Vol 18 No 10, October 2009
1674-1056/2009/18(10)/4130–06

Chinese Physics B

© 2009 Chin. Phys. Soc.
and IOP Publishing Ltd

The nonlinear Wannier function in square Krönig–Penney model*

Xue Rui(薛 锐)[a], Liang Zhao-Xin(梁兆新)[b], and Li Wei-Dong(李卫东)[a]†

[a] *Institute of Theoretical Physics and Department of Physics, Shanxi University, Taiyuan 030006, China*

[b] *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China*

(Received 5 March 2009; revised manuscript received 17 April 2009)

The nonlinear Wannier functions in square Krönig-Penney potential are investigated with the help of a set of exact nonlinear Bloch solutions. The nonlinear interaction makes the Wannier functions fall off as non-exponential law with distance and enhances the tunneling coupling between the neighbor sites.

Keywords: exact nonlinear Bloch solution, nonlinear Wannier function
PACC: 0365, 7115B

1. Introduction

One of the project of Bose-Einstein condensates (BECs), as a quantum simulator, is loading it into optical lattice to test the basic concepts in solid state physics. Since the experiment realization for superfluid-Mott insulator transition,[1] the Josephson oscillation[2] and bright gap solitons,[3] the theoretical research on this object has been extensively explored such as the loop structures,[4] dynamical instabilities,[5] transport of BECs,[6] etc. In the point of theoretical view, the tight-binding approximation plays an important role in constructing Bose-Hubbard model,[7] discrete nonlinear Schrödinger,[8] and further understanding the physics of BECs in lattice.

To apply the tight-binding (t-b) approximations into a periodic system, one has to find the Wannier functions (WFs), which form the orthogonal and complete set basis. It has been extensively proved that WFs play an important role in expressing localized states in crystalline solids and developing the electron theory of solids. Therefore, they are extensively studied in solid-state physics[9−13] in the past several decades. The key property of the Wannier function is that they are localized around the site[14] and somewhat similar to atomic wave function at the same site. Similarly, the WFs are also very important in nonlinear case, the Bose-Hubbard model and discrete nonlinear Schrödinger are obtained by assuming there exists a complete WFs.[7,8]

In this paper, we are going to study the lowest nonlinear Wannier functions in square Krönig–Penney (KP) potential, based on a set of exact nonlinear Bloch solutions. The linear Schröinger equation with this potential, exactly solved in the 1930s, presents a clearing physical picture to understand the solid theory.[15,16] It is interesting to note that the nonlinear Schrödinger equation (NLSE), with the same KP external potential, can be derived analytically. In the frame of mean-field theory, Bloch states of a BEC in a Krönig–Penney potential, which is composed of a lattice of δ function, have been reported in Refs.[17], [18] and [19]. Here we extend these δ functions to the square potentials, called as square Krönig–Penney potential. Since the properties of WFs are determined by its phase changing, we are going to find the one special Wannier function, suggested by Kohn in 1959.[9] For each Bloch band there exists a unique WF possessing the following basic properties; (i) it is symmetric to either $x = 0$ or $x = T/2$; (ii) it is real, and (iii) it is falling off exponentially with distance.[9] After that, we calculate the two important parameters in the Bose-Hubbard model, the on-site interaction U and the corresponding hopping terms J.

*Project supported by the National Natural Science Foundation of China (Grant No 10674087), 973 Program (Grant Nos 2006CB921603 and 2008CB317103), the Natural Science Foundation of Shanxi Province of China (Grant No 200611004), NCET (NCET-06-0259) and IMR SYNL-T.S. Kê Research Fellowship.

†Corresponding author. E-mail: wdli@sxu.edu.cn

This paper is structured as follows. In Section 2, we review the basic properties of Wannier function. In Section 3, the exact Bloch solutions of NLSE with a square KP potential are presented. And then, we obtain the nonlinear Wannier function for various potential depth and nonlinear interaction in Section 4. Section 5 concludes this paper.

2. Wannier function

For a 1D crystal with lattice period T along x axis, the Bloch function satisfies[20]

$$\psi_{lq}(x) = \mathrm{e}^{\mathrm{i}\,qx}\phi_{lq}(x), \tag{1}$$

where $\phi_{lq}(x)$ is a periodic function and it satisfies the condition $\phi_{lq}(x) = \phi_{lq}(x+T)$, q is the quasimomentum of the state and l is the band index.

