Cylindrical quantum dots with hydrogen-bonded materials

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Abstract
The properties of cylindrical quantum dots are analysed in this paper. Energies of elementary excitations as well as one-particle wavefunctions are found for this structure. For cylindrical quantum wires the temperature of phase transition is found. The behaviour of electric susceptibility in the paraelectric phase is investigated. It is shown that the entropy of cylindrical quantum dots is a quantity depending on two indices. The arithmetical average value of all elements of this matrix is less than the entropy of the corresponding ideal structure.

Introduction
Cylindrical structures are often used in practice (electrical conductors, water tubes). On the other hand these structures appear in animated matter (nerves, blood vessels etc). Therefore the permanent interest in investigations of these structures is understandable.

The goals of our investigation are micro and nano cylindrical structures. The basic characteristics of cylindrical quantum wires will be analysed. Quantum wires will be considered as sufficiently long to make boundary conditions negligible and therefore these will be treated as translation invariant along their axis. In hollow quantum tubes molecules are located in the shell of a cylinder. One cross-section of the tube contains a relatively small number of molecules which is of the order of 5–15 molecules.

In quantum dots the number of molecules along the length is relatively small so boundary conditions must be taken into account. The number of molecules in cross-sections (discs) is of the order of ten.

The main characteristic of cylindrical structures is cyclical invariance in discs. The consequences of this invariance are series of interesting effects which are sometimes of practical interest.

In the first part of this paper, the Hamiltonian of hydrogen-bonded quantum wires will be formulated and dynamical as well as thermodynamical properties will be analysed.

In the second part, energies of elementary excitations in quantum dots will be investigated. The entropy characteristic will be analysed, too.
as follows:

\[
H = \frac{i}{\hbar} \sum_{m,n} \left( J_{m,n,m+1,n} + J_{m,n,m-1,n} + I_{m,n,m,n+1} + I_{m,n,m,n-1} \right)
\]

\[
\times \left( P^*_{m,n} P_{m,n} - \frac{1}{2} \sum_{n'} \left( Y_{m,n,m+1,n'} P_{m+1,n} + Y_{m,n,m-1,n'} P_{m-1,n} + W_{m,n,m,n+1} P_{m+1,n+1} + W_{m,n,m,n-1} P_{m-1,n-1} \right) \right)
\]

\[
+ \frac{1}{2} \sum_{n'} \left( J_{m,n,m+1,n'} P_{m+1,n+1} + J_{m,n,m-1,n'} P_{m-1,n-1} - \frac{i}{2} \sum_{n''} P^*_{m,n} P_{m,n} \right)
\]

\[
- \frac{1}{2} \left( J_{m,n,m+1,n} P_{m+1,n+1} + J_{m,n,m-1,n} P_{m-1,n-1} - \frac{i}{2} \sum_{n'} P^*_{m,n} P_{m,n} \right).
\]

It should be pointed out that the mentioned approximation has been successfully applied in a series of problems [8–10].

Taking into account the approximation used we can write

\[
\{ P_{m,n}, H \} \approx \{ B_{m,n}, H \}.
\]

So the approximate equation of motion is

\[
\hbar \dot{B}_{m,n} = E B_{m,n} = \sigma (J + 1) B_{m,n} - \frac{1}{2} \sigma Y (B_{m+1,n} + B_{m-1,n}) - \frac{1}{2} \sigma W (B_{m,n+1} + B_{m,n-1})
\]

\[
(1.9)
\]

where \( E \) is the energy of elementary excitations.

The one-particle wavefunction of the considered system is

\[
|\psi\rangle = \sum_{m,n} A_{m,n} B^*_{m,n} |\psi\rangle.
\]

(1.10)

From the condition \( \langle \psi | \psi \rangle = 1 \) it follows that

\[
\sum_{m,n} |A_{m,n}|^2 = 1.
\]

(1.11)

In order to find coefficients \( A_{m,n} \) one has to apply the operator

\[
EF - \{ B_{m,n}, H \} = 0
\]

to wavefunction (1.10). In this way the system of equations

\[
\{ E - \sigma (J + 1) A_{m,n} + \frac{1}{2} \sigma Y (A_{m+1,n} + A_{m-1,n}) + \frac{1}{2} \sigma W (A_{m,n+1} + A_{m,n-1}) \} = 0
\]

(1.12) is obtained.

