

The Dispersion Function of a Quasi Two-Dimensional Periodic Sandwich using a Dirichlet-to-Neumann Map

N.T. Bagraev¹, G.J. Martin², B.S. Pavlov^{2,3}, A.M. Yafyasov³
 L.I. Goncharov³ and A.V. Zubkova³

¹Ioffe Physical-Technical Institute, Russian Academy of Sciences
 St. Petersburg, Russia

²New Zealand Institute of Advanced Study
 Massey University, Albany, Auckland, New Zealand

³V.A. Fock Physical Institute
 Department of Physics, St. Petersburg University, Russia

Abstract

A quasi two-dimensional periodic B-Si-B sandwich structure reveals surprising properties, including high-temperature superconductivity at 145 K⁰ [3]. This effect can be interpreted as superconductivity-gap (SC-gap) enhancing resulting from hybridisation of Bloch-functions of the weakly interacting Boron's doped upper and low plates of the sandwich, resulting in the restructuring of systems of spectral band/gaps, similarly to [1]. In this paper we suggest a soft model of a two-dimensional periodic lattice and a quasi two-dimensional periodic sandwich and calculate the typical dispersion function of the objects based on a rational approximation of the corresponding Dirichlet-to-Neumann maps (DN-maps). The rational approximations are interpreted as DN -maps of the corresponding fitted solvable models, which reveal some interesting physical properties such as Landau-Zener enhancing of the SC gap which may imply the high temperature superconductivity phenomenon.

Keywords: periodic structures, Dirichlet-to-Neumann map, fitted zero-range model.

1 Dispersion equation of a quasi-2D the periodic lattice in the resonance area

Bloch waves with real quasi-momentum play a role of eigenfunctions of continuous spectrum of the periodic lattice. In the case of a one-dimensional periodic lattice they are obtained as linear combinations of standard solutions of the Cauchy problem for the corresponding 1D Schrödinger equation $-u'' + q(x)u = \lambda u$, $q(x+a) = q(x)$. The quasi-momentum exponential $e^{ipa} \equiv \mu$ and the corresponding dispersion function $\lambda = \lambda(p)$ are found from the quadratic equation $\mu + \mu^{-1} = \text{Tr } T$ containing the trace of

the transfer-matrix \mathcal{T} . The Cauchy problem approach to calculation of the dispersion function fails in the case of 2D Schrödinger equation, because the Cauchy problem for the 2D Schrödinger equation is ill-posed. Vice versa, the approach based on the boundary problem is efficient, see [2, 4] for 2D Schrödinger equation $-\Delta u + q(x)u = \lambda u$, $q(x_1 + m^1 a_1, x_2 + m^2 a_2) = q(x)$, $m_1, m_2 = 0, \pm 1, \pm 2, \dots$. In [2] we presented the corresponding approach based on Dirichlet-to-Neumann map on the period Ω , $\mathcal{DN} : u|_{\partial\Omega} \longrightarrow \frac{\partial u}{\partial n}|_{\partial\Omega}$. The role of basic solutions of the boundary problem for the 2D Schrödinger equation on a square lattice with the period $\Omega \equiv (0, a) \times (0, a)$ play the solutions Ψ_l of the special boundary problem, obtained as extension from the “active” part Γ of the boundary $\partial\Omega$ of the period, where the exchange of the electrons between two neighboring periods is maximal. In the case when the active zone Γ is well localized on the side of the square period Ω , and the electron’s density on the period is supported by a proper sub-domain Ω_{in} we can consider the Schrödinger equation on Ω_{in} imposing zero boundary conditions on $\partial\Omega_{in} \setminus \Gamma$ and quasi-periodic matching conditions on Γ . Thus we can substitute the original period Ω by the “romboidal” period Ω_{in} with contacts Γ , see Fig. 1. For periodic lattices composed of “romboidal” periods, with relatively small contact zones Γ , spectral characteristics can be calculated via analytic perturbation procedure based on rational approximation of the corresponding DN-map. The matrix elements of the DN-map are obtained from the Green formula, based on extension of an orthogonal basis $\{\psi_l\} \subset L_2(\Gamma)$ on the “romboidal” period as solutions of the boundary problem:

$$-\Delta \Psi_l + q(x)\Psi_l = \lambda \Psi_l, \quad \Psi_l \Big|_{\Gamma} = \psi_l, \quad \Psi_l \Big|_{\partial\Omega \setminus \Gamma} = 0, \quad (1)$$

see for instance [6]:

$$\langle \mathcal{DN} \psi_l^\Gamma, \psi_m^\Gamma \rangle = \int_{\Omega} [\nabla \bar{\Psi}_l \nabla \Psi_m + q \bar{\Psi}_l \Psi_m - \lambda \bar{\Psi}_l \Psi_m] d\Omega. \quad (2)$$

This serves, together with a similar formula for the inverse $\mathcal{ND} = \mathcal{DN}^{-1}$, a base for practical calculation of the dispersion and the Bloch functions, see [4]. In the case of the square period $(0, a) \times (0, a)$ the boundary bases $\{\Psi_l\}$ are selected on the contacts $\Gamma_\alpha^i \subset \partial\Omega_\alpha^i$, $i = 1, 2, \alpha = 0, a, \cup_{i,\alpha} \Gamma_\alpha^i = \Gamma \subset \partial\Omega$, see for instance Fig. 1 below. Then the DN-map is represented by the block-matrix

$$\mathcal{DN} = \{\mathcal{DN}_{\alpha,\alpha'}\}, \quad \{\alpha, \alpha'\} = \{0, a\},$$

with blocks mapping the data $\vec{u}_a \equiv (u|_{\Gamma_a^1}, u|_{\Gamma_a^2})$, $\vec{u}_0 = (u|_{\Gamma_0^1}, u|_{\Gamma_0^2})$ into

$$\frac{\partial \vec{u}_a}{\partial n} \equiv \left(\frac{\partial u}{\partial n} \Big|_{\Gamma_a^1}, \frac{\partial u}{\partial n} \Big|_{\Gamma_a^2} \right), \quad \frac{\partial \vec{u}_0}{\partial n} \equiv \left(\frac{\partial u}{\partial n} \Big|_{\Gamma_0^1}, \frac{\partial u}{\partial n} \Big|_{\Gamma_0^2} \right).$$

The 0-components of the Bloch function can be eliminated based on the quasi-periodic conditions $\vec{u}_0 = \mu^{-1} \vec{u}_a$, $\frac{\partial \vec{u}_0}{\partial n} = -\mu^{-1} \frac{\partial \vec{u}_a}{\partial n}$, which imply the following linear homogeneous system for vector-functions $(\vec{u}_a, \frac{\partial \vec{u}_a}{\partial n})$.

$$\begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ -\mu^{-1} \frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \begin{pmatrix} \mathcal{DN}_{aa} & \mathcal{DN}_{a0} \\ \mathcal{DN}_{0a} & \mathcal{DN}_{00} \end{pmatrix} \begin{pmatrix} \vec{u}_a \\ \mu^{-1} \vec{u}_a \end{pmatrix}. \quad (3)$$

A nontrivial solution of the equation (3) exists if and only if zero is an eigenvalue of the relevant operator:

$$[\mu \mathcal{DN}_{00} \mu^{-1} + \mu \mathcal{DN}_{0a} + \mathcal{DN}_{a0} \mu^{-1} + \mathcal{DN}_{aa}] \vec{u}_a = 0. \quad (4)$$

Then the dispersion function is obtained as a connection between the energy λ and the quasi-momentum $\vec{p} = (p_1, p_2)$ or the quasi-momentum exponentials $\mu = \text{diag}(\mu_1, \mu_2) \equiv (e^{ip_1 a}, e^{ip_2 a})$ defined by the condition (4) for the quasi-periodic solutions of the corresponding Schrödinger equation, see [2]. The “quadratic equation” (4) is, in fact, an infinite-dimensional linear system. Neither elementary tools of linear algebra, nor the straightforward computing are sufficient to construct a solution of this system.

