Effect of periodicity restrictions on the ground state of quantum systems with periodic potentials

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We investigate the effect of periodicity restrictions on the ground state of a quantum system. For a system whose potential is periodic in L and whose wave function is restricted to be periodic in nL, where n is an integer such that $n \geqslant 1$, we prove that observables periodic in L calculated at zero temperature are independent of the value of n. As a result the winding number may be restricted to a value of $w=0$ in ground state calculations, as has been suggested by the numerical results of Henelius *et al.* [Phys. Rev. B **57**, 13 382 (1998)].

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Periodic systems in quantum mechanics have always been of great interest. An example that has received considerable attention recently is the quantum anisotropic planar rotor (QAPR) model [1], developed in an effort to understand the quantum effects in the orientational ordering of diatomic adsorbates on inert surfaces. The model consists of rigid diatomic molecules that are constrained to rotate on a plane due to the presence of the surface. Another system that can be described by a lattice of coupled one-dimensional rotors is that of coupled Josephson oscillators [2]. The list provided here is far from complete, other examples abound in the literature [3].

A system of rotors is distinct from a general periodic system in that there is a periodicity restriction on the wave function. In the case of molecular rotors, the periodicity of the potential is such that it satisfies the periodicity restriction on the wave function, but the value in which the potential is periodic may in general be different from the value in which the wave function is restricted to be periodic (e.g., homonuclear diatomic molecules). For systems such as an electron in the field of a periodic lattice, the potential is periodic, but there is no periodicity restriction on the wave function.

In this report, we concentrate on a particular class of periodic systems. We restrict the potential energy of a system to be periodic in L for all coordinates. Furthermore, we restrict the wave function to be periodic in nL, where n is an integer such that $n \geqslant 1$. Many examples of periodic systems fall into this class of systems (e.g., molecules performing one-dimensional rotation, an electron in a periodic lattice). Although observables may be defined arbitrarily, in most cases observables that characterize the class of systems defined above are periodic in L.

In the study of one-dimensional rotation a helpful concept is that of the winding number. In the Feynman description of quantum statistical mechanics [4], the partition function is obtained by integrating over all cyclic paths in configuration space. In Cartesian space cyclic paths are all deformable into each other. This is not so in the case of one-dimensional rotation. Paths that wind around the circle a different number of times are not deformable into each other. They fall into different homotopy classes, each class labeled by a different value of the winding number. Paths in the same homotopy class are deformable into each other. The value of the winding number for a given path may be defined as the net number of times the path winds around the circle [3,5]. The winding number incorporates the effect of the periodicity restriction on the wave function into the path-integral representation.

Schulman has shown [5] that for systems whose paths fall into different homotopy classes, the partition function may be evaluated by path-integrating in each homotopy class, and then summing over each resulting contribution.

In calculating the properties of periodic systems, care must be taken in incorporating the periodicity restrictions on the wave function. For general quantum many-body systems at finite temperatures, numerical results may be obtained by the path-integral Monte Carlo [6–8] (PIMC) method. The winding number may be incorporated into the PIMC in several different ways [9,10]. Thus, finite temperature simulations of coupled rotors is possible. In the limit of zero temperature it has been conjectured based on numerical evidence by Henelius *et al.* [11] that the winding number may be fixed at $w=0$. Proof for this assertion was only provided for the case of free rotors. Fixing the winding number at $w=0$ corresponds to simulating a system that does not have periodicity restrictions on its wave function. If it was proven that the winding number can be fixed at $w=0$, then zero-temperature methods such as the diffusion Monte Carlo (DMC) [12–14] method or the Green's function Monte Carlo (GFMC) [17,18] would not need to be modified to account for periodicity restrictions due to rotation.

The purpose of this Brief Report is to investigate the assertion of Henelius *et al.* mentioned above, and the role of winding numbers for periodic systems at zero temperature. We prove that restricting the winding number to $w=0$ (i.e., neglecting the periodicity restriction on the wave function) is appropriate in the calculation of observables at zero temperature. The proof consists of two steps. First, we write the partition function of a periodic system as defined above in terms of the winding number, and argue that in the $n=\infty$ case the winding number may be fixed at $w=0$ for any temperature. Second, we prove that in the ground state observables are independent of n.

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Consider a particle with mass m in a potential that is periodic in L and whose wave function is restricted to be periodic in nL, where n is an integer such that $n \geqslant 1$. We treat a one-dimensional system here, but the concepts are trivially generalizable to the many-dimensional case. Based on the considerations above, and based on the results of Schulman [5], we may write the partition function as

$$Q = \sum_{w=-\infty}^{\infty} Q_w, \tag{1}$$

where Q_w is the contribution to the partition function from one homotopy class,

$$Q_w = \int dx \int_x^{x+wnL} \mathcal{D}x(\tau) \exp(-S), \tag{2}$$

where S is the Euclidean action

$$S = \int_0^\beta d\tau \left[\frac{m}{2} \left(\frac{\partial x(\tau)}{\partial \tau} \right)^2 + Vx(\tau) \right]. \tag{3}$$

In the above equations, x denotes the coordinate of the particle, w denotes the winding number, and β denotes the inverse temperature. Note that the paths contributing to Q_w are not cyclic, unless the winding number is zero.

