbf{P} = -i\hbar \int_{\Omega} \hat{\psi}^\dagger(\mathbf{r})\nabla\hat{\psi}(\mathbf{r})d\Omega,
\]

with \( d\Omega = dr_1 \cdots dr_d \), and satisfy the commutation relations:

\[
[i\hbar \delta_{\mu\nu} \mathbf{P}, \hat{N}] = i\hbar \delta_{\mu\nu} \hat{N}
\]

\[
[i\hbar \delta_{\mu\nu} \mathbf{R}, \hat{N}] = [\mathbf{P}, \hat{N}] = 0
\]

From \([6], [7], \) and \([8] \), we can derive additional commutation relations:

\[
[\mathbf{R}, \hat{\psi}^\dagger(\mathbf{r})] = \mathbf{r}\hat{\psi}^\dagger(\mathbf{r})
\]

\[
[\mathbf{R}, \hat{\psi}(\mathbf{r})] = -\mathbf{r} \hat{\psi}(\mathbf{r})
\]

C. Calculation of the normal and the superfluid densities in the general case

We consider a \( d \)-dimensional system of identical particles of mass \( m \) in a \( L_1 \times \cdots \times L_d \) box with periodic boundary conditions that is moving at low velocity \( \mathbf{v} \) with respect to the lab frame \( F \). In the frame \( F' \) of the moving walls the system is at rest. Thus, in this frame, the Hamiltonian is independent of the velocity \( \mathbf{v} \), and is a
functional $\Phi$ of the creation and annihilation field operators:

$$\hat{H}_0 = \Phi[\hat{\psi}^\dagger(r), \hat{\psi}(r)]$$  \hspace{1cm} (15)

Defining the partition function $Z_o = \text{Tr} e^{-\beta \hat{H}_o}$ where $\beta$ is the inverse temperature, the average total momentum in $F'$ is given by

$$\langle \tilde{P} \rangle_{F'} = \frac{1}{Z_o} \text{Tr} \hat{P} e^{-\beta \hat{H}_o}$$  \hspace{1cm} (16)

Since $F$ moves at velocity $-\tilde{v}$ with respect to $F'$, the total momentum in the lab frame can be obtained from the above expression by performing an inverse Galilean transformation with velocity $\tilde{v}$. For this purpose, it is useful to define the unitary operator:

$$\hat{U} = e^{-i\frac{\pi}{2} \cdot \vec{\tilde{v}} \cdot \vec{\tilde{R}}}$$  \hspace{1cm} (17)

By using (11), it is straightforward to check that:

$$\hat{U}^\dagger \vec{P} \hat{U} = \vec{P} - \hat{m} \vec{v} \hat{N}$$  \hspace{1cm} (18)

$$\hat{U}^\dagger \vec{R} \hat{U} = \vec{R}$$  \hspace{1cm} (19)

Thus, $\hat{U}$ is the operator that performs a Galilean transformation (at time $t = 0$) with velocity $\tilde{v}$, and the total momentum operator in $F$ is given by the inverse transformation, $\hat{U} \vec{P} \hat{U}^\dagger$. Since the density matrix $e^{-\beta \hat{H}_o} / Z_o$ describes probabilities of states, it remains unchanged when going to the lab frame. As a result, the average total momentum in $F$ takes the form

$$\langle \vec{P} \rangle_F = \frac{1}{Z_o} \text{Tr} \hat{U} \vec{P} \hat{U}^\dagger e^{-\beta \hat{H}_o}$$

$$= \frac{1}{Z_o} \text{Tr} \vec{P} e^{-\beta \hat{H}_o} \hat{U} \hat{U}^\dagger$$

$$= \frac{1}{Z_o} \text{Tr} \vec{P} e^{-\beta \hat{H}_\tilde{v}}$$  \hspace{1cm} (20)

where we have used the invariance of the trace under cyclic permutations, and we have defined:

$$\hat{H}_\tilde{v} = \hat{U}^\dagger \hat{H}_o \hat{U}$$  \hspace{1cm} (21)

From the correspondence principle, the classical momentum of the fluid must be equal to the quantum average of the momentum operator $\vec{P}$. Since in $F$ only the normal fluid with mass $M_n = \rho_n \Omega$ spins, we have:

$$\rho_n \Omega \tilde{v} = \frac{1}{Z_o} \text{Tr} \vec{P} e^{-\beta \hat{H}_\tilde{v}}$$  \hspace{1cm} (22)

Calculating the divergence of (22) with respect to $\tilde{v}$, we get:

$$\vec{\nabla} \tilde{v} \cdot (\rho_n \Omega \tilde{v}) = \Omega (\vec{\nabla} \tilde{v} \rho_n) \cdot \tilde{v} + \rho_n \Omega \vec{d}$$

$$= -\frac{1}{Z_o} \text{Tr} \vec{P} \int_0^\beta e^{-(\beta - \tau) \hat{H}_\tilde{v}} \vec{\nabla} \tilde{v} \hat{H}_\tilde{v} e^{-\tau \hat{H}_\tilde{v}} d\tau$$  \hspace{1cm} (23)

From (17) and (21), the gradient of $\hat{H}_\tilde{v}$ with respect to $\tilde{v}$ can be expressed as:

$$\vec{\nabla}_\tilde{v} \hat{H}_\tilde{v} = \frac{i}{\hbar} \frac{m}{\hbar} \hat{U}^\dagger [\vec{R}, \hat{H}_o] \hat{U}$$  \hspace{1cm} (24)

Injecting (24) in (23) and taking the limit $\tilde{v} \rightarrow 0$, we get the general expression of the normal density:

$$\rho_n = -i \frac{m}{\hbar \Omega d} \int_0^\beta \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_\tilde{v}} [\vec{R}, \hat{H}_o] e^{-\tau \hat{H}_\tilde{v}} d\tau$$  \hspace{1cm} (25)

As a result, the general expression of the superfluid density takes the form:

$$\rho_s = \rho + i \frac{m}{\hbar \Omega d} \int_0^\beta \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_\tilde{v}} [\vec{R}, \hat{H}_o] e^{-\tau \hat{H}_\tilde{v}} d\tau$$  \hspace{1cm} (26)

The above expressions of $\rho_n$ and $\rho_s$ can be evaluated with path-integrals methods, such as the Stochastic Green Function (SGF) algorithm (see paragraphs VI and VII C for concrete examples).