Fortunately the spectral problems on the physically meaningful square periodic lattices correspond to effectively narrow conductivity channels ω_α^i , $\alpha = 0, a$; $i = 1, 2$, or “covalent bonds” connecting neighboring periods. According to analysis presented in [5] for the Helmholtz resonator with narrow channels connecting the outer and the inner spaces, the channel actually *filters* the signals exiting from the inner space or entering the inner space of the resonator. The connecting channel transmits the part of the signal filtered to the cross-section subspace N of the oscillating modes in the channel, but weakens the component of the signal in the orthogonal subspace N^\perp , corresponding to the exponentially growing or decreasing modes. In this paper we achieve essential simplification of the original transmission problem via imposing partial matching condition (quasi-periodic matching condition- in actual case) in the contact subspace N and partial zero condition on N^\perp . Correspondingly we use the “partial” DN-map of the model Schrödinger equation with Dirichlet zero boundary condition on the complementary subspace $L_2(\Gamma) \ominus N \equiv N^\perp$ and partial Dirichlet boundary condition in the contact space N

$$-\Delta u + qu = \lambda u, P_N^\perp u \Big|_\Gamma = 0, P_N u \Big|_\Gamma = u_\Gamma^N \in N \quad (5)$$

is obtained via framing of the standard DN-map by projections P_N onto the contact space N .

$$\mathcal{DN}^N \equiv P_N \mathcal{DN} P_N.$$

Actually selection of an appropriate contact space defines the main free parameter of our model. In real physical situations the contact space may be associated with cross-section subspaces of electron’s conductivity channels or the covalent bonds, see more comments below. But once the contact subspace is selected, the dispersion equation of the model is obtained in the same form (4) via substitution of the standard DN- map by the corresponding finite-dimensional “partial” DN map

$$[\mu \mathcal{DN}_{00}^N \mu^{-1} + \mathcal{DN}_{aa}^N + \mathcal{DN}_{a0}^N \mu^{-1} + \mu \mathcal{DN}_{0a}^N] \vec{u}_a \equiv \mathcal{D}(\lambda, \mu) \vec{u}_a = 0. \quad (6)$$

The ultimate equation (6), contrary to (4), is a finite-dimensional one, which allows to obtain the dispersion equation for the model periodic quasi-2D lattice in explicit form.

Selecting appropriate contacts Γ and the contact spaces N allows to substitute the original periodic Schrödinger problem by a soluble zero-range model with spectral

properties as close to the original system, as required on a given temperature interval, for given temperature.

We guess that the contact zones and contact spaces can be interpreted as a mathematical notions for description of covalent bonds and conductivity channels in quantum chemistry. Both mathematically and physically they are bridging orbitals of neighboring periods of the lattice. If the contact zones are relatively small, we say that the corresponding periods are “romboidal” see a simplest example below , Fig. 1. For low temperature there exist, generically, only one resonance eigenvalue $\lambda_1^D \approx \Lambda^F$ (Fermi level) of the Dirichlet problem on a “romboidal” period, and the cross-section of the branch of the hybrid wave -function bridging the unperturbed orbitals φ_1^D of neighboring periods has a simplest possible structure, characterized by a 1D contact space $N^1 = N_0^1 = N_a^1$, $N^2 = N_0^2 = N_a^2$ on each contact zone $\Gamma_0^{1,2}$, $\Gamma_a^{1,2}$, $N^1 \oplus N^2 = N$.

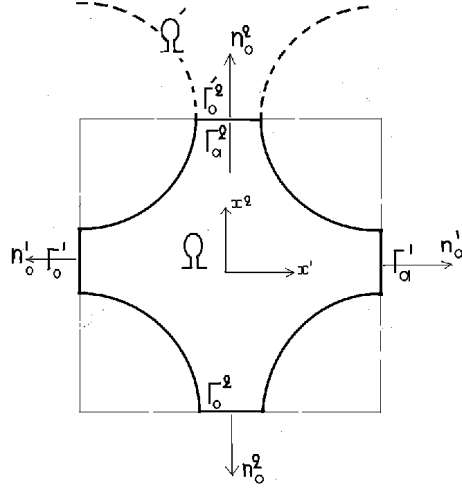


Figure 1: “Romboidal” period. Contact sections Γ_τ^i , $i = 1, 2$, $\tau = 0, a$

In fact all physically essential details of the electron’s dynamics are developed on a **resonance area** in the spectral domain - on the temperature interval near to the Fermi level $[\Lambda^F - 2m\kappa T\hbar^{-2}, \Lambda^F + 2m\kappa T\hbar^{-2}]$. Hence, in attempt to further simplification of the original spectral problem we can substitute the DN-map on the resonance area by an appropriate rational approximation . In the simplest case it can be represented as a sum of a one-dimensional polar term and a correcting term

$$\mathcal{DN}^N \approx \frac{P_N \frac{\partial \varphi_1^D}{\partial n}}{\lambda - \lambda_1} \langle P_N \frac{\partial \varphi_1^D}{\partial n} | + P_N B P_N \equiv \mathcal{D}(\lambda, \mu) = A \frac{Q}{\lambda - \lambda_1} + B, \quad (7)$$

with a 1D orthogonal projection $Q = e_q \langle e_q |, |e_q\rangle_{L_2(\Gamma)} = 1$, and the corresponding normalizing coefficient $A = |P_N \frac{\partial \varphi_1^D}{\partial n}|_{L_2(\Gamma)}^2$. Taking into account that $\dim N^1 = \dim N^2 = 1$, we represent $P_N \mathcal{DN} P_N$ by a 2×2 matrix with respect to the decomposition

of $N = \sum_{i=1,2} N(\Gamma_0^i) = \sum_{i=1,2} N(\Gamma_a^i)$. Then elimination of the variable $P^N \frac{\partial v}{\partial n} \Big|_{\Gamma_a}$ gives a (finite-dimensional !) equation for $P^N v \Big|_{\Gamma_a}$ similar to one above, see (4)

$$\begin{aligned} & A [\mu Q_{0a}^N + \mu Q_{00}^N \mu^{-1} + Q_{aa}^N + \mu Q_{a0}^N \mu^{-1}] \vec{u}_a + \\ & (\lambda - \lambda_1^D) [\mu B_{0a}^N + \mu B_{00}^N \mu^{-1} + B_{aa}^N + B_{a0}^N \mu^{-1}] \vec{u}_a = \\ & [A\mathcal{D}_Q(\lambda, p) + (\lambda - \lambda_1^D)\mathcal{D}_B(\lambda, p)] \vec{u}_a = 0, \end{aligned} \quad (8)$$

with $\mu = (\mu_1, \mu_2) = (e^{ip_1 a}, e^{ip_2 a})$. The determinant condition of existence of a non-trivial solution of the ultimate equation (1) with partial quasi-periodic matching conditions gives the dispersion equation $\lambda = \lambda(p_1, p_2)$ for the corresponding *model periodic lattice* L_N :

$$\det \mathcal{D}(\lambda, \mu) = 0.$$

In the case of a single resonance eigenvalue, on the resonance area on the spectral domain near the Fermi level, we obtain, with use of the above rational approximation (8), the determinant condition for $\lambda = \lambda(p)$, $\mu_s = e^{ip_s}$, $s = 1, 2$:

$$\det [A\mathcal{D}_Q(p) + (\lambda - \lambda_1^D)\mathcal{D}_B(\lambda, p)] = 0. \quad (9)$$

For small temperature one can substitute $\mathcal{D}_B(\lambda, p)$ by the value of it at the Fermi level $\lambda_1^D \approx \Lambda^F$, which implies the approximate determinant condition

$$\det [A\mathcal{D}_Q(p) + (\lambda - \lambda_1^D)\mathcal{D}_B(\lambda_1^D, p)] = 0, \quad (10)$$

which defines the shape of the dispersion function on the resonance area in terms of the corresponding resonance parameters: the resonance eigenfunction of the Dirichlet Schrödinger operator on the period and the resonance eigenvalue, as well as an averaged effect of others neighboring eigenvalues represented by the correcting term B . Naturally our approach can be easily modified in case of a few eigenvalues on the resonance area and improved via taking into account a polynomial approximation of the correcting term. A major modification would arise when the contact area and contact spaces are extended. We guess that this important work should be not done in a general case, but for lattices composed of special materials. Our approach easily admits the corresponding modification. In particular it can be used as a tool of design of artificial periodic structures, with prescribed transport properties. In particular, for mathematical design of sandwich structures.