Since the quantum wire is translation invariant along the \( z \) axis we can take the coefficients \( A_{m,n} \) in the form

\[
A_{m,n} = F_n e^{\imath nk}\sigma
\]

(1.13)

where \( \sigma \) is the lattice constant in the \( z \) direction and \( k \) is the wavevector. After substitution of (1.13) into (1.12) one obtains

\[
F_{n+1} + F_{n-1} + \rho F_n = 0 \quad n = 0, 1, 2, \ldots, N
\]

(1.14)

where

\[
\rho = \frac{E - \{ \sigma (J + 1) - \sigma Y \cos \phi \}}{\frac{1}{2} \sigma W}.
\]

(1.15)

Coefficients \( F \) are related to disc molecules and, consequently, they must satisfy the cyclicity condition:

\[
F_{N+1} = F_k \quad k = 0, \pm 1, \pm 2, \ldots
\]

(1.16)

where \( N \) is the total number of molecules in one disc.

We shall look for the solution of (1.14) in the form

\[
F_n = \Phi \cos n\varphi.
\]

(1.17)

From (1.17) it follows that

\[
F_{n+1} + F_{n-1} = F_n \sin 2 \varphi.
\]

(1.18)

This means that the system is satisfied if

\[
\rho = - \varphi.
\]

(1.19)

The value of parameter \( \varphi \) will be determined from the cyclicity condition by substituting (1.17) into (1.16). In such a way we obtain

\[
\sin \frac{N + 1}{2} \varphi \sin \frac{N + 1}{2} \varphi = 0.
\]

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The last is satisfied if
\[ \varphi = \frac{2\pi \nu}{N+1}, \quad \nu = 1, 2, 3, \ldots, N+1. \] (1.20)

Combining (1.20) and (1.15) we obtain the following formula for the energies of the micro-tube elementary excitations:
\[ E_{k\nu} = \sigma(J+I) - \sigma Y \cos \frac{2\pi \nu}{N+1}. \] (1.21)

The function \( F \) is given by the formula
\[ F_n = \Phi \cos \frac{2\pi \nu}{N+1} n \] (1.22)
while the coefficients \( A_{m,n} \) are given by
\[ A_{m,n} = \Phi e^{im\pi \nu} \cos \frac{2\pi \nu}{N+1} n. \] (1.23)

The normalizing condition (1.11) has to be applied in two different ways. If \( \frac{2\pi \nu}{N+1} \) is integer the sum over index \( n \) is equal to \( N+1 \). If \( \frac{2\pi \nu}{N+1} \) is not integer, the sum over index \( n \) is equal \( \frac{N+1}{2\pi \nu} \). Consequently, we obtain a double formula for the wavefunction
\[ |\psi_{k\nu}\rangle = \sum_{m,n} B_{m,n}^+ |0\rangle \] (1.24)

It is clear that the following is valid:
\[ |\psi_{k\nu}\rangle = B_{k\nu}^+ |0\rangle. \] (1.25)

Using this formula and (1.24) we can connect operators acting in momentum space \( B_{k\nu}^+ \) with operators acting in configurational space \( B_{m,n}^+ \) with operators acting in configurational space \( B_{m,n}^+ \) with the following relations:
\[ B_{k\nu}^+ = B_{m,n}^+ \] (1.26)
\[ B_{m,n}^+ = B_{k\nu}^+ \] (1.27)

and the function depending on \( m \) and \( n \) is the following:
\[ |\psi_{m,n}\rangle = \sum_{n,n} B_{m,n}^+ |0\rangle \] (1.28)