**D. Relationship between the superfluid density and the free energy**

There exists a particular class of Hamiltonians for which the superfluid density can be directly related to the Laplacian $\Delta_{\vec{v}}$ of the free energy associated to the Hamiltonian $\hat{H}_\tilde{v}$.

$$F_{\vec{v}} = -\frac{1}{\beta} \ln Z_{\vec{v}}$$  \hspace{1cm} (27)

with $Z_{\vec{v}} = \text{Tr} e^{-\beta \hat{H}_\vec{v}}$. This class is defined by Hamiltonians $\hat{H}_o$ for which the commutator with the position operator satisfies:

$$[\vec{R}, \hat{H}_o] = i \frac{\hbar}{m} \vec{P}$$  \hspace{1cm} (28)

The most common example of Hamiltonian that belongs to this class is given by $\hat{H}_o = \hat{T} + \hat{V}$, where $\hat{V}$ is a potential that satisfies $[\vec{R}, \hat{V}] = 0$ and $\hat{T}$ is the kinetic energy:

$$\hat{T} = -\frac{\hbar^2}{2m} \int_\Omega \hat{\psi}^\dagger(\vec{r}) \Delta_{\vec{v}} \hat{\psi}(\vec{r}) d\Omega$$  \hspace{1cm} (29)

For any Hamiltonian that satisfies (28), the gradient (24) takes the form

$$\vec{\nabla}_\tilde{v} \hat{H}_\tilde{v} = -\frac{1}{\hbar} m \vec{v} \hat{N}$$  \hspace{1cm} (30)

from which $\vec{P}$ can be extracted and injected into (22), leading to:

$$\rho_n \Omega \tilde{v} = -\frac{1}{Z_o} \text{Tr} (\vec{\nabla}_\tilde{v} \hat{H}_\tilde{v} - m \vec{v} \hat{N}) e^{-\beta \hat{H}_\tilde{v}}$$

$$= -\frac{Z_{\vec{v}}}{Z_o} \vec{\nabla}_\tilde{v} F_{\vec{v}} + \frac{m \vec{v}}{Z_o} \text{Tr} \hat{N} e^{-\beta \hat{H}_\tilde{v}}$$  \hspace{1cm} (31)
From the divergence of the above expression in the limit $\vec{v} \to 0$, we get for the superfluid density the expression:

$$\rho_s = \lim_{\vec{v} \to 0} \frac{1}{14d} \Delta_{\vec{v}} F_{\vec{v}}$$  \hspace{1cm} (32)

At this point, it is useful to determine how the creation and annihilation field operators transform under $\hat{U}$. Using (13) and (14), we find:

$$\hat{U} \hat{\psi}(\vec{r}) \hat{U} = \hat{\psi}(\vec{r}) e^{i \frac{\vec{v}}{h} \cdot \vec{r}}$$ \hspace{1cm} (33)

$$\hat{U} \hat{\phi}(\vec{r}) \hat{U} = \hat{\phi}(\vec{r}) e^{-i \frac{\vec{v}}{h} \cdot \vec{r}}$$ \hspace{1cm} (34)

As a result, performing a Galilean transformation with velocity $\vec{v}$ is equivalent to applying a phase boost $\varphi(\vec{r}) = \frac{\vec{v}}{h} \cdot \vec{r}$ to the creation and annihilation field operators. This allows us to relate the superfluid density to the response of the free energy to a boundary phase-twist. For this, consider a vector $\vec{L} = n_1 L_1 \hat{r}_1 + \cdots + n_d L_d \hat{r}_d$ where $n_1, \ldots, n_d$ are integers. The phase-twist at the tips of the vector $\vec{L}$ that results from the velocity $\vec{v}$ is $\varphi = \frac{\vec{v}}{h} \cdot \vec{L}$. This allows us to rewrite (32) as:

$$\rho_s = \lim_{\vec{v} \to 0} \frac{m^2 \vec{L}^2}{h^2 \beta} \frac{\partial^2 F_{\vec{v}}}{\partial \varphi^2}$$ \hspace{1cm} (35)

It is clear that the free energy cannot depend on the sign of the velocity or the phase-twist. This implies:

$$\lim_{\vec{v} \to 0} \frac{\partial^2 F_{\vec{v}}}{\partial \varphi^2} = \lim_{\vec{v} \to 0} \frac{2 \partial F_{\vec{v}}}{\partial \varphi}$$ \hspace{1cm} (36)

Therefore, the superfluid density is directly related to the response of the free energy to a boundary phase-twist:

$$\rho_s = \lim_{\vec{v} \to 0} \frac{2m^2 \vec{L}^2}{h^2 \beta} \frac{\partial F_{\vec{v}}}{\partial \varphi}$$ \hspace{1cm} (37)

While equations (32), (35), and (37) are well known, it is important to keep in mind that they are valid only for Hamiltonians that satisfy Eq. (28).

### E. Relationship between the superfluid density and the winding number

As in the previous subsection, we assume here that the Hamiltonian satisfies the condition (28). In addition, we add the constraint that the Hamiltonian conserves the number of particles, $[\hat{H}, \hat{N}] = 0$. Performing a Taylor expansion and introducing a complete set of states $|\Psi_k\rangle$ in the position occupation number representation, the partition function $Z_{\vec{v}}$ can be written as:

$$Z_{\vec{v}} = \sum_{n \geq 0} \frac{(-\beta)^n}{n!} \sum_{\Psi_{n+1}} \prod_{k=1}^{n} \langle \Psi_{k+1} | \hat{H}_{\vec{v}} | \Psi_k \rangle,$$ \hspace{1cm} (38)

with the convention $|\Psi_{n+1}\rangle = |\Psi_1\rangle$. From (21), we have:

$$\prod_{k=1}^{n} \langle \Psi_{k+1} | \hat{H}_{\vec{v}} | \Psi_k \rangle = \prod_{k=1}^{n} \langle \Psi_{k+1} | \hat{H}_0 | \Psi_k \rangle \times e^{i \frac{\vec{v}}{h} \cdot \sum_{j} L_j W_{j}^{\Psi} \hat{r}_j},$$ \hspace{1cm} (39)

where $W_j^{\Psi}$ counts the number of particles that cross the boundaries of the system in the direction $\hat{r}_j$ while evolving over the sequence of states $|\Psi_k\rangle$. Therefore the partition function $Z_{\vec{v}}$ can be written as:

$$Z_{\vec{v}} = \sum_{n \geq 0} \frac{(-\beta)^n}{n!} \sum_{\Psi_{n+1}} \prod_{k=1}^{n} \langle \Psi_{k+1} | \hat{H}_0 | \Psi_k \rangle e^{i \frac{\vec{v}}{h} \cdot \sum_{j} L_j W_{j}^{\Psi} \hat{r}_j},$$ \hspace{1cm} (40)

where $W_j^{\Psi}$ are the components of the winding number operator $\hat{W}$ that take the eigenvalues $\Psi_j$. Injecting (40) into (27), and using (32), the superfluid density becomes directly related to the fluctuations of the winding number:

$$\rho_s = \frac{m^2 \vec{L}^2 - d}{h^2 \beta} \langle \Psi^2 \rangle$$ \hspace{1cm} (41)

For a hypercubic system, $\Omega = L^d$, the above expression becomes:

$$\rho_s = \frac{m^2 \vec{L}^{2-d}}{h^2 \beta} \langle \Psi^2 \rangle$$ \hspace{1cm} (42)

Here too, it is important to keep in mind that while Eq. (42) is well known, it cannot be applied to Hamiltonians that do not satisfy Eq. (28). In addition, the conservation of the number of particles is required for the winding number to be well defined. For Hamiltonians that do not satisfy these conditions, only equations (26) and (27) are valid.