2 Dirichlet-to-Neumann approach to calculation of the dispersion function of a quasi-2D sandwich

The recent discovery of quasi-relativistic behavior of terms in man-made bi-layer periodic quasi-2D sandwich structures, see [5], suggests that the weak interaction of two-dimensional periodic lattices can be used as a source of various artificial structures

with interesting and useful transport properties. Study of the Landau-Zener transformation, see [7], in the 2D case requires new analytic machinery, since the 1D technique, based on the transfer-matrix, fails because the Cauchy problem for Schrödinger equation on a square period is ill-posed. We consider a periodic 2D sandwich based on Dirichlet-to-Neumann technique developed in previous section.

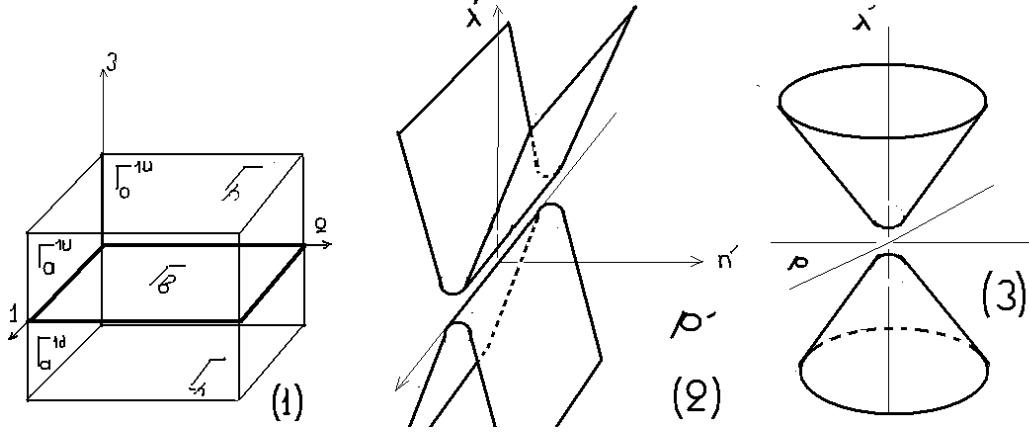


Figure 2: Two-storied period of the periodic quasi-2D sandwich lattice (1). Landau-Zener 2D phenomenon as a blowup of crossing of two surfaces (2). Blowup of a light cone can't be obtained as a 2D Landau-Zener effect (3)

Consider 2-storied period, see Fig 2, with the partial quasi-periodic boundary conditions on the vertical walls $\Gamma_{i,\alpha}^{u,d}$, $i = 1, 2$, $\alpha = 0, a$, with the contact subspaces $N_{1,2}$, zero boundary conditions on the upper and lower lids Γ_h, Γ_{-h} and a bilateral potential barrier Γ_b^{ud} , emulating the layer of pure Silicon in B-Si-B sandwich, squeezed between two Boron's doped Silicon plates Σ_u, Σ_d , see [3].

Selecting the contact subspace N_b on the barrier and denoting by $n_b^{d,u}$ the outer normals on both sides Γ_b^{ud} of the barrier, we impose the boundary condition on Γ_b on a jump of the normal derivative $\frac{\partial V^u}{\partial n^u} \Big|_{\Gamma_b^u} + \frac{\partial V^d}{\partial n^d} \Big|_{\Gamma_b^d} \equiv \left[\frac{\partial V}{\partial n} \right] \Big|_{\Gamma_b}$

$$P_{N_b} \left[\frac{\partial V^u}{\partial n^u} \Big|_{\Gamma_b^u} + \frac{\partial V^d}{\partial n^d} \Big|_{\Gamma_b^d} \right] + \beta V_b = 0, \text{ or } \left[\frac{\partial V}{\partial n} \right] \Big|_{\Gamma_b} + \beta V_b = 0, \quad (11)$$

under continuity condition imposed on the value of the N_b projection $P_{N_b} V^u \Big|_{\Gamma_b^u}$ of the wave-function on the barrier.

$$V_b = P_{N_b} V^d \Big|_{\Gamma_b^d} = P_{N_b} V^u \Big|_{\Gamma_b^u}, \quad (12)$$

Once the magnitude of the tunneling constant β is fixed, we could consider the DN-map of the two-storied period with the joint vertical walls $\Gamma_{i,\alpha} = \Gamma_{i,\alpha}^u \cup \Gamma_{i,\alpha}^d$, and

$N_i = N_i^u \cup N_i^d$. Then the dispersion equation for the 2D sandwich is obtained based on the previous formulae (6,8).

It is interesting to observe the behavior of the dispersion surfaces in dependence of the tunneling parameter β . To do that we consider the relative DN-maps of the upper and the lower storeys Ω^u, Ω^d of the whole 2-storied period Ω of the sandwich. Denote by N_i^u, N_i^d, N_b the contact subspaces associated with the corresponding walls $\Gamma_{\alpha,i}^u, \Gamma_{\alpha,i}^d, \Gamma_b$ and by $N_i^{u,\perp}, N_i^{d,\perp}, N_b^\perp$ the relevant orthogonal complements in the spaces of square-integrable functions on the walls.

$$\mathcal{DN}^u = \begin{pmatrix} \mathcal{DN}_{aa}^u & \mathcal{DN}_{a0}^u & \mathcal{DN}_{ab}^u \\ \mathcal{DN}_{0a}^u & \mathcal{DN}_{00}^u & \mathcal{DN}_{0b}^u \\ \mathcal{DN}_{ba}^u & \mathcal{DN}_{b0}^u & \mathcal{DN}_{bb}^u \end{pmatrix}, \quad (13)$$

with 2×2 block

$$\mathcal{DN}^u = \begin{pmatrix} \mathcal{DN}_{aa}^u & \mathcal{DN}_{a0}^u \\ \mathcal{DN}_{0a}^u & \mathcal{DN}_{00}^u \end{pmatrix}$$

and $2 \times 1, 1 \times 2$ and 1×1 blocks

$$\mathcal{DN}_{\alpha,b}^u = \begin{pmatrix} \mathcal{DN}_{ab}^u \\ \mathcal{DN}_{0b}^u \end{pmatrix}, \quad \mathcal{DN}_{b,a}^u = (\mathcal{DN}_{ba}^u; \mathcal{DN}_{b0}^u), \quad \mathcal{DN}_{bb}^u = P_b^u \mathcal{DN}_{bb}^u,$$

squeezed by projections onto appropriate contact spaces. Similar representation is valid for \mathcal{DN}^d . The joint DN-map \mathcal{DN}_{2D} of the period with continuity condition in the contact space N_b on $\Gamma_b : P_{N_b} V \Big|_{\Gamma_b^u} = P_{N_b} V \Big|_{\Gamma_b^d}$ and the tunneling condition on the barrier

$$\left[P_{N_b} \frac{\partial V}{\partial n} \right] + \beta P_{N_b} V \Big|_{\Gamma_b} = 0,$$

is given by the block-matrix acting on the vector $(V_a^u, V_0^u, V_b, V_0^d, V_a^d)$, with 2D components

$$V_a^u \equiv (V_{a1}^u, V_{a2}^u), \quad V_0^u \equiv (V_{01}^u, V_{02}^u), \\ V_a^d \equiv (V_{a1}^d, V_{a2}^d), \quad V_0^d \equiv (V_{01}^d, V_{02}^d)$$

and 1D component V_b .