Taking into account the fact that the part of the wavefunction corresponding to disc molecules is a real one it can be concluded that the probability current exists only in the \( z \)-direction,
\[ j = \frac{\hbar}{2m^*} \left( \frac{\partial}{\partial (\rho m a)} |\psi\rangle - \frac{\partial}{\partial (\rho m a)} \langle\psi| \right) = \hbar k_0 \cos 2\pi \frac{m}{N+1}. \] (1.29)

At the end of this part two things will be noticed. The first of these is the fact that in quantum tubes containing \( 2^n \) molecules in a disc \( n \geq 2 \), some specific selection rules take place. These rules prohibit the appearance of some excitations on the determining string of the tube. The same is valid for probability currents: some of them cannot flow along some of the determining strings of the tube.

The second objection is rather of formal character. The usual approach to solving the system of difference equations (1.18) is writing this system in developed form and equating the determinant system with zero \([11, 12]\). In the given case determinants are of Fibonacci type.

Equating to zero (1.29) one finds \( \rho \) and \( \varphi \). This calculation is sometimes complicated, as seen in this section. It is not necessary to look for the solution of the Fibonacci equation. It is sufficient to analyse the cylindricity condition and therefrom the values of \( \rho \) and \( \varphi \) immediately follow.

2. Thermodynamics of quantum wire (ferro- and paraelectric phase transitions)

Thermodynamical properties of quantum tubes will be analysed by the method of a two-time Pauli Green function.
\[ \langle P_{m,n}(t)|P_{m,n}^+(0) \rangle = \Theta(t) [P_{m,n}(t), P_{m,n}^+(0)]. \] (2.1)

In this formula \( \Theta(t) \) is Heaviside’s step function:
\[ \Theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases}. \] (2.2)

Differentiating (2.1) over \( t \) and using the equations of motion of the Pauli operator we come to the following equation:
\[ \frac{\text{d}}{\text{d}t} \langle (P_{m,n}(t)) P_{m',n'}(0) \rangle = \imath \hbar \delta_{m,m'} \delta_{n,n'} \delta(t) 
+ \langle (P_{m,n}(t), H) | P_{m',n'}^*(0) \rangle. \] (2.3)

After the substitution of commutator (1.5) into (1.3) we obtain
\[ \frac{\text{d}}{\text{d}t} \langle (P_{m,n}(t)) P_{m',n'}(0) \rangle = \imath \hbar \sigma \delta_{m,m'} \delta_{n,n'} \delta(t) 
+ (J + I) \langle (P_{m,n}(t)) P_{m',n'}^*(0) \rangle 
- \frac{1}{2} Y \langle (P_{m+1,n}(t)) P_{m',n'}^*(0) \rangle + \langle (P_{m-1,n}(t)) P_{m',n'}^*(0) \rangle 
- \frac{1}{2} W \langle (P_{m,n+1}(t)) P_{m',n'}^*(0) \rangle + \langle (P_{m,n-1}(t)) P_{m',n'}^*(0) \rangle 
+ Y \langle (P_{m,n}^*(t)) P_{m+1,n}^*(0) \rangle 
+ Y \langle (P_{m,n}^*(t)) P_{m-1,n}^*(0) \rangle 
+ W \langle (P_{m,n+1}^*(t)) P_{m',n'}^*(0) \rangle 
+ W \langle (P_{m,n-1}^*(t)) P_{m',n'}^*(0) \rangle. \] (2.4)

Applying to (2.4) Tyablikov's approximation which was described in section 1,
\[ \langle (P_{m,n}^*(t)) P_{m,n}^*(0) \rangle \approx \frac{1 - \sigma}{2} \langle (P_{m,n}^*(t)) P_{m,n}^*(0) \rangle \] (2.5)

