Statistical Mechanics:

Algorithms and Computations

Werner Krauth

(see Fig. 3.5). The normalized and mutually orthogonal sine functions in eqn (3.20) have a periodicity $2L$, not L, unlike the wave functions in a box with periodic boundary conditions.

Using the plane waves in eqn (3.20) and their energies $E_n = \frac{1}{2}(n\pi/L)^2$, we find the following for the density matrix in the box:

$$
\rho^{\text{box},[0, L]}(x, x', \beta)
$$
$$
= \frac{2}{L} \sum_{n=1}^{\infty} \sin\left(\frac{\pi}{L}nx\right) \exp\left(-\beta\frac{\pi^2 n^2}{2L^2}\right) \sin\left(\frac{\pi}{L}nx'\right)
$$
$$
= \frac{1}{L} \sum_{n=-\infty}^{\infty} \sin\left(n\pi\frac{x}{L}\right) \exp\left(-\beta\frac{\pi^2 n^2}{2L^2}\right) \sin\left(n\pi\frac{x'}{L}\right). \quad (3.21)
$$

We can write the product of the two sine functions as

$$
\sin\left(n\pi\frac{x}{L}\right) \sin\left(n\pi\frac{x'}{L}\right)
$$
$$
= \frac{1}{4}\left[\exp\left(in\pi\frac{x - x'}{L}\right) + \exp\left(-in\pi\frac{x - x'}{L}\right)\right.
$$
$$
\left. - \exp\left(in\pi\frac{x + x'}{L}\right) - \exp\left(-in\pi\frac{x + x'}{L}\right)\right]. \quad (3.22)
$$

Using eqn (3.22) in eqn (3.21), and comparing the result with the formula for the periodic density matrix in eqn (3.11), which is itself expressed in terms of the free density matrix, we obtain

$$
\rho^{\text{box},[0, L]}(x, x', \beta) = \rho^{\text{per},2L}(x, x', \beta) - \rho^{\text{per},2L}(x, -x', \beta)
$$
$$
= \sum_{w=-\infty}^{\infty} \left[\rho^{\text{free}}(x, x' + 2wL, \beta) - \rho^{\text{free}}(x, -x' + 2wL, \beta)\right]. \quad (3.23)
$$

This intriguing sum over winding numbers is put together from terms different from those of eqn (3.21). It is, however, equivalent, as we can easily check in an example (see Fig. 3.6).

In conclusion, we have derived in this subsection the density matrix of a free particle in a box either with periodic boundary conditions or with walls. The calculations were done the hard way—explicit mathematics—using the Poisson sum formula and the representation of products of sine functions in terms of exponentials. The final formulas in eqns (3.18) and (3.23) can also be derived more intuitively, using path integrals, and they are more generally valid (see Subsection 3.3.3).

3.1.4   Density matrix in a rotating box

In Subsection 3.1.3, we determined the density matrix of a free quantum particle in a box with periodic boundary conditions. We now discuss the physical content of boundary conditions and the related counter-intuitive behavior of a quantum system under slow rotations. Our discussion is
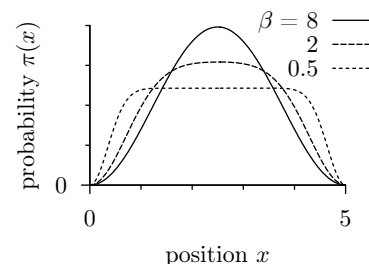
Fig. 3.6 Probability of being at position x for a free particle in a box with walls (from eqn (3.21) or eqn (3.23), with $L = 5$).

a prerequisite for the treatment of superfluidity in quantum liquids (see Subsection 4.2.6), but also for superconductivity in electronic systems, a subject beyond the scope of this book.
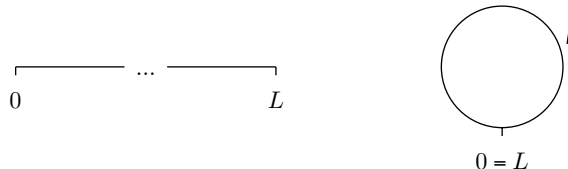

Fig. 3.7 A one-dimensional quantum system on a line of length L (*left*), and rolled up into a slowly rotating ring (*right*).

Let us imagine for a moment a complicated quantum system, for example a thin wire rolled up into a closed circle of circumference L, or a circular tube filled with a quantum liquid, ideally ^{4}He (see Fig. 3.7). Both systems are described by wave functions with periodic boundary conditions $\psi_n(0) = \psi_n(L)$. More precisely, the wave functions in the lab system for N conduction electrons or N helium atoms satisfy

$$\psi_n^{\text{lab}}(x_1, \ldots, x_k + L, \ldots, x_N) = \psi_n^{\text{lab}}(x_1, \ldots, x_k, \ldots, x_N). \qquad (3.24)$$

These boundary conditions for the wave functions in the laboratory frame continue to hold if the ring rotates with velocity v, because a quantum system—even if parts of it are moving—must be described everywhere by a single-valued wave function. The rotating system can be described in the laboratory reference frame using wave functions $\psi_n^{\text{lab}}(x, t)$ and the time-dependent Hamiltonian $H^{\text{lab}}(t)$, which represents the rotating crystal lattice or the rough surface of the tube enclosing the liquid.