$$\mathcal{DN}_{2D} = \begin{pmatrix} \mathcal{DN}_{aa}^u & \mathcal{DN}_{a0}^u & \mathcal{DN}_{ab}^u & 0 & 0 \\ \mathcal{DN}_{0a}^u & \mathcal{DN}_{00}^u & \mathcal{DN}_{0b}^u & 0 & 0 \\ \mathcal{DN}_{ba}^u & \mathcal{DN}_{b0}^u & [\mathcal{DN}_{bb}^u + \mathcal{DN}_{bb}^d] & \mathcal{DN}_{b0}^d & \mathcal{DN}_{ba}^u \\ 0 & 0 & \mathcal{DN}_{0b}^d & \mathcal{DN}_{00}^d & \mathcal{DN}_{0a}^d \\ 0 & 0 & \mathcal{DN}_{ab}^d & \mathcal{DN}_{a0}^d & \mathcal{DN}_{aa}^d \end{pmatrix}. \quad (14)$$

Due to partial zero condition on the walls and the lids with selected entrance subspaces $N_1^u, N_2^u, N_1^d, N_2^d, N_b$ of the open channels, the components of the boundary vectors are selected from these subspaces and the matrix elements are framed by projections onto $N_1^u, N_2^u, N_1^d, N_2^d, N_b$. We omit the projections in the formula (14) for the

DN-map. The quasi-periodic boundary conditions are represented, with the diagonal matrices $\mu_u = [\mu_1^u, \mu_2^u]$ and $\mu_d = [\mu_1^d, \mu_2^d]$ on the boundary vectors, as

$$\mathcal{DN}_{2D} \begin{pmatrix} V_a^u \\ \mu_u^{-1} V_a^u \\ V_b \\ \mu_d^{-1} V_a^d \\ V_a^d \end{pmatrix} = \begin{pmatrix} \frac{\partial V_a^u}{\partial n} \\ -\mu_u^{-1} \frac{\partial V_a^u}{\partial n} \\ -\beta V_b \\ -\mu_d^{-1} \frac{\partial V_a^d}{\partial n} \\ \frac{\partial V_a^d}{\partial n} \end{pmatrix} \quad (15)$$

The roles of independent variables in this equation are played by the vectors $V_a^u = (V_{a1}^u, V_{a2}^u) \in N_1^u \oplus N_2^u$, $V_a^d = (V_{a1}^d, V_{a2}^d) \in N_1^d \oplus N_2^d$ and $\frac{\partial V_a^u}{\partial n} = (\frac{\partial V_{a1}^u}{\partial n}, \frac{\partial V_{a2}^u}{\partial n}) \in N_1^u \oplus N_2^u$ and $\frac{\partial V_a^d}{\partial n} = (\frac{\partial V_{a1}^d}{\partial n}, \frac{\partial V_{a2}^d}{\partial n}) \in N_1^d \oplus N_2^d$ and vector $V_b \in N_b$. The vectors $\frac{\partial V_a^u}{\partial n}$, $\frac{\partial V_a^d}{\partial n}$ enter only into the right side of the equation (15) and can be easily eliminated, resulting in a homogeneous finite-dimensional linear system, which has a non-trivial solution under appropriate determinant condition. We prefer more explicit condition of existence of a non-trivial solution. Via multiplication of the first pair of equations of the system (15) by the 2×2 matrix $\begin{pmatrix} 1 & 0 \\ 0 & \mu_u \end{pmatrix}$ and the last pair of equations by the 2×2 matrix $\begin{pmatrix} 1 & 0 \\ 0 & \mu_d \end{pmatrix}$, and subsequent adding the pairs, the terms with normal derivatives are eliminated, so that the system is reduced to three equations with respect to the variables $\vec{V}^u, V_b, \vec{V}^d$

$$\begin{pmatrix} \mathbf{D}^u & \mathbf{D}_b^u & 0 \\ [\mathbf{D}_b^u]^+ & \mathcal{DN}_{bb}^u + \mathcal{DN}_{bb}^d + \beta I & [\mathbf{D}_b^d]^+ \\ 0 & \mathbf{D}_b^d & \mathbf{D}^d \end{pmatrix} \begin{pmatrix} \vec{V}^u \\ V_b \\ \vec{V}^d \end{pmatrix} = 0. \quad (16)$$

Here we are using the notations:

$$\mathbf{D}^u \equiv \mathcal{DN}_{aa}^u + \mathcal{DN}_{a0}^u \mu_u^{-1} + \mu_u \mathcal{DN}_{0a}^u + \mu_u \mathcal{DN}_{00}^u \mu_u^{-1},$$

$$\mathbf{D}^d \equiv \mathcal{DN}_{aa}^d + \mathcal{DN}_{a0}^d \mu_d^{-1} + \mu_d \mathcal{DN}_{0a}^d + \mu_d \mathcal{DN}_{00}^d \mu_d^{-1}.$$

$$\mathbf{D}_b^u \equiv \mathcal{DN}_{ab}^u + \mu_u \mathcal{DN}_{0b}^u, \quad [\mathbf{D}_b^u]^+ \equiv \mathcal{DN}_{ba}^u + \mathcal{DN}_{b0}^u \mu_u^{-1},$$

$$\mathbf{D}_b^d \equiv \mathcal{DN}_{ab}^d + \mu_d \mathcal{DN}_{0b}^d, \quad [\mathbf{D}_b^d]^+ \equiv \mathcal{DN}_{ba}^d + \mathcal{DN}_{b0}^d \mu_d^{-1}.$$

Via elimination of \vec{V}^u, \vec{V}^d based on the first and third equations

$$\vec{V}^u = -[\mathbf{D}^u]^{-1} \mathbf{D}_b^u V_b, \quad \vec{V}^d = -[\mathbf{D}^d]^{-1} [\mathbf{D}_b^d]^{-1} V_b,$$

we obtain a homogeneous equation for V_b

$$[\mathbf{D}_b^u]^+ [\mathbf{D}^u]^{-1} \mathbf{D}_b^u V_b + [\mathbf{D}_b^d]^+ [\mathbf{D}^d]^{-1} \mathbf{D}_b^d V_b = [\mathcal{DN}_{bb}^u + \mathcal{DN}_{bb}^d + \beta I] V_b. \quad (17)$$

This is a scalar equation, if the original Schrödinger equation disregards the spin of electron, hence V_b is scalar. But if the spin is taken into account, then V_b is the spinor, and (17) is a vector (spinor) equation.

In the resonance area, on the temperature interval near the Fermi level, we are able to substitute the DN-map by the rational approximation

$$\mathcal{DN}^{u,d} = A^{u,d} \frac{Q_{u,d}}{\lambda - \lambda_1^{u,d}} + B^{u,d} \quad (18)$$

and, correspondingly, the matrices \mathbf{D}^u , \mathbf{D}^d , \mathbf{D}_b^u , \mathbf{D}_b^d by the corresponding rational approximation (18)

$$\begin{aligned} \mathbf{D}^u &\approx A^u \frac{\mu Q_{0a}^u + \mu Q_{00}^u \mu^{-1} + Q_{aa}^u + \mu Q_{a0}^u \mu^{-1}}{\lambda - \lambda_1^u} + [\mu B_{0a}^u + \mu B_{00}^u \mu^{-1} + B_{aa}^u + B_{a0}^u \mu^{-1}] \equiv \\ &\equiv A^u \frac{\mathbf{D}_Q^u(\lambda, \mu)}{(\lambda - \lambda_1^u)} + \mathbf{D}_B^u(\lambda, \mu). \end{aligned} \quad (19)$$

$$\begin{aligned} \mathbf{D}^d &\approx A^d \frac{\mu Q_{0a}^d + \mu Q_{00}^d \mu^{-1} + Q_{aa}^d + \mu Q_{a0}^d \mu^{-1}}{\lambda - \lambda_1^d} + [\mu B_{0a}^d + \mu B_{00}^d \mu^{-1} + B_{aa}^d + B_{a0}^d \mu^{-1}] \equiv \\ &\equiv A^d \frac{\mathbf{D}_Q^d(\lambda, \mu)}{(\lambda - \lambda_1^d)} + \mathbf{D}_B^d(\lambda, \mu), \end{aligned} \quad (20)$$

$$\mathbf{D}_b^u \approx A^u \frac{Q_{ab}^u + \mu^u Q_{0b}^u}{\lambda - \lambda_1^u} + B_{ab}^u + \mu^u B_{0b}^u \equiv A^u \frac{\mathbf{Q}_b^u}{\lambda - \lambda_1^u} + \mathbf{B}_b^u, \quad (21)$$

$$\mathbf{D}_b^d \approx A^d \frac{Q_{ab}^d + \mu^d Q_{0b}^d}{\lambda - \lambda_1^d} + B_{ab}^d + \mu^d B_{0b}^d \equiv A^d \frac{\mathbf{Q}_b^d}{\lambda - \lambda_1^d} + \mathbf{B}_b^d. \quad (22)$$