The dynamics of particles moving in the lowest lying well separated bands can also be described by Wannier functions. The Wannier functions, localized at lattice site x_i, could be found by Fourier transformation

$$W_l(x-x_i) = \frac{T}{2\pi}\int_{-\pi/T}^{\pi/T}\psi_{lq}(x)\mathrm{e}^{-\mathrm{i}\,q\cdot x_i}\mathrm{d}q. \tag{2}$$

These Wannier functions are complete sets of orthogonal normalized real mode functions for each band l,

$$\int \mathrm{d}x W_l^*(x-x_i)W_{l'}(x-x_{i'}) = \delta_{ll'}\delta_{ii'}. \tag{3}$$

The normalization in Eq.(3) presupposes that the Bloch functions are normalized in a unit cell of the lattice:

$$\int_{\mathrm{cell}} |\psi_{lq}(x)|^2\,\mathrm{d}x = 1. \tag{4}$$

Kohn proved that for each Bloch band there exists a unique Wannier function $W_n(x)$ with the following three properties: they are symmetric, real, and decay exponentially.[9]

For the nonlinear case, one expected that there are the nonlinear Wannier functions in Refs.[7] and [8] and the orthogonality of them has been proved in Ref.[27].

3. Model and the solution

To have the nonlinear Wannier function, we consider the following one-dimensional (1D) stationary NLSE (or Gross–Pitaevskii equation), which has been proved to describe the dynamics of BEC's at ultra-low temperature [21,22]

$$\mu\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{\mathrm{pot}}(x) + gnT \mid \psi(x)\mid^2\right) \times \psi(x), \tag{5}$$

where μ is the chemical potential, $g = 4\pi\hbar^2 a_{\mathrm{s}}/m$ is the nonlinear coupling constant and a_{s} is 1D reduced s-wave scattering length. The square KP potential is given by

$$V_{\mathrm{pot}}(x) = \sum_{n=-\infty}^{+\infty} V_{\mathrm{q}}(x-nT) \tag{6}$$

with

$$V_{\mathrm{q}} = \begin{cases} 0, & -a < x < a, \\ V_0, & a < x < a+b. \end{cases}$$

After introducing $\psi(x) = r(x)\exp(-\mathrm{i}\,\Theta(x))$ (in dimensionless units), equation (5) can be rewritten as

$$\left(\frac{\partial\rho(x)}{\partial x}\right)^2 = 2\eta\rho(x)^3 + 4(\mu - V_{\mathrm{pot}})\rho(x)^2 - \beta\rho(x) - 4\alpha^2, \tag{7}$$

and

$$\Theta = \int \mathrm{d}x\frac{\alpha}{\rho(x)}, \tag{8}$$

where $\rho(x) = r^2(x)$, is the density of the state and β is an integral constant. α is another integral constant and has a simple physical meaning: the current of the quantum state. In our paper, we measure lengths in units of T/π, where $T = 2a + b$ is the period of the external potential, and energies in units of the recoil energy $E_{\mathrm{R}} = \hbar^2 q_{\mathrm{B}}^2/2m$, with the Bragg momentum $q_{\mathrm{B}} = \pi/T$. $\eta = gnT/E_{\mathrm{R}}$ represents the nonlinear interaction and n is the average density.

It has been proven that the solution of Eq.(7) can be written in terms of the Jacobi elliptic functions (SN, SC and NC).[23–26] Generally, we can have two different solutions depending on the relation of the chemical potential and the barrier height. Firstly for $\mu > V_0$,

$$\rho_1(x) = A/8K^2 - \left(A/8K^2 - 128K^4\alpha^2/A\left(16K^4 + A\eta\right)\right)\mathrm{SN}^2(Kx+\delta, n_1).$$

For $\mu < V_0$, we have two different solutions, depending on the number (only 0 or 1) of the nodes within the barrier. For the case without nodes in the barrier region, the solution is

$$\rho_2(x) = B/8Q^2 + (B/8Q^2 + 128Q^4\alpha^2/B\left(16Q^4 - B\eta\right))\mathrm{SC}^2(Qx+\gamma, n_2).$$