we reduce (2.4) to
\[ \frac{d}{dt} \langle (P_{m,n}(t)) P_{m,n}(0) \rangle = \imath \hbar \sigma \delta_{m,m'} \delta_{n,n'} \delta(t) 
+ (J + I) \langle (P_{m,n}(t)) P_{m,n}^*(0) \rangle 
- \frac{1}{2} Y \langle (P_{m+1,n}(t)) P_{m,n}^*(0) \rangle + \langle (P_{m-1,n}(t)) P_{m,n}^*(0) \rangle 
- \frac{1}{2} W \langle (P_{m,n+1}(t)) P_{m,n}^*(0) \rangle + \langle (P_{m,n-1}(t)) P_{m,n}^*(0) \rangle 
+ Y \langle (P_{m,n}^*(t)) P_{m+1,n}^*(0) \rangle 
+ Y \langle (P_{m,n}^*(t)) P_{m-1,n}^*(0) \rangle 
+ W \langle (P_{m,n+1}^*(t)) P_{m,n}^*(0) \rangle 
+ W \langle (P_{m,n-1}^*(t)) P_{m,n}^*(0) \rangle. \] (2.6)

After transformations
\[ \langle (P_{m,n}(t)) P_{m,n}^*(0) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{M(N+1)} \text{d} \omega \times \sum_{k,\psi} \langle (P|P^*) \rangle_{k,\psi} \text{e}^{\imath k(n-m') + \imath \psi(n-n')} \] (2.7)

we obtain the following equation for the Green function:
\[ E - \sigma (J + I) + \sigma Y \cos \alpha \kappa + \sigma W \cos \frac{2\pi \nu}{N+1} \times G_{k,v}(\omega) = \frac{\sigma}{2\pi} \] (2.8)

where
\[ N = M(N+1) \]
\[ F_k = J + I - Y \cos \alpha \kappa - W \cos \frac{2\pi \nu}{N+1} \] (2.10)
\[ \Theta = k_B T. \]

Since the ordering parameter \( \sigma \) is close to zero in the vicinity of the transition temperature, the following approximation can be used:
\[ \coth \sigma \approx \frac{1}{\frac{1}{e} + \frac{1}{3}.} \] (2.11)

Applying (2.11) to (2.9) we obtain
\[ \sigma = \sqrt{L} \sqrt{1 - \frac{\Theta}{\Theta_c}} \] (2.12)

where
\[ L = \frac{6\lambda M(N+1)}{\sum_{k,v} \frac{1}{f_k}} \] (2.13)

and
\[ \Theta_c = \frac{1}{M(N+1)} \sum_{k,v} \frac{1}{f_k}. \] (2.14)

Taking into account that \( Y \) and \( W \) are noticeably less than \( J \) and \( I \) one can write the function \( \frac{1}{\sigma} \) in (2.14) as a geometric progression exact up to the quadratic term. After simple calculations one can obtain the phase transition temperature:
\[ \Theta_c = \frac{1}{2} \left( J + I - \frac{1}{2} Y^2 + W^2 \right). \] (2.15)

The transition from the ferroelectric to paraelectric phase is a second kind phase transition since the derivative of the internal energy over temperature is infinite at the phase transition temperature.

Analysis of the behaviour of a quantum tube in the paraelectric phase requires inclusion of the energy of the external field \( pE \), where \( p \) is the dipole momentum.
\[ \sigma = 1 - \frac{2\sigma}{M(N+1)} \int_{-\infty}^{\infty} \exp(\sigma \frac{p E(x)}{2\Theta}) - 1 \]
\[ = \theta \left( \frac{p E}{2\Theta} + \frac{J + I}{2\Theta} \right). \] (2.16)

In the analysis small terms \( Y \) and \( W \) will be neglected [13]. After these approximations and applications of the formula (2.9) it follows that
\[ \sigma \approx \frac{p E}{2\Theta} + \frac{\sigma(J + I)}{2\Theta} \frac{1}{\text{ch}^2 \frac{p E}{2\Theta}} \]

wherefrom
\[ \sigma \left( 1 - \frac{J + I}{2\Theta} \frac{1}{\text{ch}^2 \frac{p E}{2\Theta}} \right) = \Theta \frac{p E}{2\Theta}. \] (2.17)

Since the electric susceptibility is defined as
\[ \chi = \lim_{E \rightarrow 0} \frac{\partial \sigma}{\partial E} \] (2.18)
one has to differentiate $\sigma$ over field $E$ with $E$ tending to zero. In this way one obtains
\[
\chi = \frac{p}{2} \frac{1}{\Theta - \Theta_0^{(0)}} \tag{2.19}
\]
where
\[
\Theta_0^{(0)} = \frac{J + 1}{2} \tag{2.20}
\]
It is clear from (2.19) that electric susceptibility tends to infinity when the temperature of the paraelectric phase tends to $\Theta_0^{(0)}$.