The substitution of the rational approximations (19,20,21,22) yields an approximate dispersion equation of the sandwich on the resonance spectral domain (on the temperature interval near the Fermi level). Neglecting $(\lambda - \lambda_1)\mathbf{B}_b$ compared with \mathbf{Q}_b , but still keeping all terms in the denominators u, d :

$$Q = A\mathbf{D}_Q(\lambda, \mu) + (\lambda - \lambda_1)\mathbf{D}_B(\lambda, \mu)$$

we obtain an approximate dispersion equation of the sandwich in the resonance domain:

$$\begin{aligned} \frac{|A^u|^2}{(\lambda - \lambda_1^u)^2} [\mathbf{Q}_b^u]^+ \frac{I}{\mathbf{D}^u} \mathbf{Q}_b^u V_b + \frac{|A^d|^2}{(\lambda - \lambda_1^d)^2} [\mathbf{Q}_b^d]^+ \frac{I}{\mathbf{D}^d} \mathbf{Q}_b^d V_b = \\ \left[A_{bb}^u \frac{Q_{bb}^u}{\lambda - \lambda_1^u} + A_{bb}^d \frac{Q_{bb}^d}{\lambda - \lambda_1^d} + B_{bb}^u + B_{bb}^d + \beta \right] V_b. \end{aligned} \quad (23)$$

The inverse $[\mathbf{D}]^{-1}$ is easily calculated because $\dim N_1 = \dim N_2 = 1$:

$$[\mathbf{D}^u]^{-1} = \frac{\begin{pmatrix} \mathbf{D}_{22} & -\mathbf{D}_{12} \\ -\mathbf{D}_{21} & \mathbf{D}_{11} \end{pmatrix}}{\det \mathbf{D}^u} \equiv \frac{\mathbf{R}}{\det \mathbf{D}^u}.$$

In spinless theory this yields a scalar dispersion equation with the coefficients

$$\begin{aligned} \left[\mathbf{Q}_b^{u,d} \right]^+ \frac{\mathbf{R}^{u,d}}{\mathbf{Q}_b^{u,d}} &\equiv \mathbf{F}^{u,d} : \\ |A^u|^2 \frac{\mathbf{F}^u}{(\lambda - \lambda_1^u)^2 \det \mathbf{D}^u} + |A^d|^2 \frac{\mathbf{F}^d}{(\lambda - \lambda_1^d)^2 \det \mathbf{D}^d} &= \\ A_{bb}^u \frac{Q_{bb}^u}{\lambda - \lambda_1^u} + A_{bb}^d \frac{Q_{bb}^d}{\lambda - \lambda_1^d} + B_{bb}^u + B_{bb}^d + \beta. \end{aligned}$$

For large β (weak connection between the upper and lower plates of the sandwich) the dispersion equation describes the transformation of the intersection of terms $(\lambda - \lambda_1^u)^2 \det \mathbf{D}^u = (\lambda - \lambda_1^d)^2 \det \mathbf{D}^d = 0$ into quasi-intersection. Vice versa, taking into account spin, we obtain a similar vector equation, with 2×2 matrix coefficients $\mathbf{F}^u, \mathbf{F}^d$ and singular coefficients. This may exhibit pure crossing shape even for $\beta \rightarrow \infty$. For instance, the 2D equation

$$\left[\frac{Q_b^u(\mu)}{A^u Q^u + (\lambda - \lambda_1) Q_B^u} + \frac{Q_b^d(\mu)}{A^d Q^d + (\lambda - \lambda_1) Q_B^d} \right] \vec{V} = \beta \vec{V}$$

with mutually orthogonal projections $Q_b^{u,d}, Q_b^u + Q_b^d = I$, equivalent $\lambda_1^u = \lambda_1^d = \lambda_1$ and one-dimensional blocs Q^u, Q_B^u, Q^d, Q_B^d , - reveals pure crossing shape of the terms for any large β .

More interesting physical picture arises when the barrier possess resonance properties, taken into account by the energy-dependence of the coefficient β , see [4]. The resonance properties may be caused by the size quantization on the space-charge region near the surface of the emitter, see for instance [9].

3 Straightforward calculation of the dispersion equation for a 2D lattice and a sandwich

The semi-analytic approach to calculation of the dispersion of the 2D periodic lattice or sandwich opens a way to numerous interesting spectral problems for one-body Schrödinger operator. Some of them are sketched above, for a fitted solvable model constructed for given contacts and contact subspaces. One of most important questions is one about selection of the contact domains Γ_σ^i on the sides the period and selection of the contact subspaces N_1, N_2 . We calculate the dispersion as a function of the modulo $|p|$ of the quasi-momentum, depending on the direction ν of the quasi-momentum, based on general finite-dimensional equation for the dispersion function $\lambda(p) = \lambda(|p|, \nu)$. Consider a typical example of a 2D lattice generated by a non-dimensional Schrödinger operator with real periodic potential obtained via restriction of Yukawa potential on the romboidal period framed by the arcs of circles radius 0.05 centered on the corners of the square 1.1×1.1 and by the central intervals Γ_α^i length δ

on the sides of the period. We choose the contacts Γ_α^i in form of intervals $0 < \gamma < \delta^i$ centered at the mid-points 0_α^i of the corresponding sides of the square period and span the contact spaces by $\sqrt{2/\delta^i} \sin l\pi\gamma/\delta^i$ and use the basic equation (6). The direction of vector ν is defined by the angle $\varphi = 0, 15^\circ, 30^\circ, 45^\circ$ between the orth e_1 and ν . For strong Yukawa potential the dispersion function $\lambda(|p|)$ with 3D contact spaces $l = 1, 2, 3$ on the on the contacts is calculated for selected angles and is represented by (3) based on straightforward computing for the corresponding DN-map. Our numer-

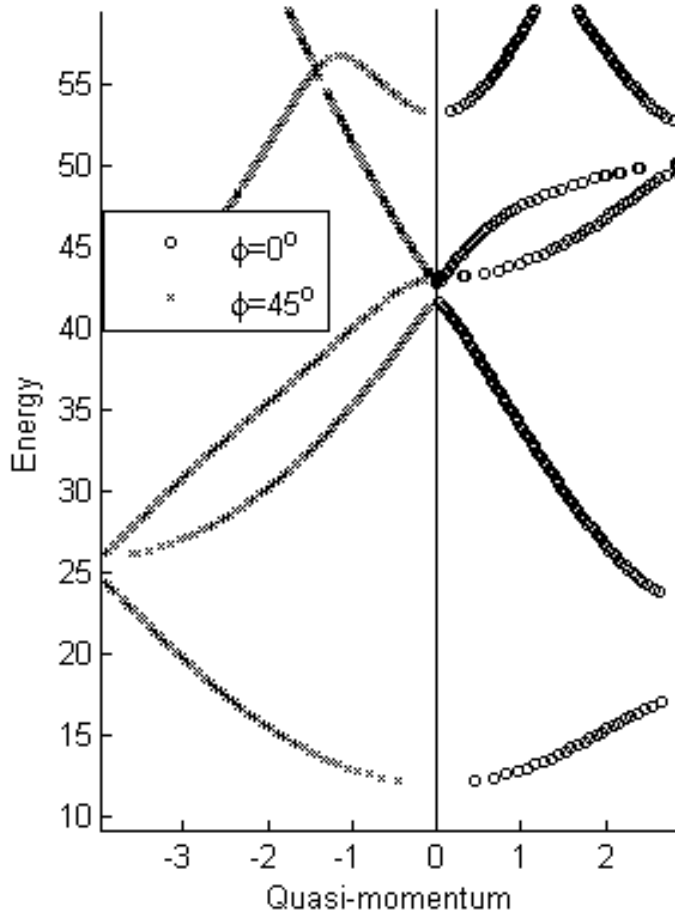


Figure 3: The sections of the dispersion surface of the periodic Schrödinger operator on a at the corners of the square period.

ical experiments showed that beginning from $\dim N = 3$ the shape of the dispersion function in the domain of low energy reveals clear features of stability, which gives a good reason to assume that the finite dimension of the contact subspace already allows to construct a realistic soluble model of the Schrödinger operator with Yukawa potential on the above square lattice.