### IV. THE SUPERFLUID DENSITY IN LATTICES

Determining the expression of the superfluid density in lattices is not as straightforward as it looks like. In particular, simply replacing the continuous-space operators by their discrete-space equivalents into (26) leads to inconsistencies. The reason is that some of the usual commutation rules between the operators $\hat{N}$, $\hat{R}$, $\hat{P}$, and $\hat{T}$ are no longer valid when these operators are discretized. It is therefore necessary to proceed carefully with the discretization of space.

#### A. Discretization of space

We start by noticing that (5) represents a dimensionless quantity. This implies that the dimension of the creation and annihilation field operators is the inverse square-root of a $d$-dimensional volume:

$$[\hat{\psi}^\dagger(\vec{r})] = [\hat{\psi}(\vec{r})] = L^{-\frac{d}{2}}$$ \hspace{1cm} (43)
Performing for each component of \( \vec{r} \) the change variable \( r_j = l y_j \), where \( l \) is a positive parameter with the dimension of a length and \( y_j \) is the new dimensionless variable, we can define the dimensionless creation and annihilation operators

\[
a^\dagger_{\vec{y}} = t^{d/2} \psi^\dagger (l \vec{y}), \\
a_{\vec{y}} = t^{d/2} \psi (l \vec{y}),
\]

which satisfy the commutation relations:

\[
[a_{\vec{y}}, a^\dagger_{\vec{y}}]_\zeta = [a_{\vec{y}}, a^\dagger_{\vec{y}}]_\zeta = 0 \\
[a_{\vec{y}}, a^\dagger_{\vec{y}}]_\zeta = \delta(\vec{y} - \vec{y}')
\]

Using these dimensionless operators, Eq. (8) can be rewritten as:

\[
N = \int_\Omega a^\dagger_{\vec{y}} a_{\vec{y}} d\vec{y}_1 \cdots d\vec{y}_d
\]

Because of the relation \( d r_j = l d y_j \), working in the limit \( l \rightarrow 0 \) implies \( d y_j \rightarrow 1 \). In this case, the components of \( \vec{y} \) vary by steps of 1, the integral over \( \Omega \) becomes discrete, and \( l \) becomes the lattice constant. In this limit, Eq. (47) becomes:

\[
[a_{\vec{y}}, a^\dagger_{\vec{y}}]_\zeta = \delta(\vec{y} - \vec{y}')
\]

Defining \( \hat{n}_\vec{y} = a^\dagger_{\vec{y}} a_{\vec{y}} \), the number operator takes the well-known form:

\[
\hat{N} = \sum_\vec{y} \hat{n}_\vec{y}
\]

Applying the same discretization to the position operator, we get:

\[
\hat{R} = l \sum_\vec{y} \vec{y} \hat{n}_\vec{y}
\]

By using for the first-order derivative the symmetrical prescription

\[
\frac{\partial}{\partial y_j} a_{\vec{y}} = \frac{1}{2} (a_{\vec{y}+\vec{y}_j} - a_{\vec{y}+\vec{y}_j})
\]

where \( \vec{y}_j \) is a unit vector in the \( j \) direction, the discrete momentum operator takes the form

\[
\hat{\mathbf{p}} = -i \sqrt{m t/2} \sum_{(p,q)} (a^\dagger_{\vec{y}_p} a_{\vec{y}_q} - H.c.) (\vec{y}_q - \vec{y}_p),
\]

where we have defined \( t = \frac{\hbar^2}{2 m^2} \) and the sum \( \sum_{(p,q)} \) is over all pairs of distinct neighboring sites \( p \) and \( q \). In a similar way, using for the second-order derivative the symmetrical prescription

\[
\frac{\partial^2}{\partial y_j \partial y_{j'}} a_{\vec{y}} = \frac{1}{2} (a_{\vec{y}+\vec{y}_j} + a_{\vec{y}-\vec{y}_j} + a_{\vec{y}+\vec{y}_{j'}} + a_{\vec{y}-\vec{y}_{j'}} - a_{\vec{y}+\vec{y}_j} - a_{\vec{y}-\vec{y}_j} - a_{\vec{y}+\vec{y}_{j'}} - a_{\vec{y}-\vec{y}_{j'}} - 2 a_{\vec{y}})
\]

the discrete kinetic operator takes the form:

\[
\hat{T} = -t \sum_{(p,q)} (a^\dagger_{\vec{y}_p} a_{\vec{y}_q} + H.c.) + 2 t \hat{N}
\]

Note that the second term in (55) is usually dismissed, as it only gives rise to a shift of the chemical potential and does not change the physics. In our case, we explicitly take it into account in order to ease the connection with the continuous case. It is useful in the following to rewrite (55) as \( T = \sum_j T_j \), where \( T_j \) is defined as:

\[
T_j = -i \sum_{\vec{y}} (a^\dagger_{\vec{y}} a_{\vec{y}+\vec{y}_j} + H.c.) + 2 t \hat{N}
\]

**B. The normal and superfluid densities in the general case**

With the previous discrete operators, it is easy to check that the commutator (11) becomes:

\[
[\mathcal{R}_\mu, \mathcal{P}_\nu] = i \hbar \delta_{\mu,\nu} \left( \hat{N} - \frac{1}{2 t} \hat{T}_\mu \right)
\]

As a result, as opposed to the continuous case, the discrete operator \( \hat{R} \) is not the generator of infinitesimal translations in momentum space. It actually translates the quasi-momentum. Therefore the unitary operator \( \hat{U} = e^{-i \frac{\pi}{2 t} \vec{v} \cdot \hat{R}} \) is no longer the operator that performs a Galilean transformation with velocity \( \vec{v} \). This implies that Eq. (20) is not applicable in the discrete case and needs to be modified. To this end, it is useful to determine how the momentum \( \mathcal{P} \) transforms under \( \hat{U} \) at first order in \( \vec{v} \). Using (57) we find:

\[
\hat{U} \hat{P} \hat{U}^\dagger = \hat{P} + m \vec{v} \hat{N} - \frac{m}{2 t} \sum_j v_j \hat{y}_j \hat{T}_j + \mathcal{O}(\vec{v}^2)
\]

This implies that new terms proportional to \( \langle \hat{T}_j \rangle \) must be introduced when discretizing (20):

\[
\langle \hat{P}_f \rangle = \frac{1}{2 \alpha} \operatorname{Tr} \hat{P} e^{-\beta \hat{H}_\alpha} + \frac{m}{2 t} \sum_j v_j \hat{y}_j \langle \hat{T}_j \rangle + \mathcal{O}(\vec{v}^2)
\]

As before, the correspondence principle requires the above quantum average of the momentum to be equal to the classical momentum, which in \( \mathcal{F} \) is due to the normal fluid only, \( \rho_n \vec{v} \). Calculating the divergence of this equality and taking the limit \( \vec{v} \rightarrow 0 \), we deduce the expression of the normal density for a general lattice Hamiltonian:

\[
\rho_n = \frac{m}{2 t \hbar \Omega d} \langle \hat{T} \rangle - i \frac{m}{\hbar \Omega d} \left( \hat{P} \cdot \int_0^\beta e^{\tau \hat{H}_\alpha} [\mathcal{R}, \hat{H}_\alpha] e^{-\tau \hat{H}_\alpha} d\tau \right)
\]

As a result, the expression of the superfluid density for a general lattice Hamiltonian is:

\[
\rho_s = \rho - \frac{m}{2 t \hbar \Omega d} \langle \hat{T} \rangle + i \frac{m}{\hbar \Omega d} \left( \hat{P} \cdot \int_0^\beta e^{\tau \hat{H}_\alpha} [\mathcal{R}, \hat{H}_\alpha] e^{-\tau \hat{H}_\alpha} d\tau \right)
\]
Comparing (26) and (61), we see that not only have the continuous-space operators been replaced by their discrete-space equivalents, but a new term proportional to the kinetic energy also appeared. Of course, in the limit \( l \to 0 \), we have \( t \to +\infty \) and (61) converges to (26).