3. Wavefunction and energy spectrum in quantum dots

The conditions valid for a quantum wire are the same in discs of quantum dots, but index $m$, determining the positions of the discs along the $z$ axis, takes the relatively small set of values $m = 0, 1, 2, \ldots, M$, where $M$ is of the order of ten.

Taking this into account we can write the Hamiltonian of quantum dots as follows:
\[
H = \sum_{m=0}^{M} \sum_{n=0}^{N} \sigma (I + J) B_{m,n}^* B_{m,n} - \frac{1}{2} \sigma Y \sum_{n=0}^{N} B_{m,n}^* (B_{m,n+1} + B_{m,n-1}) - \frac{1}{2} \sigma W \sum_{m=0}^{M} B_{m,n}^* (B_{m,n+1} + B_{m,n-1}) \tag{3.1}
\]
The one-particle wavefunction
\[
|\psi\rangle = \sum_{m=0}^{M} \sum_{n=0}^{N} A_{mn} B_{m,n}^* |0\rangle \tag{3.2}
\]
is normalized by the condition $\langle \psi | \psi \rangle = 1$ wherefrom it follows that
\[
\sum_{m,n} |A_{mn}|^2 = 1. \tag{3.3}
\]
Coefficients $A_{mn}$ satisfy the system of difference equations
\[
[E B_{m,n} - [B_{m,n}^* H]] |\psi\rangle = 0. \tag{3.4}
\]
Since the commutator $[B_{m,n}, H]$ is:
\[
[B_{m,n}, H] = \sigma (I + J) B_{m,n} - \frac{1}{2} \sigma Y (B_{m+1,n} + B_{m-1,n}) - \frac{1}{2} \sigma W (B_{m,n+1} + B_{m,n-1}) \tag{3.5}
\]
equation (3.4) goes over to
\[
[E - \sigma (I + J)] A_{mn} + \frac{1}{2} \sigma Y A_{mn+1} + \frac{1}{2} \sigma W (A_{m+1,n} + A_{m,n-1}) = 0. \tag{3.6}
\]
The method of separation of variables will be used in solving system (3.6), i.e. it will be taken that
\[
A_{mn} = \Phi_{m} F_{n}. \tag{3.7}
\]
After substitution of (3.7) into (3.6) the latter becomes
\[
[E - \sigma (I + J)]\Phi_{m} F_{n} + \frac{1}{2} \sigma Y \Phi_{m} F_{n+1} + \frac{1}{2} \sigma W (F_{n+1} + F_{n-1}) = 0. \tag{3.8}
\]
It should be noticed that for $\Phi_{m}$ and $F_{n}$ given by
\[
\Phi_{m} = \sum_{s} \alpha_{s} \sin(m + s) \tag{3.9}
\]
it follows that
\[
\Phi_{m+1} + \Phi_{m-1} = \Phi_{m} 2 \cos ak \tag{3.10}
\]
Combining (3.10) and (3.8) we obtain
\[
[E - \sigma (I + J) + \sigma Y \cos ak + \sigma W \cos \varphi] \Phi_{m} F_{n} = 0 \tag{3.11}
\]
wherefrom we find the expression for energy:
\[
E = \sigma (I + J) - \sigma Y \cos ak - \sigma W \cos \varphi. \tag{3.12}
\]
The parameter $\varphi$ has to be determined from the cyclicity condition over discs. This was done in the previous section and the result obtained is
\[
\varphi = \frac{2\pi v}{N + 1} \quad v = 1, 2, 3, \ldots, N + 1. \tag{3.13}
\]
The values of parameters $ak$ will be determined from boundary equations for coefficients $\Phi$ in the $z$ direction. These boundary equations are
\[
\Phi_{-1} = 0 \tag{3.14}
\]
\[
\Phi_{M+1} = 0. \tag{3.15}
\]
The two boundary conditions require function $\Phi_{m}$ with two undetermined coefficients $\lambda_{1}$ and $\lambda_{2}$:
\[
\Phi_{m} = \lambda_{1} \sin mak + \lambda_{2} \sin(m-1)ak. \tag{3.16}
\]
Function (3.16) has to satisfy the conditions (3.14) and (3.15) for
\[
ak \neq 0; \quad \sin ak \neq 0. \tag{3.17}
\]
In this case we obtain the following system of equations, determining $\lambda_{1}$ and $\lambda_{2}$:
\[
\lambda_{1} \sin(M + 1)ak - \lambda_{2} \sin Mak = 0 \tag{3.18}
\]
\[
\lambda_{1} + 2\lambda_{2} \cos ak = 0. \tag{3.19}
\]
The determinant of this system is equal to zero when parameters $ak$ take values
\[
ak = \frac{\pi \mu}{M + 2}; \quad \mu = 1, 2, \ldots, M + 1. \tag{3.20}
\]
If condition (3.20) is satisfied the coefficients $\Phi_{m}$ are given by
\[
\Phi_{m} = \alpha \sin(m + 1)ak = \alpha \sin (m + 1) \pi \mu \tag{3.21}
\]
where $\alpha$ is an arbitrary constant. In the previous section it was obtained that
\[
F_{n} = \beta \cos \frac{2\pi v}{N + 1} \tag{3.22}
\]
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where $\beta$ is an arbitrary constant. Combining (3.21), (3.22) and (3.7) we obtain