Interesting resonance properties are revealed by Heine-Abarenkov potential constructed on a period as a potential well surrounded by the thick wall. The Dirichlet problem on the "romboidal" period for the corresponding Schrödinger operator has a single simple isolated eigenvalue, the DN-map has a corresponding polar term and a regular correcting term. The rational approximation of the corresponding DN-map framed by the projections on the corresponding 1D contact spaces N_1, N_2 , spanned by $\sqrt{2/\delta^i} \sin l\pi\gamma/\delta^i$, $l = 1$, for low temperature on the corresponding small temperature interval centered at the lowest resonance eigenvalue λ_1 has a form

$$A \frac{Q}{\lambda - \lambda_1} + B = A_1 \frac{\begin{pmatrix} Q_{aa} & Q_{a0} \\ Q_{0a} & Q_{00} \end{pmatrix}}{\lambda - \lambda_1} + \begin{pmatrix} B_{aa} & B_{a0} \\ B_{0a} & B_{00} \end{pmatrix}$$

with an one-dimensional projection orthogonal projection Q and a constant Hermitian matrix. We select

$$Q_{aa} = \frac{1}{2} \begin{pmatrix} \nu_1 \langle \nu_1 & 0 \\ 0 & 0 \end{pmatrix}; Q_{a0} = \frac{1}{2} \begin{pmatrix} 0 & \nu_1 \langle \nu_2 \\ 0 & 0 \end{pmatrix}; \quad (24)$$

$$Q_{0a} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ \nu_2 \langle \nu_1 & 0 \end{pmatrix}; Q_{00} = e_0 \langle e_0 = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & \nu_2 \langle \nu_2 \end{pmatrix}, \quad (25)$$

see Fig. 4. The regular term B depends on the upper eigenvalues and eigenfunctions. We consider an example selecting the regular term as

$$B = \begin{pmatrix} B_{aa} & B_{a0} \\ B_{0a} & 0 \end{pmatrix},$$

where

$$B_{00} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad B_{aa} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$B_{a0} = b_{a0} \begin{pmatrix} 0 & \nu_1 \langle \nu_2 \\ \nu_2 \langle \nu_1 & 0 \end{pmatrix}, \quad B_{0a} = b_{0a} \begin{pmatrix} 0 & \nu_2 \langle \nu_1 \\ \nu_1 \langle \nu_2 & 0 \end{pmatrix},$$

Elimination of the variables u'_0, u'_a, u_0 as suggested in (8), gives an equation for the 2-vector u_a :

$$\frac{A}{\lambda - \lambda_1^D} [\mu Q_{0a}^N + \mu Q_{00}^N \mu^{-1} + Q_{aa}^N + \mu Q_{a0}^N \mu^{-1}] \vec{u}_a +$$

$$[\mu B_{0a}^N + \mu B_{00}^N \mu^{-1} + B_{aa}^N + B_{a0}^N \mu^{-1}] \vec{u}_a \equiv \left[\frac{AD_Q(\lambda, p)}{\lambda - \lambda_1^D} + \mathcal{D}_B(\lambda, p) \right] \vec{u}_a = 0. \quad (26)$$

The corresponding equation (26) has a nontrivial solution \vec{u}_a if the determinant of the corresponding 2×2 matrix

$$AD_Q + (\lambda - \lambda_1^D) \mathcal{D}_B(\lambda, p)$$

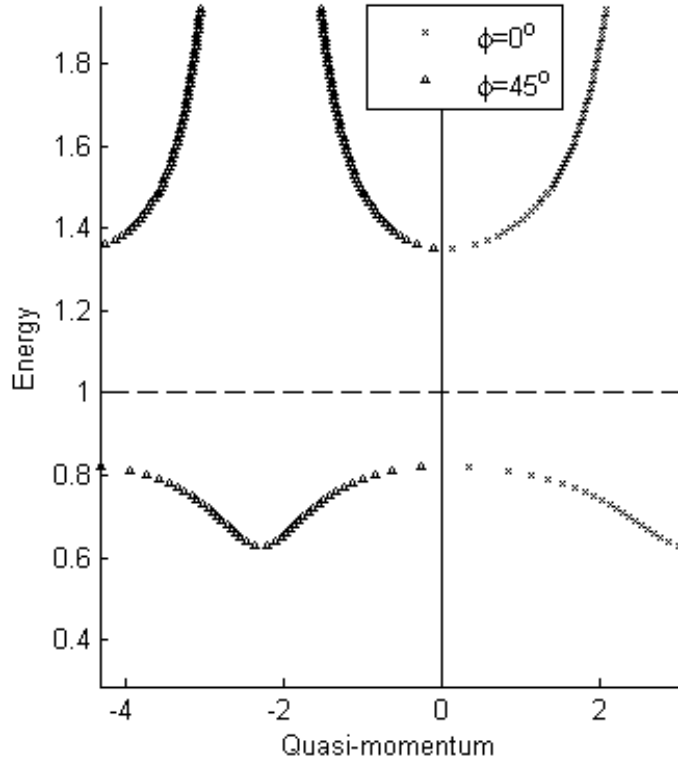


Figure 4: Sections of the dispersion surface of an abstract model emulating Heine-Abarenkov potential with the lower resonance eigenvalue $\lambda_1 = 1$ (punctured line).

vanishes. This condition yields the dispersion equation $\lambda = \lambda(\vec{p})$, with the quasi-momentum \vec{p} defined by the quasi-momentum exponentials $\mu = \text{diag}(\mu_1, \mu_2) = \text{diag}(e^{ip_1}, e^{ip_2})$.

In the case when the Heine-Abarenkov potential well is deep enough, there are several eigenvalues with eigenfunctions localized in the well. In particular, there is an eigenfunction symmetric with respect to reflection in the line connecting the mid-points of Γ_0^1, Γ_a^1 and antisymmetric with respect to reflection in the line connecting the mid-points of Γ_0^2, Γ_a^2 , or vice versa. The corresponding eigenvalue is non-degenerated if the potential is not symmetric with respect to the change of the variables $1 \rightarrow 2, 2 \rightarrow 1$. The corresponding DN-map is characterized by the polar term AQ with the projection

$$Q = \frac{1}{2} \begin{pmatrix} \nu_1 \langle \nu_1 & 0 & -\nu_1 \langle \nu_1 & 0 \\ 0 & 0 & 0 & -\nu_1 \langle \nu_1 \\ -\nu_1 \langle \nu_1 & 0 & 0 & 0 \\ 0 & -\nu_1 \langle \nu_1 & 0 & \nu_1 \langle \nu_1 \end{pmatrix}$$

If the correcting term is selected as above, we obtain the dispersion curves in various direction as shown one Fig. 5:

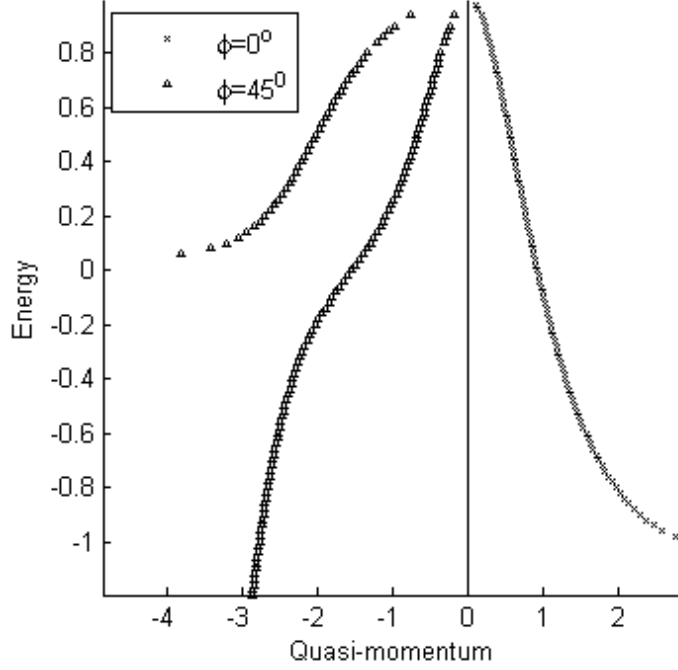


Figure 5: Sections of the dispersion surface of the abstract model emulating Heine-Abarenkov potential with resonance eigenvalue $\lambda_2 > \lambda_1$.