But for the case having one node in barrier,

$$\rho_2(x) = -B/8Q^2 + \left(Q^2/\eta + B/8Q^2 - Q\sqrt{BQ^2 - 16\alpha^2\eta}/\sqrt{B}\eta\right)\mathrm{NC}^2(Qx+\gamma, n_2).$$

According to the Bloch theory, one can find the Bloch solutions and the corresponding energy spectrum for KP potential. Imposing the continuity of the wave function and continuity of the first derivative of the wave function at $x = a$, and the Bloch periodic condition, we have

$$\rho_1(a) = \rho_2(a), \tag{9}$$

$$\partial_x\rho_1(a) = \partial_x\rho_2(a), \tag{10}$$

$$\rho_1(-a) = \rho_2(T), \tag{11}$$

$$\partial_x\rho_1(-a) = \partial_x\rho_2(T), \tag{12}$$

and

$$\Theta_2(T) - (\Theta_1(-a) - qT) = 2n\pi. \tag{13}$$

Since the nonlinearity, we need another two conditions: the continuity of chemical potential

$$\mu_1 = \mu_2, \tag{14}$$

and the normalization of wave function

$$\int_{-a}^{a}\rho_1(x)\,\mathrm{d}x + \int_{a}^{T}\rho_2(x)\,\mathrm{d}x = 1. \tag{15}$$

Principally, we can fix the free parameters A, B, K, Q, δ, γ, α by simultaneous solving Eqs.(9)–(15). For example, given the well width $2a = 0.8$ and barrier width $b = 0.2$ (will be used throughout this paper), the lowest Bloch states ($l = 0$) for $q = 0.5\pi$ in different system parameters are plotted in Fig.1. The shaded part denotes the barrier region in all the figures. Since the Bloch wave functions are complex, the real part and the imaginary part of Bloch wave functions ψ_q, for given interatomic interaction ($gn = 0.1E_\mathrm{R}$) and different potential depth ($V_0 = 10E_\mathrm{R}$, $30E_\mathrm{R}$, $60E_\mathrm{R}$), are presented in Figs.1(a) and 1(c) respectively. Meanwhile, for given potential ($V_0 = 60E_\mathrm{R}$) and different interatomic interactions ($gn = 0, 5E_\mathrm{R}$, $10E_\mathrm{R}$), they are plotted in Figs.1(b) and 1(d) respectively. It is easy to see that increasing the potential depth and the nonlinear interaction makes the Bloch wave function locate within the well. The difference between these two cases is the response of the wave functions. For increasing the potential depth, it becomes sharper and sharper (see Figs.1(a) and 1(c)). While for increasing the nonlinear interaction, it becomes broader and broader (see Figs.1(b) and 1(d)).