$$A_{m,n} = A_0 \sin \frac{\pi \mu}{M + 2} (m + 1) \cos \frac{2\pi v}{N + 1} n$$

$m = 0, 1, 2, \ldots, M; n = 0, 1, 2, \ldots, N$.

$\mu = 1, 2, \ldots, M + 1; \nu = 1, 2, \ldots, N + 1$. (3.23)

The normalizing coefficients $A_0$ differ for the cases if $\frac{2\mu}{M + 1}$ is integer and if $\frac{2\nu}{N + 1}$ is not integer.

The total wavefunction is the result of the direct product of the particle wavefunctions depending on the couples of subindices $(\mu, \nu)$ and those depending on the couples of subindices $(m, n)$. Consequently, we obtain a split formula for the wavefunction:

$$|\xi_{\mu,\nu}\rangle =$$

$$= l \text{ (integer)}$$

$$= l \text{ (integer)}$$. (3.24)

The function depending on configurational indices $m$ and $n$ is also given by a split formula:

$$|\xi_{m,n}\rangle =$$

$$= l \text{ (integer)}$$

$$= l \text{ (integer)}$$. (3.25)

From (3.12), (3.13) and (3.20) one can obtain the expression for the energy of elementary excitations in cylindrical quantum dots

$$E = \sigma (j + 1) - \sigma Y \cos \frac{\pi \mu}{M + 2} - \sigma W \cos \frac{2\pi v}{N + 1} \mu = 1, 2, \ldots, M + 1; \nu = 1, 2, \ldots, N + 1$$. (3.26)