C. The superfluid density as a function of the free energy and the winding number

As for the continuous-space case, the superfluid density can be related to the free energy if the Hamiltonian satisfies \( [\vec{R}, \hat{H}_a] = i \frac{\hbar}{m} \vec{p} \). In this case, the gradient \( \vec{\nabla} \hat{H}_a = -i \hat{\psi} \hat{\psi}^\dagger \) is given by the opposite of the inverse transformation of (58):

\[
\vec{\nabla} \hat{H}_a = -\vec{p} + m \vec{v} \hat{\nabla}^2 - \frac{m}{2t} \sum_j v_j \hat{\nabla}_j + \mathcal{O}(\hat{\psi}^2) \tag{62}
\]

Extracting \( \vec{p} \) from the above expression and injecting it into (59), we get:

\[
\langle \vec{P} \rangle_x = -\frac{Z_o}{Z_o^s} \vec{\nabla} F_{\vec{p}} + m \vec{v} \frac{1}{Z_o} \vec{\nabla} e^{-\beta \hat{H}_a} - \frac{m}{2t} \sum_j v_j \hat{\nabla}_j + \mathcal{O}(\hat{\psi}^2) \tag{63}
\]

Calculating the divergence of (63) and taking the limit \( \vec{v} \to 0 \), the terms in \( \vec{\nabla} \) cancel out. Thus, the expression of \( \rho_s \) as a function of the free energy in discrete space is the same as in continuous space (62), and so are the expressions of \( \rho_s \) as the response of the free energy to a phase boost (37), and as a function of the winding number (41).

D. Dimensionless superfluid density

For lattice systems, it is common to work with the dimensionless superfluid density \( \tilde{\rho}_s \), defined as the superfluid fraction \( \eta_s = \rho_s / \rho \) times the dimensionless density \( \tilde{\rho} = \langle \hat{N} \rangle / S_{\text{tot}} \), where \( S_{\text{tot}} = S_1 \times \cdots \times S_d \) is the total number of lattice sites. This can be written as:

\[
\tilde{\rho}_s = \frac{\rho_s \Omega}{m S_{\text{tot}}} \tag{64}
\]

Injecting (61) into (64), the dimensionless superfluid density takes the general form:

\[
\tilde{\rho}_s = \tilde{\rho} - \frac{1}{2t d S_{\text{tot}}} \langle \hat{\tau} \rangle + i \frac{1}{\hbar d S_{\text{tot}}} \langle \vec{p} \cdot \int_0^\beta e^{i \hat{R}_a} [\vec{R}, \hat{H}_a] e^{-i \hat{R}_a} d\tau \rangle \tag{65}
\]

V. LATTICES WITH NON-ORTHONORMAL PRIMITIVE VECTORS

In order to obtain the correct expressions of the superfluid density in lattices with non-cubic primitive cells, it is necessary to perform a careful change of basis when discretizing space.

A. Change of basis

We consider an orthonormal basis, \( B_r = \{ \hat{r}_1, \cdots, \hat{r}_d \} \), and a transformation \( A \) that changes \( B_r \) into a general basis, \( B_q = \{ \hat{q}_1, \cdots, \hat{q}_d \} \). We denote by \( A \) the matrix representation of \( A \) in the basis \( B_r \). Position vectors are contravariant, thus their coordinates \( (q^1, \cdots, q^d) \) in \( B_q \) are obtained from their coordinates \( (r^1, \cdots, r^d) \) in \( B_r \) by the inverse transformation,

\[ q^i = A_{ij} r^j, \tag{66} \]

where we have used Einstein’s summation convention. On the contrary, the derivatives with respect to the coordinates are covariant,

\[ \frac{\partial}{\partial q_j} = A_{ij} \frac{\partial}{\partial r_i}, \tag{67} \]

thus the Laplacian in the basis \( B_q \) takes the form:

\[ \Delta_q = A_{ik} A_{jk}^{-1} \frac{\partial^2}{\partial q_i \partial q_j} \tag{68} \]

Defining the metric tensor \( g_{\mu\nu} = \hat{q}_\mu \cdot \hat{q}_\nu \), the dot-product in the basis \( B_q \) of two vectors \( \vec{u} = (u^1, \cdots, u^d) \) and \( \vec{v} = (v^1, \cdots, v^d) \) takes the form:

\[ \vec{u} \cdot \vec{v} = g_{\mu\nu} u^\mu v^\nu \tag{69} \]

B. Discretization of space in non-orthonormal coordinates

For the sake of simplicity, we assume in the remainder of this section that the Hamiltonian is of the form \( \hat{\mathcal{H}}_a = \hat{T} + \hat{V} \), so (41) applies. A condition for the discretization to be valid is that the discretized Hamiltonian should reproduce quantitatively the same physics as its continuous space analog when the lattice constants go to zero. By performing the change of variables (66), the continuous-space kinetic operator (29) can be rewritten as

\[ \hat{T} = -\frac{\hbar^2}{2m} \sum_{\mu=1}^d \sum_{\nu=1}^d \frac{\partial^2}{\partial q_\mu \partial q_\nu} \hat{\psi}^\dagger \hat{\psi} dQ, \tag{70} \]

where \( |J| \) is the Jacobian determinant,

\[ |J| = \left| \frac{\partial (r^1, \cdots, r^d)}{\partial (q^1, \cdots, q^d)} \right|, \tag{71} \]
and $dQ = dq_1 \cdots dq_d$. Performing a second change of variables for each coordinates, $q_j = l_jy_j$, where $l_j$ has the dimension of a length and $y_j$ is the new dimensionless variable, the kinetic operator becomes

$$\hat{T} = -\frac{\hbar^2 |J|A_{jk}^{-1}A_{jk}^{-1}}{2mll_j} \int_{\Omega} a_y^\dagger \frac{\partial^2}{\partial y_j \partial y_j} a_y \, dy_1 \cdots dy_d,$$  

(72)

where we have generalized the previous definitions of the dimensionless creation and annihilation operators:

$$a_y^\dagger = \sqrt{l_1} x \cdots \sqrt{l_d} x y_1, \ldots, l_1 y_d, \quad a_y = \sqrt{l_1} x \cdots \sqrt{l_d} x y_1, \ldots, l_1 y_d$$  

(73)