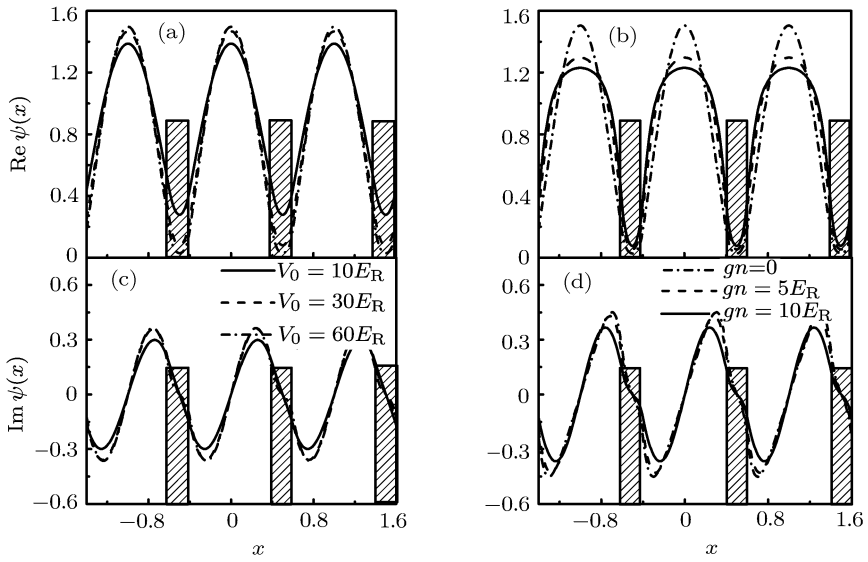


Fig.1. (a), (b) $\mathrm{Re}\,\psi_q(x)$ with $V_0 = 10E_\mathrm{R}$, $30E_\mathrm{R}$, $60E_\mathrm{R}$ for $q = 0.5\pi$, $gn = 0.1E_\mathrm{R}$ and with $V_0 = 60E_\mathrm{R}$ for $q = 0.5\pi$, $gn = 0, 5E_\mathrm{R}, 10E_\mathrm{R}$ respectively. (c), (d) $\mathrm{Im}\,\psi_q(x)$ with $V_0 = 10E_\mathrm{R}$, $30E_\mathrm{R}$, $60E_\mathrm{R}$ for $q = 0.5\pi$, $gn = 0.1E_\mathrm{R}$ and with $gn = 0, 5E_\mathrm{R}, 10E_\mathrm{R}$ for $q = 0.5\pi$, $V_0 = 60E_\mathrm{R}$.

4. Nonlinear Wannier function

Following the above calculation, our Bloch function can be written in the following form

$$\psi_{lq}(x) = \mathrm{e}^{\mathrm{i}\,qx}\sqrt{\rho(x)}\mathrm{e}^{-\mathrm{i}\,\Theta(x)}, \tag{16}$$

where $\sqrt{\rho(x)}\mathrm{e}^{-\mathrm{i}\,\Theta(x)}$ corresponds to the periodic function $\phi_{lq}(x)$ in Eq.(1).

Although the expression for a Wannier function in terms of the Bloch function is well-known, the calculation of the Wannier function is different because it depends upon the choice of the Bloch function phase.[11] According to the definition of the Wannier function (2) and using the Bloch function (16), our Wannier function can be written in the form of

$$W_0(x) = \frac{T}{2\pi}\int_{-\pi/T}^{\pi/T}\sqrt{\rho(x)}\mathrm{e}^{-\mathrm{i}\,\Theta(x)}\mathrm{e}^{\mathrm{i}\,qx}\mathrm{d}q, \tag{17}$$

where the lowest band ($l = 0$) and $x_i = 0$ have been considered.

For BECs in periodic potential, all particles populate in the lowest bands of the lattice. We can expand the field operator in terms of the Wannier basis $\psi(x) = \sum_i a_i W_0(x - x_i)$, then the standard Bose-Hubbard Hamiltonian [7] is written in the form of $H = -J\sum_{\langle i,j\rangle} a_i^\dagger a_j + U/2\sum_i \widehat{n}_i\,(\widehat{n}_i - 1) + \sum_i \epsilon_i \widehat{n}_i$, here $a_i, a_i^\dagger$ are the annihilation and creation operators for a particle on site x_i and $\widehat{n}_i = a_i^\dagger a_i$. $\langle i,j\rangle$ denotes the sum over nearest neighbors and ϵ_i describes the energy offset of each lattice site. The hopping parameter J , on-site interaction U are defined by

$$J = -\int \mathrm{d}x W_0^*(x - x_i)\Big\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_{\mathrm{pot}}(x)\Big\} \times W_0(x - x_j), \tag{18}$$

and

$$U = \frac{4\pi a_{\mathrm{s}}\hbar^2}{m}\int \mathrm{d}x\,|W_0(x - x_i)|^4\,. \tag{19}$$

As pointed out in Ref.[7], U and J play a crucial role to determine the properties of the system. Therefore, we are going to calculate these parameters, to understand the reason of quantum phase transition.

With the help of the obtained Bloch wave functions, as shown in Fig.1, the Wannier functions (defined by Eq.(17)) are plotted in Fig.2. Obviously, the WFs satisfy the three basic requirements of Kohn.[9] For a given nonlinear interaction, with increasing the potential depth V_0 (see Fig.2(a)) the Wannier function $W_0\,(x)$ becomes more localized around zero. This is the same as the linear case: the t-b approximation is good for the deep potential. While for a fixed potential depth V_0, the Wannier function ($W_0\,(x)$) becomes broader and broader with the increasing of interatomic interaction gn (see Fig.2(b)). Therefore, the nonlinear interaction makes the Wannier functions fall off as non-exponential law with distance. This means that the nonlinear interaction makes the t-b approximation bad for the same potential depth. This is because the nonlinear interaction usually increases the coupling between the neighbour sites (see Fig.3).[28] Furthermore, this might be the reason of the 'screening effect' of nonlinearity on the lattice.[29]