At the end of this section the entropy properties of cylindrical quantum dots will be analysed. For clarity the entropy of an ideal structure will be analysed first. The one-particle wavefunction of the structure, depending on $\mu$ and $\nu$, is given by

$$|\xi_{\mu,\nu}\rangle_{id} = \frac{1}{\sqrt{(M + 1)(N + 1)}} e^{i\mu(\mu + \nu)v} B_{m,n}^{*}[0]$$

wherefrom the probability of experimental registration of excitation with energy $E_{\mu,\nu}$ is given by

$$V_{m,n}^{\mu,\nu} = \frac{1}{\sqrt{(M + 1)(N + 1)}} e^{i\mu(\mu + \nu)v} B_{m,n}^{*}[0]$$

so that the probability of excitation registration is the same as (3.28). The entropies calculated using the found possibilities are given by

$$S_{m,n}^{\mu,\nu} = - \sum_{m,n} V_{m,n}^{\mu,\nu} \ln V_{m,n}^{\mu,\nu} = S_{m,n}$$

$$= - \sum_{m,n} V_{m,n}^{\mu,\nu} \ln V_{m,n}^{\mu,\nu} = \ln (M + 1)(N + 1) \text{ (3.30)}$$

As can be seen in ideal structures the entropies of the configurational distribution of excitations and of the momentum one are usually mutually equal (equal to one another) and equal to the number of molecules of the structure.

For cylindrical quantum dots the possibility of registration of excitation at the point $(m, n)$ is

$$\Pi_{m,n}^{\mu,\nu} =$$

$$\frac{2}{(M + 2)(N + 1)} \sin^2 \frac{\pi \mu}{M + 2} \frac{2\nu}{N + 1} = l \text{ (integer)}$$

$$\times \cos^2 \frac{2\pi v}{N + 1} za \frac{2n}{N + 1} \neq l \text{ (integer)}$$. (3.31)

Since

$$\sum_{m=0}^{M} \sum_{n=0}^{N} \Pi_{m,n}^{\mu,\nu} = 1$$

the entropies of the momentum distribution of excitations are given by

$$S_{m,n}^{\mu,\nu} = - \sum_{m,n} \Pi_{m,n}^{\mu,\nu} \ln \Pi_{m,n}^{\mu,\nu} \text{ (3.33)}$$

It is seen that in general entropy is a rectangular matrix. This means that different values of the entropy exist depending on the indices used, i.e. depending on the state occupied by the particle.

From (3.25) can be found the probability of registrations of the excitations with energy $E_{\mu,\nu}$

$$R_{m,n}^{\mu,\nu} =$$

$$\frac{2}{(M + 2)(N + 1)} \sin^2 \frac{\pi \mu}{M + 2} \frac{2\nu}{N + 1} = l \text{ (integer)}$$

$$\times \cos^2 \frac{2\pi v}{N + 1} za \frac{2n}{N + 1} \neq l \text{ (integer)}$$. (3.34)
In this case it is valid that
\[ \sum_{m=0}^{M} \sum_{n=0}^{N} R_{m,n}^{\mu,\nu} = 1. \] (3.35)

The entropy of the configurational distribution of excitations can be found as
\[ S_{m,n} = -\sum_{m,n} R_{m,n}^{\mu,\nu} \ln R_{m,n}^{\mu,\nu}. \] (3.36)

The entropy of the configurational distribution is also a rectangular matrix.
The matrices \( S_{m,n}^{\mu,\nu} \) and \( S_{m,n} \) are not equal. They are symmetric with each other with respect to the secondary diagonal.

To make this clear, some illustrative examples will be quoted. The entropy of the ideal structure with \( (3 \times 3) \) molecules is
\[ S_{id} = \ln 9 = 2.20. \] (3.37)

The entropy of the momentum distribution of excitations in cylindrical quantum dots with \( N = 2 \) is given by
\[ (S^{\mu,\nu})_{3 \times 3} = \begin{pmatrix} 1.91 & 1.56 & 1.91 \\ 1.91 & 1.56 & 1.91 \\ 2.14 & 1.79 & 2.14 \end{pmatrix}. \] (3.38)

while the entropy of the configurational distribution has the form
\[ (S_{m,n})_{3 \times 3} = \begin{pmatrix} 2.14 & 1.91 & 1.91 \\ 1.79 & 1.56 & 1.56 \\ 2.14 & 1.91 & 1.91 \end{pmatrix}. \] (3.39)

The symmetry of configurational and momentum matrices with respect to the secondary diagonal is obvious. If the elements of the configurational matrix change places across the secondary diagonal the momentum matrix is obtained. This symmetry is valid for all quadratic entropy matrices.