Q_w is defined as the integral over all paths that end at a value that is displaced by wnL compared to their starting point. The set of all such paths can be generated from the set of all cyclic paths by the transformation [16]

$$x(\tau) = \tilde{x}(\tau) + \frac{nL\tau}{\beta} w, \tag{4}$$

where $\tilde{x}(\tau)$ denotes a member of the set of cyclic paths. The transformation of Eq. (4) allows us to write the partition function in a different form,

$$Q = \sum_{w=-\infty}^{\infty} \exp\left(-\frac{mw^2n^2L^2}{2\beta} \right) \int dx \int_x^x \mathcal{D}\tilde{x}(\tau) \exp(-S_w), \tag{5}$$

where

$$S_w = \int_0^\beta d\tau \left[\frac{m}{2} \left(\frac{\partial \tilde{x}(\tau)}{\partial \tau} \right)^2 + V\left(\tilde{x}(\tau) + \frac{nL\tau}{\beta} w \right) \right]. \tag{6}$$

Note, that the paths that enter the Euclidean action S_w are the cyclic paths $\tilde{x}(\tau)$.

Upon inspecting the Gaussian term $\exp(-mw^2n^2L^2/2\beta)$ in Eq. (5), we can deduce the behavior of the system in various limits. At high temperatures ($\beta \to 0$), only the $w=0$ term contributes to the partition function [Eq. (5)]. In this temperature range, the periodicity restriction on the wave function may be neglected. As the temperature is lowered, winding numbers other than zero begin to contribute and the periodicity restriction can no longer be neglected. In the $\beta \to \infty$ (zero temperature) limit, all winding numbers of a given coordinate contribute with equal probabilities to the Gaussian term. For this reason, the assertion of Henelius *et al.* [11] is not obvious.

In the limit $n \to \infty$ only the $w=0$ winding number contributes to the partition function [Eq. (5)], and we recover the partition function of a system whose wave function is not restricted to be periodic. We now prove that ground state observables are independent of n.

Theorem: Consider a many-body Hamiltonian operator

$$H = T + V.$$

Let V be the potential energy operator, and assume that this operator is periodic in L for all coordinates. Let T be the kinetic energy operator. Let Φ be an observable that is periodic in L for all coordinates. Consider the following two systems, both of which have Hamiltonian H: *System A*, the wave function is restricted to be periodic in nL for all coordinates, where n is an integer and $n \geqslant 1$; *System B*, the wave function is restricted to be periodic in L for all coordinates.

If these conditions hold, then the expectation value of Φ taken over the ground state of system A is equal to the expectation value Φ taken over the ground state of system B. Note that the Hilbert space of system B is a subspace of the Hilbert space of system A.

Proof: Let Ψ_g denote the ground state wave function of system A. We may write

$$H\Psi_g(\mathbf{x}) = E_g \Psi_g(\mathbf{x}), \tag{7}$$

where E_g is the ground state energy, and the vector $\mathbf{x}$ represents the coordinates of the system collectively.

Let R_m^i denote the operator that translates the ith coordinate by mL, where m is an integer. Operating on Ψ_g with R_m^i produces a new function that satisfies Eq. (7).

We construct a new function

$$\Psi'(\mathbf{x}) = C \sum_{m_1=1}^{n}, \ldots, \sum_{m_N=1}^{n} R_{m_1}^1, \ldots, R_{m_N}^N \Psi_g(\mathbf{x}), \tag{8}$$

where C is the normalization constant. By construction, the function Ψ' is periodic in L for all coordinates, and is therefore a member of the Hilbert space of system B. Furthermore, Ψ' satisfies

$$H\Psi'(\mathbf{x}) = E_g \Psi'(\mathbf{x}). \tag{9}$$

Since the space of all functions that are periodic in L is a subspace of all functions that are periodic in nL, the ground state energy of the system that is restricted to be periodic in L cannot be less than the ground state energy of the system periodic in nL. Since Ψ' is periodic in L, and its energy is E_g, it follows that E_g is the ground state energy of system B. The ground state energy of the two systems A and B are therefore equal.

For observables periodic in L, one can couple the observable to a constant field [15] and add it to the Hamiltonian. Since the observable is periodic in L, the theorem also holds for the ground state energy of the system that is coupled to the field. Since the expectation value of the observable in the ground state is equal to the derivative of the ground state energy of the coupled system at zero field, it follows that observables are also equal for systems A and B.

In making the connections between physical systems and cases relevant to the theorem we need to consider the meaning of the parameter n. In the simplest case $n=1$ the periodicity associated with the rotation and the periodicity of the potential are equal. A physical example of an $n=1$ system is adsorbed heteronuclear diatomics on a surface constrained to rotate on the plane. A system composed of homonuclear diatomics that are allowed to interconvert between *ortho*- and *parastates* corresponds to the case $n=2$. In this case the periodicity of the rotation is twice the periodicity of the potential. An electron in an infinite periodic lattice is also subject to a periodic potential, but there are no restrictions on its wave function due to periodicity. Hence, the $n=\infty$ case corresponds to particles in infinite periodic lattices.

An important implication of the theorem concerns ground state simulation methods. The $n=\infty$ case of the theorem corresponds to systems with no periodicity restrictions on the wave function. As we have pointed out earlier, in this case only the $w=0$ term contributes to the partition function. It follows that in the zero-temperature limit, the winding number can be neglected in a simulation. This is in contrast to finite temperature simulation methods, where the winding number needs to be included in the simulation. The assertion of Henelius *et al.* is therefore true, provided that the symmetry of the observables in question are the same as the symmetry of the potential.

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