As before, the above change of variables is valid for any positive values of $l_j$ and, because of the relation $dq_j = l_j dy_j$, working in the limit $l_j \to dq_j$ implies $dy_j \to 1$. In this case, integrals become discrete, $l_j$ becomes the lattice constant in the $y_j$ direction, and the kinetic operator takes the form:

$$\hat{T} = -\frac{\hbar^2 |J|A_{jk}^{-1}A_{jk}^{-1}}{2mll_j} \sum_{y \in \Omega} a_y^\dagger \frac{\partial^2}{\partial y_j \partial y_j} a_y,$$  

(75)

It is important to keep in mind that the volume $\Omega$ is a hyperrectangle. However, if the basis $B_\text{c}$ is not orthogonal, summing over a hyperparallelipped turns out to be more convenient. As a result, instead of a hyperrectangle of volume $\Omega = \prod_l L_j$, we consider a hyperparallelipped of volume $\tilde{\Omega} = |J| \prod_l L_j$. Since the volume $\tilde{\Omega}$ is scaled by a factor $|J|$ with respect to $\Omega$, the same energy can be recovered by multiplying it by the inverse factor. Therefore, the Jacobian determinant disappears and the kinetic operator is equivalent to

$$\hat{T} = -\frac{\hbar^2 A_{jk}^{-1}A_{jk}^{-1}}{2mll_j} \sum_{y \in \tilde{\Omega}} a_y^\dagger \frac{\partial^2}{\partial y_j \partial y_j} a_y,$$  

(76)

where the summation is over all vectors $\vec{y}$ in the volume $\tilde{\Omega}$ with the components $y_j$ varying over $S_j = L_j/l_j$ lattice sites. We can use for the second-order derivative the previous symmetrical prescription (54). The discretization of the potential term $\hat{V}$ can be done in a similar way, and does not affect the following conclusions.

C. Application to Bravais lattices

We give here some examples of application of the above discretization to some common Bravais lattices, and we emphasize the differences between our expressions for the superfluid density and the expressions that are usually improperly used.

1. Hypercubic lattice

In the case of a hypercubic lattice with $S_1 \times \cdots \times S_d$ sites, the basis of the primitive cell is orthogonal, and the lattice constants $l_j$ are all equal to the same value $t$. Using the identity transformation for $A$ and defining $t = \frac{\hbar^2}{2mll_j}$, Eq. (76) leads to the previous discrete form of the kinetic energy:

$$\hat{T} = -t \sum_{p,q} \left( a_p^\dagger a_q + H.c. \right) + 2t N'$$  

(77)

In this simple case, the metric tensor $g_{\mu\nu}$ is just the identity, and combining (42) and (64) leads to

$$\hat{\rho}_s = \frac{S^{2-d}}{2t_3 l_3} \left( W_1^2 + \cdots + W_d^2 \right),$$  

(78)

where we have assumed the same number of lattice sites $S_j = S$ in each of the primitive directions. For this case, we recover the well-known expression. A common mistake arises when applying (78) to non-cubic lattice geometries, as we show below.

2. Triangular lattice

We address here the case of a $S \times S$ triangular lattice (Fig. 3). The transformation matrix $A$ that changes the orthonormal basis $B_\text{c} = \{ \tilde{r}_1, \tilde{r}_2 \}$ into the basis $B_q = \{ \vec{q}_1, \vec{q}_2 \}$ and the metric tensor $g_{\mu\nu}$ are given by:

$$A = \begin{pmatrix} 1 & 1/2 \\ 0 & \sqrt{3}/2 \end{pmatrix}, \quad g = \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}$$  

(79)

with the energy scale $t' = \frac{\hbar^2}{3 ml' t}$. As a result, using (69) for the square of the winding number operator, the dimensionless superfluid density is:

$$\hat{\rho}_s = \frac{1}{6t' \beta} \left( W_1^2 + W_2^2 + W_3 W_2 \right)$$  

(81)

The above expression computed with the energy scale $t' = 1$ differs significantly from the quantity (78) that is usually improperly applied with $t = 1$. Doing so not only introduces an energy scale mismatch between the simulated Hamiltonian and the computed superfluid density, but some winding correlations are missed too.
The transformation matrix $A$ and the metric tensor $g_{uv}$ associated to the primitive cell of a face-centered cubic lattice (Fig. 4) are given by:

$$A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}, \quad g = \begin{pmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1 \end{pmatrix}$$ (82)

FIG. 4. (Color online) Face-centered cubic lattice. The basis $B_s$ is changed to $B_q$ by the transformation $[82]$.

With this transformation, Eq. (76) becomes

$$\tilde{T} = -t'' \sum_{(p,q)} \langle a_p | a_q + H.c. \rangle + 12t'' \tilde{N},$$ (83)

with the energy scale $t'' = \frac{\hbar^2}{4m^2}$. Thus, for a $S \times S \times S$ lattice, the dimensionless superfluid density takes the form:

$$\tilde{\rho}_s = \frac{\langle W_1^2 + W_2^2 + W_3^2 + W_1 W_2 + W_2 W_3 + W_3 W_1 \rangle}{12t'' \beta S}$$ (84)

Once again, the above expression computed with the energy scale $t'' = 1$ differs significantly from the quantity (78) that is usually improperly applied with $t = 1$.

D. Application to non-Bravais lattices

A non-Bravais lattice can be described as a basis of points that is reproduced at each point of an underlying Bravais lattice. Another possible description is to consider it as a Bravais lattice with smaller lattice constants and missing points. The advantage of this latter description is that we already know how to discretize continuous space and obtain a Bravais lattice with the associated expression of the superfluid density. By adding to the Hamiltonian an infinite potential at the locations of the missing points, we can prevent the particles from occupying those positions and generate the corresponding non-Bravais lattice. This mathematical “trick” allows us to determine the expression of the superfluid density.

A honeycomb lattice (Fig. 5) is usually seen as a two-point basis $(p_1, p_2)$ that is reproduced at each point of a triangular lattice generated by a basis $B_q$. In our case, it is more convenient to describe it as a triangular lattice generated by a second basis $B_u$, to which we remove all points generated by the basis $B_q$.

At this point, it is useful to consider the Hamiltonian $\hat{H} = \hat{T} + \hat{V}$ with $\hat{T}$ given by (29) and $\hat{V}$ by

$$\hat{V} = \int_\Omega \hat{\psi}^\dagger (\vec{r}) \hat{V}(\vec{r}) \hat{\psi}(\vec{r}) d\Omega,$$ (85)

with

$$V(\vec{r}) = U \hbar^2 \sum_{j_1, j_2} \delta (\vec{r} - j_1 \vec{q}_1 - j_2 \vec{q}_2),$$ (86)

where $U$ is a parameter with the dimension of an energy and $h = ||\vec{q}_1|| = ||\vec{q}_2||$. Injecting (86) into (85) and using the previously defined dimensionless creation and annihilation operators (73) and (74), the potential becomes:

$$\hat{V} = U \sum_{j_1, j_2} \hat{n}_{j_1 j_1} \hat{n}_{j_2 j_2}$$ (87)