For the case \( M = N = 3 \) the entropy of the ideal structure is
\[ S_{id} = \ln 16 = 2.77. \] (3.40)

The entropy matrix for the configurational distribution of excitations in corresponding quantum dots is
\[ (S_{m,n})_{4 \times 4} = \begin{pmatrix} 2.67 & 1.98 & 2.67 & 1.98 \\ 2.67 & 1.98 & 2.67 & 1.98 \\ 2.67 & 1.98 & 2.67 & 1.98 \\ 2.67 & 1.98 & 2.67 & 1.98 \end{pmatrix}. \] (3.41)

The entropy matrix of the momentum distribution is
\[ (S^{\mu,\nu})_{4 \times 4} = \begin{pmatrix} 1.97 & 1.97 & 1.91 & 1.97 \\ 2.67 & 2.67 & 2.67 & 2.67 \\ 1.97 & 1.97 & 1.97 & 1.97 \\ 2.67 & 2.67 & 2.67 & 2.67 \end{pmatrix}. \] (3.42)

Symmetry with respect to the secondary diagonal appears here too.
As an example for a rectangular matrix quantum dot having four molecules in the disc 12 molecules along the \( z \) axis will be taken. It is interesting to note that the configurational matrix has four columns and 12 rows while the momentum matrix has 12 columns and four rows.

The mentioned matrices are given by the formulae (3.43) and (3.44):
\[ (S^{\mu,\nu})_{4 \times 12} = \begin{pmatrix} 2.95 & 2.95 & \cdots & 2.95 \\ 3.64 & 3.64 & \cdots & 3.64 \\ 2.95 & 2.95 & \cdots & 2.95 \\ 3.64 & 3.64 & \cdots & 3.64 \end{pmatrix} \] (3.43)

\[ (S_{m,n})_{12 \times 4} = \begin{pmatrix} 3.64 & 2.95 & 3.64 & 2.95 \\ 3.64 & 2.95 & 3.64 & 2.95 \\ \cdots & \cdots & \cdots & \cdots \\ 3.64 & 2.95 & 3.64 & 2.95 \end{pmatrix}. \] (3.44)

At the end of these considerations the entropies of ideal structures will be compared to arithmetical averages of matrix elements of the corresponding entropy matrices of quantum dots. The numerical values are the following. For the ideal structures we have
\[ (S)_{3 \times 3} = \ln 9 = 2.20 \]
\[ (S)_{4 \times 4} = \ln 16 = 2.77 \] (3.45)
\[ (S)_{4 \times 12} = \ln 48 = 3.87. \]

The average values of matrix elements are equal for configurational entropy and momentum entropy. So we have
\[ \langle S \rangle_{3 \times 3} = 1.76 \]
\[ \langle S \rangle_{4 \times 4} = 2.32 \] (3.46)
\[ \langle S \rangle_{4 \times 12} = 3.30. \]

It should be pointed out that cylindrical quantum dots in all cases have average entropy lower than the entropy of corresponding ideal structures. This leads to the conclusion that quantum dots are more ordered systems than the corresponding ideal structures.

4. Conclusion

The analysis of cylindrical quantum dotss has shown that these structures possess a series of interesting properties whose application can lead to new physical results. The most interesting is the fact that in a geometrical regular structure energetical defects and vacancies appear.

The authors have made an effort to give a wide picture of cylindrical hydrogen bonded structures. The wavefunctions, energies of elementary excitations, phase transitions and entropy properties have been investigated.

Finally it should be pointed out that the references which have been quoted up to now were mainly used to explain some starting formulae.

Investigation of micro and nano cylindrical structures has been very popular for several years so that citation of all attempts in this domain are practically impossible. We wish to note that most papers are dedicated to carbon nano-tubes which obey high transfer properties (see for example [20, 21]).
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