Our aim in previous section was to construct a convenient semi-analytic bridge between the structure of orbitals on the period in the resonance spectral domain and the shape of the dispersion surface in the resonance domain. The "analytic" part of the bridge was already constructed, ending by the formula (23), assuming that the one-pole rational approximation (28) for the DN-map on the 2D lattice or sandwich (18) on the resonance spectral domain is selected. The examples considered in this section show typical behavior of the dispersion in the resonance domain. In fact our proposal has a softer nature (in the sense of V. Arnold), due to the freedom of selection of the rational approximation (probably a multi-pole-approximation) for the real material lattice or sandwich on the resonance domain,

$$\mathcal{DN} \approx \sum_{s \leq m} A_s \frac{Q_s}{\lambda - \lambda_s} + P_m(\lambda), \quad (27)$$

the choice of the contacts/contact subspaces and temperature (interval of energies) We guess that this problem, though looks as a mathematical one, lies outside of mathematics, - on the border with quantum chemistry, with its specific system of notions (covalent bonds, etc...) and methods.

According to our previous analysis the derivation of the dispersion equation of the sandwich composed of two 2D periodic lattices separated by a weakly transparent barrier includes the 2D dispersion of the layers $\mathcal{D}^u, \mathcal{D}^d$ as basic details. Contrary to

above analysis of a 2D lattice we base on the DN-maps $\mathcal{DN}^u, \mathcal{DN}^d$ of the upper and lower parts of the two-storied period. Besides the components (28), connecting the Dirichlet data on $\Gamma_\alpha^i, i = 1, 2; \alpha = a, 0$ the DN-map of the upper/lower half of the period includes the components connecting the Dirichlet data on Γ_b with Neumann data on Γ_α^i and vice versa, subject to filtering by the appropriate contact subspace N_b . Assuming that the temperature is low, we considered in (13) the $2 \times 1, 1 \times 2$ and 1×1 blocks substituted by the corresponding rational approximations, based on our previous assumption

$$\mathcal{DN}_b \approx \frac{\left(\begin{array}{c} P_N \frac{\partial \varphi_1^D}{\partial n} \Big|_{\Gamma_a} \\ P_N \frac{\partial \varphi_1^D}{\partial n} \Big|_{\Gamma_0} \end{array} \right) \left\langle P_{N_b} \frac{\partial \varphi_1^D}{\partial n} \Big|_{\Gamma_b} \right\rangle}{\lambda - \lambda_1} + B_b \left(\begin{array}{c} e_b^a \\ e_b^0 \end{array} \right) \equiv \mathcal{D}_b(\lambda, \mu) = A_b \frac{Q_b}{\lambda - \lambda_1} + \vec{B}_b. \quad (28)$$

Here due to (24, 25)

$$\left(\begin{array}{c} P_N \frac{\partial \varphi_1}{\partial n} \Big|_{\Gamma_a} \\ P_N \frac{\partial \varphi_1}{\partial n} \Big|_{\Gamma_0} \end{array} \right) \left\langle P_{N_b} \frac{\partial \varphi_1^D}{\partial n} \right\rangle = \frac{A_b}{\sqrt{2}} \left[\nu_1 \Big|_{\Gamma_a} + \nu_2 \Big|_{\Gamma_0} \right] \left\langle \nu_b \right\rangle, \quad (29)$$

with a new fitting parameter $A_b^{u,d}$ for vertical blocs of the upper and lower half-periods. The horizontal blocs are connected with the vertical blocs as Hermitian adjoints. The central block is one-dimensional and contains four fitting parameters as $\frac{Q_b^{u,d}}{\lambda - \lambda_1^{u,d}} + B_{bb}^{u,d}$, see (17). Then substitution into (23) the expressions for blocks obtained via elimination all variables except V_b yields a scalar homogeneous equation, which can be used as an equation for the dispersion function depending explicitly on the fitting parameters. We postpone the discussion of this technicalities to an oncoming publication.

4 Derivation of the DN-map on the resonance spectral domain from the relevant ND map.

Calculation of the relative DN-map in the resonance domain is complicated due to instability of the solution of the boundary problem (1) for the values of the spectral parameter close to the Fermi level $\Lambda_F \approx \lambda_1^D$. In the simplest case of a single resonance eigenvalue $\lambda_1^D \equiv \lambda_1$ the polar term of the DN-map (and hence one of the relative DN-map) is calculated in terms of the resonance eigenfunction, see (28), but, to calculate the regular term B we have to use the duality

$$\mathcal{DN}_N \times \mathcal{ND}_N = I_N = \mathcal{ND}_N \times \mathcal{DN}_N \quad (30)$$

of the relative DN -map \mathcal{DN}_N and the relative ND-map \mathcal{ND}_N defined by the partial Dirichlet (31) and Neumann (31) boundary problems with the corresponding data from

the contact subspace N

$$-\Delta\Psi + q(x)\Psi = \lambda\Psi, \quad \Psi\Big|_{\Gamma} = \psi_{\Gamma} \in N, \quad \Psi\Big|_{\partial\Omega\setminus\Gamma} = 0, \quad \psi_{\Gamma} \xrightarrow{\mathcal{DN}_N} \frac{\partial\Psi}{\partial n}\Big|_{\Gamma}. \quad (31)$$

$$[-\Delta + q(x) - \lambda]\Psi = 0, \quad \Phi\Big|_{\partial\Omega\setminus\Gamma} = 0, \quad \frac{\partial\Phi}{\partial n}\Big|_{\Gamma} = \rho \in N, \quad \rho_{\Gamma} \xrightarrow{\mathcal{ND}_N} \Phi\Big|_{\Gamma}. \quad (32)$$

Due to the uniqueness theorem for the Schrödinger equation, the eigenvalues of the relative Dirichlet and Neumann problems never coincide. Hence we may assume that the partial Neumann problem has a unique solution for the values of energy λ on the temperature interval centered at the Fermi level. Hereafter we deal only with the relative DN and ND maps at the Fermi level. Correspondingly we omit the lower indices N in the notations. We also use an orthogonal decomposition of the unit operator $I_N \equiv I$ in the contact subspace $I = Q \oplus Q^{\perp}$, and consider the relevant matrix representations of \mathcal{DN} , \mathcal{ND} in the resonance domain near the Fermi level. Then, with use of the notations $B_{q,\perp} \equiv QBQ^{\perp}$, $B_{q,q} = QBQ$, $B_{\perp,\perp} \equiv Q^{\perp}BQ^{\perp}$, $B_{\perp,q} \equiv Q^{\perp}BQ$, and similar notations for the matrix elements of the partial ND-map, we represent the duality equation as

$$\begin{pmatrix} \frac{A}{\lambda-\lambda_1} + B_{q,q} & B_{q,\perp} \\ B_{\perp,q} & B_{\perp,\perp} \end{pmatrix} \begin{pmatrix} \mathcal{ND}_{q,q} & \mathcal{ND}_{q,\perp} \\ \mathcal{ND}_{\perp,q} & \mathcal{ND}_{\perp,\perp} \end{pmatrix} = \begin{pmatrix} Q & 0 \\ 0 & Q^{\perp} \end{pmatrix}. \\ \begin{pmatrix} \mathcal{ND}_{q,q} & \mathcal{ND}_{q,\perp} \\ \mathcal{ND}_{\perp,q} & \mathcal{ND}_{\perp,\perp} \end{pmatrix} \begin{pmatrix} \frac{A}{\lambda-\lambda_1} + B_{q,q} & B_{q,\perp} \\ B_{\perp,q} & B_{\perp,\perp} \end{pmatrix} = \begin{pmatrix} Q & 0 \\ 0 & Q^{\perp} \end{pmatrix}. \quad (33)$$