By discretizing $\hat{T}$ with the transformation that changes an orthogonal basis into the basis $B_u$ and defining $l = ||\vec{u}_1|| = ||\vec{u}_2||$, the Hamiltonian becomes

$$\hat{H} = -t' \sum_{(p,q)} \langle a_p | a_q + H.c. \rangle + 6t' \hat{N}$$

$$+ U \sum_{j_1, j_2} \hat{n}_{j_1 j_1} \hat{n}_{j_2 j_2}$$ (88)

where the sum $\sum_{(p,q)}$ is over all distinct pairs of first neighboring sites of the triangular lattice generated by $B_u$, and the sum $\sum_{p}$ is over all sites. Since the Hamiltonian $\hat{H}$ satisfies the condition (28), the corresponding superfluid density is given by (81), and this result applies.
for any value of the parameter $U$. In particular, it applies in the limit $U \to \infty$ where the Hamiltonian becomes equivalent to

$$\hat{H} = -t' \sum_{(p,q) \in \mathcal{B}_q} (a^*_p a_q + H.c.) + 6t' \hat{N}, \quad (89)$$

where the notations $\langle p, q \rangle - B_q$ and $p - B_q$ indicate that the points generated by $B_q$ are removed. As a result, the above Hamiltonian describes particles on a honeycomb lattice, and the expression of the superfluid density is the same as for a triangular lattice and given by (81).

### 2. Kagome lattice

A kagome lattice (Fig. 6) is formed by corner-sharing triangles, and is usually seen as a three-point basis $(p_1, p_2, p_3)$ that is reproduced at each point of a triangular lattice generated by a basis $\mathcal{B}_q$. Here again, it is more convenient to describe it as a triangular lattice generated by a second basis $\mathcal{B}_u$, to which we remove all points generated by the basis $\mathcal{B}_q$.

![Fig. 6. (Color online) A kagome lattice can be described as a three-point basis $(p_1, p_2, p_3)$ that is reproduced at each point of a triangular lattice generated by a basis $\mathcal{B}_q$, or as a triangular lattice generated by a basis $\mathcal{B}_u$ to which we remove all points generated by the basis $\mathcal{B}_q$.](image)

As before, the same reasoning as for the honeycomb and kagome lattices can be applied, and we conclude that the expression of the superfluid density is given by that of a triangular lattice (81).

### 3. Pyrochlore lattice

A pyrochlore lattice (Fig. 7) is formed by corner-sharing tetrahedrons, and is usually seen as a four-point basis $(p_1, p_2, p_3, p_4)$ that is reproduced at each point of a face-centered cubic lattice generated by a basis $\mathcal{B}_q$. In a way similar to the honeycomb and kagome lattices, it is more convenient to describe it as a face-centered cubic lattice generated by a second basis $\mathcal{B}_u$, to which we remove all points generated by the basis $\mathcal{B}_q$.

![Fig. 7. (Color online) A pyrochlore lattice can be described as a four-point basis $(p_1, p_2, p_3, p_4)$ that is reproduced at each point of a face-centered cubic lattice generated by a basis $\mathcal{B}_q$, or as a face-centered cubic lattice generated by a basis $\mathcal{B}_u$ to which the points generated by the basis $\mathcal{B}_q$ are removed.](image)

As before, the same reasoning as for the honeycomb and kagome lattices can be applied, and we conclude that the expression of the superfluid density is given by that of a face-centered cubic lattice (84).

### E. Consistency check

In this subsection, we make a consistency check that illustrates the correctness of our expressions of the superfluid density for the hypercubic (78), triangular (81), and face-centered cubic (84) lattices. Since the kinetic term of the triangular lattice (80) and the kinetic term of the face-centered cubic (83) lattice correspond to the discretization of the continuous kinetic term (29) with $d = 2$ and $d = 3$, respectively, they should give exactly the same superfluid density as the kinetic term of the hypercubic lattice (77) with the corresponding dimensionality.

In order to check this, we made use of the Stochastic Green Function (SGF) algorithm with directed updates, and performed quantum Monte Carlo simulations of the kinetic term for hard-core bosons at half-filling. The results are shown in Fig. 8. The superfluid density obtained for a $16 \times 16$ triangular lattice with $t' = 1$ is in agreement with the superfluid density obtained for a $16 \times 16$ square lattice with $t = 1$, as a function of temperature $T$, the small differences being due to finite-size effects. We get the same agreement between the superfluid density obtained for a $4 \times 4 \times 4$ face-centered cubic lattice with $t'' = 1$ and the superfluid density obtained for a $4 \times 4 \times 4$ cubic lattice with $t = 1$.

### VI. LATTICE HAMILTONIAN WITH HOPPING BETWEEN SECOND NEIGHBORS

In this section, we illustrate the usefulness of Eq. (65) by considering a Hamiltonian for which the well-known expressions of the superfluid density are not applica-
The model consists of soft-core bosons on a two-dimensional $S \times S$ square lattice described by the Hamiltonian:

$$
\hat{H}_0 = -t \sum_{\langle p,q \rangle} \left( a_p^\dagger a_q + H.c. \right) + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1) - \lambda \sum_{\langle p,q \rangle} \left( a_p^\dagger a_q + H.c. \right)
$$

The sum $\sum_{\langle p,q \rangle}$ is over all distinct pairs of second-neighboring sites $p$ and $q$. In addition to the discrete operators $[50, 51, 53, 55]$, we define the operator:

$$
\hat{Q} = -i \sqrt{mt/2} \sum_{\langle p,q \rangle} \left( a_p^\dagger a_q - H.c. \right)(\hat{q}_p - \hat{q}_q)
$$

Calculating the commutator $[\hat{R}, \hat{H}_0]$ leads to:

$$
[\hat{R}, \hat{H}_0] = i \frac{\hbar}{m} (\hat{p} + \frac{\lambda}{t} \hat{Q})
$$

Therefore, the Hamiltonian $[90]$ does not belong to the class defined by $[28]$, and the expression of the superfluid density given by $[78]$ with $d = 2$ is not applicable. Injecting $[92]$ into $[65]$ with $S_{\text{tot}} = S^2$, we get the expression:

$$
\hat{\rho}_s = \hat{\rho} - \frac{1}{4tS^2} \langle \hat{\rho} \rangle - \frac{1}{2mS^2} \left( \hat{p} \int_0^\beta e^{\tau \hat{H}_o} \left( \hat{p} + \frac{\lambda}{t} \hat{Q} \right) e^{-\tau \hat{H}_o} d\tau \right)
$$

Using the SGF algorithm $[12]$ with directed updates $[13]$, it is easy to evaluate $[93]$ for a given configuration of the particle worldlines by defining $n_\zeta$ as the number of hoppings in the direction $\zeta$, with $\zeta = \leftarrow, \rightarrow, \uparrow, \downarrow, \uparrow\downarrow, \downarrow\uparrow$, the notation being self-explanatory. Then $[93]$ takes the form:

$$
\hat{\rho}_s = \frac{1}{4t^2S^2} \left( (n_{-x} - n_{-y})(n_{-y} - n_{-x} + n_{x} - n_{x} - n_{y}) + (n_x - n_y)(n_{-x} + n_{x} + n_{y} - n_{y} - n_{x}) \right)
$$

We have simulated the Hamiltonian $[90]$ with $t = 1$, $\lambda = 0.8$, and $U = 20$, at half-filling ($\hat{\rho} = \frac{1}{2}$) as a function of temperature. Fig. 9 shows a comparison between the quantity given by the discrete form of Pollock and Ceperley’s formula $[78]$ and our expression $[94]$. This example clearly demonstrates that $[78]$ is not applicable for this Hamiltonian, since it gives a value that is greater than the total density. On the other hand, our expression $[94]$ ensures that $\hat{\rho}_s \in [0; \bar{\rho}]$.