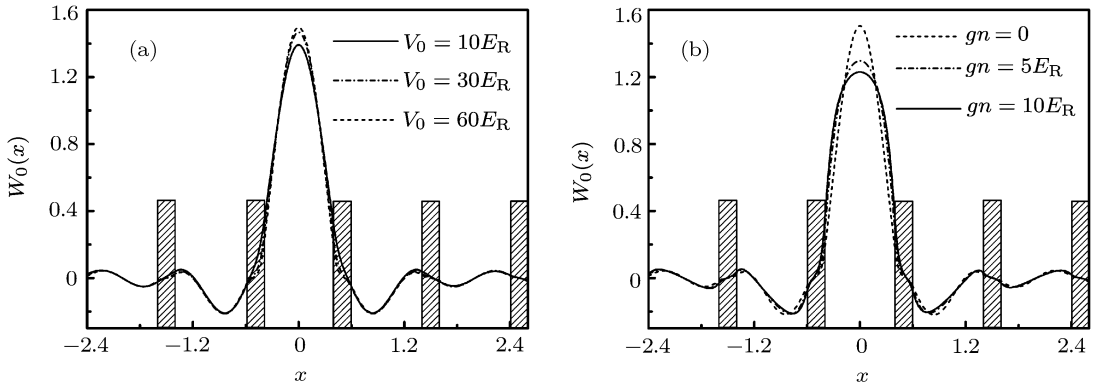


Fig.2. (a) $W_0(x)$ with $V_0 = 10E_{\mathrm{R}}$, $30E_{\mathrm{R}}$, $60E_{\mathrm{R}}$ for $gn = 0.1E_{\mathrm{R}}$. (b) $W_0(x)$ with $gn = 0$, $5E_{\mathrm{R}}$, $10E_{\mathrm{R}}$ for $V_0 = 60E_{\mathrm{R}}$.

After having the Wannier function, the on-site interaction U and the hopping parameter J (shown in Fig.3) can be calculated by Eqs.(18) and (19). For a given potential depth, the nonlinear interaction enhances the coupling between the neighbor sites (see Fig.3(a)). In contrast, the potential depth suppresses tunneling coupling J for a given nonlinear interaction. From Fig.3(b), we can see that the on-site interaction U is monotonously decreased with increasing gn and increasing the potential depth makes U increase. Considering the quantum phase transition predicted in Bose-Hubbard model,[7] the increase of nonlinear interaction will be helpful to make the system become superfluid, while the increasing of potential depth will change the system into Mott insulator.

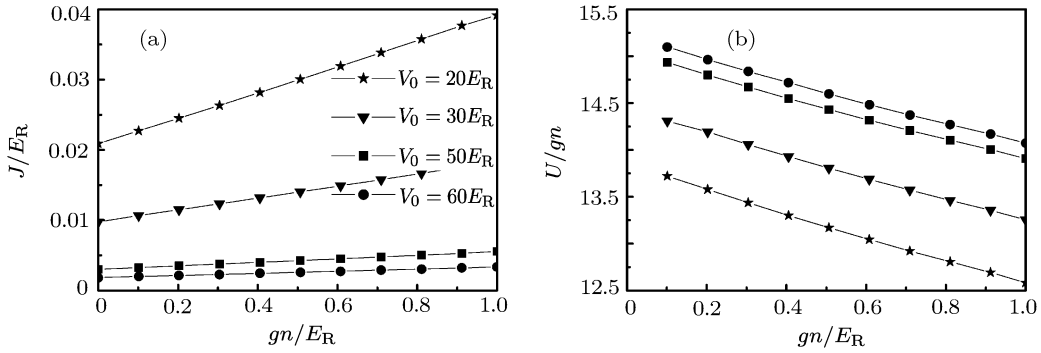


Fig.3. (a) The hopping parameter J versus nonlinear parameter gn for potential depth $V_0 = 20E_R$, $30E_R$, $50E_R$, $60E_R$. (b) The on-site interaction U as a function of the interatomic interaction for $V_0 = 20E_R$, $30E_R$, $50E_R$, $60E_R$.