Based on regularity of the \mathcal{ND} and B on the resonance domain we derive from above duality equations, that the elements of the ND-map have zeros at the resonance eigenvalue λ_1 , or, other words, the limits of the ratio's below at $\lambda \rightarrow \lambda_1$

$$\frac{\mathcal{ND}_{q,\perp}}{\lambda - \lambda_1} \equiv R_{q,\perp}(\lambda), \quad \frac{\mathcal{ND}_{\perp,q}}{\lambda - \lambda_1} \equiv R_{\perp,q}(\lambda), \quad \frac{\mathcal{ND}_{q,q}}{\lambda - \lambda_1} \equiv R_{q,q}(\lambda), \\ A \frac{\mathcal{ND}_{q,q}}{\lambda - \lambda_1} \equiv AR_{q,q} + (\lambda - \lambda_1)[R_{q,q}B_{q,q} + R_{q,\perp}B_{\perp,q}] = Q,$$

exist, the corresponding functions R are regular functions of energy on the resonance domain. Using notations introduced above we derive from the duality equations

$$B_{\perp,\perp}\mathcal{ND}_{\perp,\perp}\Big|_{\lambda=\lambda_1} = Q^{\perp}, \quad B_{\perp,q}R_{q,q} + B_{\perp,\perp}R_{\perp,q}\Big|_{\lambda=\lambda_1} = 0, \quad (34)$$

and

$$AR_{q,q} + (\lambda - \lambda_1)[R_{q,q}B_{q,q} + R_{q,\perp}B_{\perp,q}] = Q,$$

which implies

$$\frac{Q - AR_{q,q}}{\lambda - \lambda_1} = R_{q,q}B_{q,q} + R_{q,\perp}B_{\perp,q}. \quad (35)$$

These equations define the behavior of the regular B on the resonance domain. In particular, while $\mathcal{ND}_{\perp,\perp}$ is invertible, the matrix elements of $B(\lambda_1)$ can be computed based on spectral data φ_1 , λ_1 and \mathcal{ND} .

5 Conclusion: towards theoretical analysis of HTSC in B-Si-B sandwich.

The transformation of the crossing of the 2D terms into quasi-crossings - the Landau-Zener phenomenon - is similar to the 1D version discussed in [1] with the standard and flat bands overlapping. It was shown there that in the corresponding *one-dimensional model* the spectral gap δ_{LZ} , arising due to Landau-Zener gap, causes an essential enhancement of the superconductivity gap and hence high-temperature stability of the superconductivity phenomenon. Involvement of the flat band guarantees a high density of states, which permits experimental confirmation of HTSC.

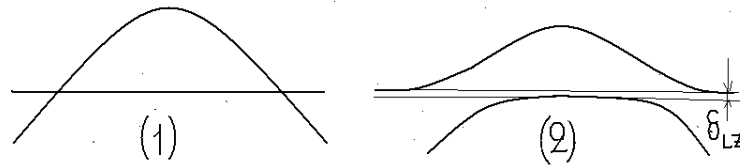


Figure 6: Enhancing of the superconductivity gap arising from a simple and flat band overlapping: transformation of the band's crossing (1) into the quasi-crossing (2) (1D schematic figure).

In [3] high-temperature superconductivity was observed in a B-Si-B sandwich. The authors interpreted it as a Josephson effect due to the interaction between the Bloch functions of the upper and lower plates of the sandwich, defined by the boundary condition on the barrier Γ_b , see Fig. 7.

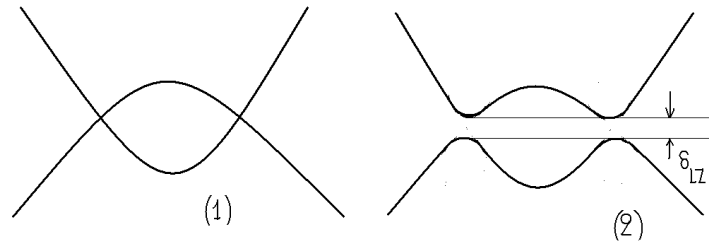


Figure 7: Additional spectral gaps arising from the 2D Landau-Zener phenomenon: transformation of the crossing of the dispersion surfaces into the quasi-crossing(2) (The 2D section of the 3D gutter).

In [3] additional electrodes were also used to manipulate the positions of the subbands in the barrier, and the stable high-temperature conductivity effect was observed.

Our above analysis is aimed on explanation observations presented in [3] in the case of quasi 2D sandwiches.

We hope that the explanation may arise as an application of the ideas [1] to the quasi-2D sandwich. Indeed the substitution of the flat band by the standard band does not destroy the Landau-Zener phenomenon, hence it is not essential for the theoretical interpretation of the superconductivity observed: the Landau-Zener gap arose due to the quasi-2D sandwich structure with a resonance barrier. On the other hand the DN approach to calculation of the dispersion function of the sandwich allows to substitute the 1D model in [1] by the 2D sandwich. An essential detail of the program is estimation of the density of states for the quasi-2D B-Si-B sandwich and the estimation of the critical temperature. We hope that it can be done based on the methods suggested above and postpone the relevant computing and analysis for an oncoming publication.

References

- [1] V. Adamyan, B. Pavlov "High-Temperature superconductivity as a result of a simple and flat bands overlapping" In Russian. *Solid state Physics* **34**, 2 (1992) pp 626-635.
- [2] N. Bagraev, G. Martin, B. Pavlov. "Landau-Zener Phenomenon on a double of weakly interacting quasi-2d lattices". In: *Progress in Computational Physics (PiCP)* (2010) pp. 61-64.
- [3] N.Bagraev, L. Klyachkin, A. Kudryavtsev, A.Malyarenko, V. Romanov "Superconductor properties for silicon nanostructures". In: "Superconductivity Theory and application". Ed. by A. Luiz, SCIVO, chapt. 4 (2010) pp. 69-92.
- [4] N. Bagraev, G. Martin, B. Pavlov, A. Yafyasov "Landau-Zener effect for quasi-2D periodic sandwich", 21 page. Accepted in "Nanosystems: Physics, Chemistry, Mathematics", to be published in December 2012.
- [5] J. Brüning, G. Martin, B. Pavlov "Calculation of the Kirchhoff coefficients for the Helmholtz resonator", *Russ. J. Math. Phys.*, **16**, (2009), no. 2, 188–207.
- [6] M. Levitin, M. Marletta "A simple calculation of eigenvalues and resonances in domains with regular ends", *Proc. Roy. Soc. Edinburgh Section., A* 138, N 5 (2008) pp.1043-1065.
- [7] C. Zener "Non-adiabatic crossing of energy -levels", *Proc. Royal Soc. A*, **137**,(1932) p.696.
- [8] B. Pavlov "it S-Matrix and Dirichlet-to-Neumann Operators" In: *Scattering and Semigroup Theory* In: *Scattering*, ed. R. Pike, P. Sabatier, Academic Press, Harcourt Science and Tech. Company (2001 pp 1678-1688
- [9] A.Yafyasov, V. Bogevolnov, G. Fursey, B. Pavlov, M. Polyakov, A. Ibragimov. "Low-treshold field emission from carbom nano-clusters", *Ultramicroscopy*,**111**(2011) pp 409-414.