![Figure 8](image)

**FIG. 8.** (Color online) The dimensionless superfluid density $\tilde{\rho}_s$ of hard-core bosons as a function of temperature $T/t$ at half-filling, for different lattice geometries. The values obtained for a triangular lattice agree with the values obtained for a square lattice, the small differences being due to finite-size effects. In the same way, the values obtained for a face-centered cubic lattice agree with the values obtained for a cubic lattice. The errorbars are smaller than the symbols’ size.

![Figure 9](image)

**FIG. 9.** (Color online) Comparison between the superfluid density (red) obtained from the general expression $[94]$ and the quantity (blue) given by $[75]$ for the Hamiltonian $[90]$. The errorbars are smaller than the symbols’ size.

### VII. Multi-Species Hamiltonians

The theory developed in sections III and IV can be directly extended to multi-species Hamiltonians in order to obtain the normal and superfluid densities of the mixture. In addition, it is possible to define and calculate those quantities for the individual species, even if inter-species conversions occur. Consider a $d$-dimensional Hamiltonian $\hat{H}_w$ with several species of particles. We denote by $m_k$ the mass of a particle of a given species $k$.

#### A. Continuous space

The continuous-space position, momentum, and kinetic operators of the mixture can be written

$$
\vec{R} = \sum_k \vec{R}_k, \quad \vec{P} = \sum_k \vec{P}_k, \quad \hat{T} = \sum_k \hat{T}_k,
$$

where $\vec{R}_k$, $\vec{P}_k$, and $\hat{T}_k$ are the position, momentum, and kinetic operators for species $k$, respectively.
where \( \vec{R}_k, \vec{P}_k, \) and \( \hat{T}_k \) are the position, momentum, and kinetic operators associated to the species \( k \), obtained by adding the index \( k \) to the creation and annihilation field operators in \([9], [10]\), and \([29]\). Performing as before a thought experiment in which the single-species fluid is replaced by the mixture, the superfluid components of all the species are observed to come to rest with respect to the lab frame \( F \), while the normal components are observed to come to rest with the frame of moving walls \( F' \). Therefore, we define the superfluid density \( \rho^s_k \) of the species \( k \) as the mass \( M^s_k \) of that species that comes to rest with respect to \( F \), divided by the volume \( \Omega \) of the system. In a similar way, we define the normal density \( \rho^n_k \) of the species \( k \) as the mass \( M^n_k \) of that species that comes to rest with respect to \( F' \), divided by \( \Omega \). We also define the total density \( \rho^s = \frac{M^s}{\Omega} \) of species \( k \), where \( M^s \) is the total mass of that species. It is easy to check that the unitary operator that performs a Galilean transformation with velocity \( \vec{v} \) of the mixture is given by:

\[
\hat{U} = e^{-i \frac{\vec{v}}{\hbar} \sum_k m_k \vec{R}_k} \quad (96)
\]

Defining as before \( \hat{H}_d = \hat{U}^\dagger \hat{H}_d \hat{U} \), its gradient with respect to \( \vec{v} \) can be written as:

\[
\nabla \hat{H}_d = \frac{i}{\hbar} \hat{U}^\dagger \sum_k m_k [\vec{R}_k, \hat{H}_d] \hat{U} \quad (97)
\]

Applying the correspondence principle to the total momentum of the species \( k \), we deduce that the normal density of that species is given by:

\[
\rho^n_k = -i \frac{\hbar}{\Omega} \sum_q m_q \left\langle \vec{P}_k \right\rangle_0^\beta e^{\vec{R}_k \cdot [\vec{R}_k, \hat{H}_d]} e^{-\vec{R}_d} d\tau \quad (98)
\]

As a result, the superfluid density of the species \( k \) is given by:

\[
\rho^s_k = \rho_k + i \frac{\hbar}{\Omega} \sum_q m_q \left\langle \vec{P}_k \cdot [\vec{R}_k, \hat{H}_d] \right\rangle_0^\beta e^{-\vec{R}_d} d\tau \quad (99)
\]

### B. Discrete space

Applying our previous definition of the dimensionless superfluid density \([64]\) to all species,

\[
\tilde{\rho}^s_k = \frac{\rho^s_k \Omega}{m_k S_{tot}}, \quad (100)
\]

the dimensionless superfluid density of the species \( k \) in discrete space is obtained in a way similar as before, by subtracting a term proportional to the kinetic energy of that species,

\[
\tilde{\rho}^s_k = \tilde{\rho}^s - \frac{1}{2 \hbar d S_{tot}} \left\langle \hat{T}_k \right\rangle + \frac{i}{\hbar m_k d S_{tot}} \sum_q m_q \left\langle \vec{P}_k \cdot [\vec{R}_k, \hat{H}_d] \right\rangle_0^\beta e^{-\vec{R}_d} d\tau \quad (101)
\]

where we have defined \( t_k = \frac{\hbar^2}{2m_k \tau} \).

### C. Application to a two-species Hamiltonian with inter-species conversion terms

We consider here a one-dimensional lattice Hamiltonian with \( S \) sites that describes atoms and molecules with inter-species conversion terms \([10,11]\) which takes the form

\[
\hat{H}_o = -t_a \sum_{(p,q)} \left( a_p^\dagger a_q + H.c. \right) - t_m \sum_{(p,q)} \left( m^a_p m_q + H.c. \right) + \frac{U_{aa}}{2} \sum_p \hat{n}_p^a (\hat{n}_p^a - 1) + \frac{U_{mm}}{2} \sum_p \hat{n}_p^m (\hat{n}_p^m - 1) + U_{am} \sum_p \hat{n}_p^a \hat{n}_p^m + D \sum_p \hat{n}_p^m + \sigma \sum_p \left( a_p^\dagger a_p m_p + H.c. \right), \quad (102)
\]

where \( a_p^\dagger \) and \( a_p \) (resp. \( m_p^a \) and \( m_p \)) are the creation and annihilation operators of an atom (resp. a molecule) on site \( p \). The operator \( \hat{n}_p^a = a_p^\dagger a_p \) (resp \( \hat{n}_p^m = m_p^a m_p \)) counts the number of atoms (resp. molecules) on site \( p \). The last term in \((102)\) converts a molecule into two atoms and vice-versa. As a result, this Hamiltonian does not conserve the number of atoms nor the number of molecules, but we can define the total density as \( \tilde{\rho}^a = \tilde{\rho}^s + \rho^m \) which is conserved. In a path-integral representation, the non-conservation of the number of atoms and molecules means that the atomic and molecular worldlines can be broken (Fig. \([10]\). As noticed in \([10,11]\) this results in the impossibility to define winding numbers for atoms and for molecules that are topologically conserved. Nevertheless, our general expression of the superfluid density \([101]\) does not rely on any definition of the winding number, and allows us to calculate the superfluid density of the atoms, \( \tilde{\rho}^s_a \), as well as the superfluid density of the molecules, \( \tilde{\rho}^s_m \). Calculating the commutators of the position operators \( R_a \) and \( R_m \) with the Hamiltonian \([102]\), we obtain

\[
[R_a, \hat{H}_o] = \frac{i}{m_a} P_a + 2C, \quad (103)
\]

\[
[R_m, \hat{H}_o] = i \frac{\hbar}{m_m} P_m - C, \quad (104)
\]

where \( C \) is given by:

\[
C = \sigma \left\langle \sum_p (a_p^\dagger a_p m_p - H.c.) \right\rangle \quad (105)
\]