The rotating system is more conveniently described in the corotating reference frame, using coordinates x^{rot} rather than the laboratory coordinates x^{lab} (see Table 3.1). In this reference frame, the crystal lattice or the container walls are stationary, so that the Hamiltonian H^{rot} is time independent. For very slow rotations, we can furthermore neglect centripetal forces and also magnetic fields generated by slowly moving charges. This implies that the Hamiltonian H^{rot} (with coordinates x^{rot}) is the same as the laboratory Hamiltonian H^{lab} at $v = 0$. However, we shall see that the boundary conditions on the corotating wave functions ψ^{rot} are nontrivial.

To discuss this point, we now switch back from the complicated quantum systems to a free particle on a rotating ring, described by a Hamiltonian

$$H^{\text{rot}} = -\frac{1}{2} \frac{\partial^2}{(\partial x^{\text{rot}})^2}.$$

We shall go through the analysis of H^{rot}, but keep in mind that the very distinction between rotating and laboratory frames is problematic for the

Table 3.1 Galilei transformation for a quantum system. E^{rot}, p_n^{rot}, and x^{rot} are defined in the moving reference frame.

Reference frame		
Lab.		Rot.
$x^{\text{lab}} = x^{\text{rot}} + vt$		x^{rot}
$p_n^{\text{lab}} = p_n^{\text{rot}} + mv$		p_n^{rot}
$E_n^{\text{lab}} = \frac{1}{2m}(p_n^{\text{lab}})^2$	$E_n^{\text{rot}} = \frac{1}{2m}(p_n^{\text{rot}})^2$	

noninteracting system, because of the missing contact with the crystal lattice or the container boundaries. Strictly speaking, the distinction is meaningful for a noninteracting system only because the wave functions of the interacting system can be expanded in a plane-wave basis. In the rotating system, plane waves can be written as

$$\psi_n^{\text{rot}}(x^{\text{rot}}) = \exp\left(i p^{\text{rot}} x^{\text{rot}}\right).$$

This same plane wave can also be written, at all times, in the laboratory frame, where it must be periodic (see eqn (3.24)). The momentum of the plane wave in the laboratory system is related to that of the rotating system by the Galilei transform of Table 3.1.

$$p_n^{\text{lab}} = \frac{2\pi}{L}n \implies p_n^{\text{rot}} = \frac{2\pi}{L}n - mv \quad (n = -\infty, \dots, \infty). \qquad (3.25)$$

It follows from the Galilei transform of momenta and energies that the partition function $Z^{\text{rot}}(\beta)$ in the rotating reference frame is

$$Z^{\text{rot}}(\beta) = \sum_{n=-\infty}^{\infty} \exp\left[-\beta E_n^{\text{rot}}\right] = \sum_{-\infty}^{\infty} \exp\left[-\frac{\beta}{2}\left(-v + 2n\pi/L\right)^2\right].$$

In the rotating reference frame, each plane wave with momentum p_n^{rot} contributes velocity p_n^{rot}/m. The mean velocity measured in the rotating reference frame is

$$\left\langle v^{\text{rot}}(\beta) \right\rangle = \frac{1}{m Z^{\text{rot}}(\beta)} \sum_{n=-\infty}^{\infty} p_n^{\text{rot}} \exp\left(-\beta E_n^{\text{rot}}\right), \qquad (3.26)$$

with energies and momenta given by eqn (3.25) that satisfy $E_n^{\text{rot}} = (p_n^{\text{rot}})^2/(2m)$. In the limit of zero temperature, only the lowest-lying state contributes to this rotating reference-frame particle velocity. The momentum of this state is generally nonzero, because the lowest energy state, the $n = 0$ state at very small rotation, E_0^{rot}, has nonzero momentum (it corresponds to particle velocity $-v$). The particle velocity in the laboratory frame is

$$\left\langle v^{\text{lab}} \right\rangle = \left\langle v^{\text{rot}} \right\rangle + v. \qquad (3.27)$$

At low temperature, this particle velocity differs from the velocity of the ring (see Fig. 3.8).

The particle velocity in a ring rotating with velocity v will now be obtained within the framework of density matrices, similarly to the way we obtained the density matrix for a stationary ring, in Subsection 3.1.3. Writing x for x^{rot} (they are the same at time $t = 0$, and we do not have to compare wave functions at different times),

$$\psi_n^{\text{rot}}(x) = \sqrt{\frac{1}{L}} \exp\left(i p_n^{\text{rot}} x\right) \quad (n = -\infty, \dots, \infty),$$

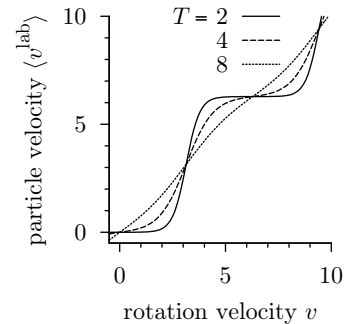$$E_n^{\text{rot}} = \frac{(p_n^{\text{rot}})^2}{2m}.$$

Fig. 3.8 Mean lab-frame velocity of a particle in a one-dimensional ring (from eqns (3.26) and (3.27) with $L = m = 1$).