5. Conclusions

The nonlinear Wannier functions in square Krönig–Penney potential are investigated, started from a set of exact nonlinear Bloch solutions. Our results show that the potential depth makes the effect on the nonlinear Wannier functions similar to that on the linear case. The nonlinear interaction makes the Wannier functions fall off as non-exponential law with distance and enhances the tunneling coupling between the neighbor sites. The t-b approximation is good for deep potential, while the increasing of interatomic interaction could make the t-b approximation bad. So the investigation on the nonlinear Wannier function provides one novel view to understand the properties of BECs in periodic potential.

Acknowledgement

We thank Biao Wu for inspiring discussion.

References

[1] Greiner M, Mandel O, Esslinger T, Hansch T W and Bloch I 2002 *Nature* (London) **415** 39

[2] Cataliotti F S, Burger S, Fort C, Maddaloni P, Minardi F, Trombettoni A, Smerzi A and Inguscio M 2001 *Science* **293** 843

[3] Eiermann B, Anker Th, Albiez M, Taglieber M, Treutlein P, Marzlin K P and Oberthaler M K 2004 *Phys. Rev. Lett.* **92** 230401

[4] Wu B and Niu Q 2000 *Phys. Rev.* A **61** 023402
Wu B, Diener R B and Niu Q 2002 *Phys. Rev.* A **65** 025601
Mueller E J 2002 *Phys. Rev.* A **66** 063603

[5] Wu B and Niu Q 2001 *Phys. Rev.* A **64** 061603(R)

[6] Rapedius K, Witthaut D and Korsch H J 2006 *Phys. Rev.* A **73** 033608

[7] Jaksch D, Bruder C, Cirac J I, Gardiner C W and Zoller P 1998 *Phys. Rev. Lett.* **81** 3108

[8] Trombettoni A and Smerzi A 2001 *Phys. Rev. Lett.* **86** 2353

[9] Kohn W 1959 *Phys. Rev.* **115** 809

[10] Bhattacharjee J and Waghmare U V 2005 *Phys. Rev.* B **71** 045106

[11] Pedersen F B, Einevoll G T and Hemmer P C 1991 *Phys. Rev.* B **44** 5470
[12] Talanina I and de Sterke C M 2000 *Phys. Rev.* A **62** 043802
[13] Bruno-Alfonso A and Nacbar D R 2007 *Phys. Rev.* B **75** 115428
[14] Wannier G H 1937 *Phys. Rev.* **52** 191
[15] Hennig D and Tsironis G P 1999 *Phys. Rep.* **307** 333
[16] Kittel C 1976 *Introduction to Solid State Physics* 5th ed. (New York: Wiley)
[17] Li W D and Smerzi A 2004 *Phys. Rev.* E **70** 016605
[18] Seaman B T, Carr L D and Holland M J 2005 *Phys. Rev.* A **71** 033622
[19] Danshita I and Tsuchiya S 2007 *Phys. Rev.* A **75** 033612
[20] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (Philadelphia: Saunders College)
[21] Dalfovo F, Giorgini S, Pitaevskii L P and Stringari S 1999 *Rev. Mod. Phys.* **71** 463
[22] Krämer M, Menotti C, Pitaevskii L and Stringari S 2003 *Eur. Phys. J.* D **27** 247
[23] Bronski J C, Carr L D, Deconinck B and Kutz J N 2001 *Phys. Rev. Lett.* **86** 1402
[24] Bronski J C, Carr L D, Deconinck B, Kutz J N and Promislow K 2001 *Phys. Rev.* E **63** 036612
[25] Li W D 2006 *Phys. Rev.* A **74** 063612
[26] Zhu J M, Ma Z Y, Fang J P, Zheng C L and Zhang J F 2004 *Chin. Phys.* **13** 798
[27] Liang Z X, Hu B B and Wu B 2009 cond-mat:0903.4058v2
[28] Jia X Y, Li W D and Liang J Q 2008 *Phys. Rev.* A **78** 023613
[29] Choi D I and Niu Q 1999 *Phys. Rev. Lett.* **82** 2022