Injecting these in \([101]\), we get the superfluid density of the atoms:

\[
\tilde{\rho}^s_a = \tilde{\rho}^s - \frac{1}{2 \hbar a S} \left\langle \hat{T}_a \right\rangle - \frac{1}{m_a S} \left\langle P_a^\beta \left( P_a(\tau) + P_m(\tau) \right) d\tau \right\rangle + \frac{2 t_m - t_a}{\hbar t_m S} \left\langle C(\tau) d\tau \right\rangle \quad (106)
\]
The superfluid density of the molecules takes the form:

\[
\tilde{\rho}_s^m = \rho^m - \frac{1}{2t_m S} \langle \hat{T}_m \rangle - \frac{1}{m_m S} \langle \hat{P}_m \int_0^\beta (\hat{P}_a(\tau) + \hat{P}_m(\tau))d\tau \rangle + \frac{2t_m - t_a}{\hbar a S} \langle \hat{P}_m \int_0^\beta \hat{C}(\tau)d\tau \rangle
\]

Evaluating (106) and (107) with the SGF method is made easy by defining \( n_L^a \) and \( n_R^a \) (resp. \( n_L^m \) and \( n_R^m \)) as the numbers of hoppings of atoms (resp. molecules) to the left and to the right in a given configuration of worldlines, and \( n_{m\to a}^p \) and \( n_{a\to m}^p \) as the numbers of conversions of molecules to atoms and atoms to molecules that occur on site \( p \). With these definitions, the superfluid densities of atoms and molecules take the final forms:

\[
\tilde{\rho}_s^a = \frac{1}{2\beta S} \langle \left( n_L^a - n_R^a \right) / t_a + \left( n_L^a - n_R^a \right) / t_m \rangle + \frac{2t_m - t_a}{2ta t_m \beta S} \langle \sum_p \left( n_{m\to a}^p - n_{a\to m}^p \right) \rangle
\]

\[
\tilde{\rho}_s^m = \frac{1}{2\beta S} \langle \left( n_L^m - n_R^m \right) / t_m + \left( n_L^m - n_R^m \right) / t_a \rangle + \frac{2t_m - t_a}{2ta t_m \beta S} \langle \sum_p \left( n_{m\to a}^p - n_{a\to m}^p \right) \rangle
\]

Figure 11 shows the densities \( \tilde{\rho}_s^a \) and \( \tilde{\rho}_s^m \) of atoms and molecules, as functions of the total density \( \tilde{\rho}_s^{tot} \). With the parameters \( t_a = 1, t_m = 0.5, \sigma = 0.5, U_{aa} = 8, U_{am} = 100, U_{am} = 12, D = 6, \) and \( \beta = 10 \), our simulations indicate that the phase is incompressible for densities \( \tilde{\rho}_s^{tot} = 1 \) and \( \tilde{\rho}_s^{tot} = 2 \), and nearly incompressible for \( \tilde{\rho}_s^{tot} = 3 \). This is consistent with the features observed in \( \tilde{\rho}_s^a \) and \( \tilde{\rho}_s^m \), and in agreement with ref. 17.

VIII. CONCLUSION

Based on real and thought experiments, we give a definition of the superfluid density for a general Hamiltonian, and we extend it to each components of multi-species Hamiltonians. We derive general expressions that allow us to calculate the superfluid density with path-integral methods. While it is well known that the superfluid density can be related to the response of the free energy to a boundary phase twist or to the fluctuations of the winding number, we show that this is true only for a particular class of Hamiltonians. Our expressions, however, can be applied to any Hamiltonian. In particular, they can be applied to Hamiltonians that do not conserve the number of particles, where the winding number is undefined. By performing a discretization of space with a general change of basis, we obtain formulae for the superfluid density for various lattice geometries. We point to some common mistakes that occur when the energy scale is not correctly reflected in the expression of the superfluid density, and when some correlations are missed because of a non-diagonal metric tensor. Finally, we give two examples of lattice Hamiltonians for which the well-known expressions of the superfluid density are not applicable. We calculate the superfluid densities for these Hamiltonians by evaluating our general expressions by means of quantum Monte Carlo simulations, using the SGF algorithm.
ACKNOWLEDGMENTS

The author would like to express special thanks to Mark Jarrell and Juana Moreno for providing support, and George Batrouni, Frédéric Hébert, and Ka-Ming Tam for enlightening discussions. This work is supported by NSF OISE-0952300.

1. P. Kapitza, Nature 141, 74 (1938).
2. J.F. Allen and A.D. Misener, Nature 141, 75 (1938).
3. M.E. Fisher, M.N. Barber, and D. Jasnow, Phys. Rev. A 8, 2 (1973).
4. E.L. Pollock and D.M. Ceperley, Phys. Rev. B 36, 8343 (1987).
5. A.J. Leggett, in Topics in Superfluidity and Superconductivity, in Low Temperature Physics, Proceedings of Blydepoort South Africa, 1991, edited by M. J. R. Hoch and R. H. Lemmer (SpringerVerlag, 1991).
6. G.G. Batrouni, Phys. Rev. B 70, 184517 (2004).
7. S. Sorella, AIP Conference Proceedings, 2006, Vol. 816 Issue 1, p265.
8. G.B. Hess and W. M. Fairbank, Phys. Rev. Lett. 19, 216 (1967).
9. S.C. Whitmore and W. Zimmermann, Jr., Phys. Rev. Lett. 15, 389 (1965).
10. D.T. Ekholm and R. B. Hallock, Phys. Rev. B 21, 3902 (1980).
11. L. Onsager, Nuovo Cimento, Suppl. 6, 249 (1949).
12. V.G. Rousseau, Phys. Rev. E 77, 056705 (2008).
13. V.G. Rousseau, Phys. Rev. E 78, 056707 (2008).
14. G.G. Batrouni and M.B. Halpern, Phys. Rev. D 30, 1775 (1984).
15. V.G. Rousseau and P.J.H. Denteneer, Phys. Rev. A 77, 013609 (2008).
16. V.G. Rousseau and P.J.H. Denteneer, Phys. Rev. Lett. 102, 015301 (2009).
17. Maria Eckholt and Tommaso Roscilde, Phys. Rev. Lett. 105, 199603 (2010).