Anomalous tunneling of bound pairs in crystal lattices

EUROPHYSICS LETTERS 1 August 2005

Europhys. Lett., **71** (3), pp. 352–358 (2005)
DOI: 10.1209/epl/i2005-10102-7

Anomalous tunneling of bound pairs in crystal lattices

V. L. Bulatov[1](*) and P. E. Kornilovitch[2](**)

[1] *2970 N. W. Christine St, Corvallis, OR 97330, USA*
[2] *2876 N. W. Audene Drive, Corvallis, OR 97330, USA*

received 13 April 2005; accepted in final form 7 June 2005
published online 14 July 2005

PACS. 03.65.Ge – Solutions of wave equations: bound states.
PACS. 03.65.Nk – Scattering theory.
PACS. 71.10.Li – Excited states and pairing interactions in model systems.

Abstract. – A novel non-perturbative method of solving scattering problems for bound pairs on a lattice is developed. Two different break-ups of the Hamiltonian are employed to calculate the full Green operator and the wave function of the scattered pair. The calculation converges exponentially in the number of basis states used to represent the non-translation–invariant part of the Green operator. The method is general and applicable to a variety of scattering and tunneling problems. As the first application, the problem of pair tunneling through a weak link on a one-dimensional lattice is solved. It is found that at the momentum values close to $\pm\pi$ the pair tunnels much easier than one particle, with the transmission coefficient approaching unity. This anomalously high transmission is a consequence of the existence of a two-body resonant state localized at the weak link.

Introduction. – The scattering of bound particle complexes has been a major subject of atomic, molecular and nuclear physics for decades. In "lattice" solid-state physics the prime system of interest has been the exciton [1, 2], in which the constituent particles, an electron and a hole, have different masses. The bound pair of two magnons in lattice magnetism is an example of a complex with equal masses [3]. In recent years, the concepts of bisolitons in one-dimensional non-linear systems [4], and bipolarons in conducting polymers [5, 6] and high-temperature superconductors [7, 8] have been developed.

Many properties of these particles derive directly from their composite nature rather than from the particulars of the binding interaction. They can therefore be studied within the framework of the "generic" two-body system, in which a model potential is introduced to ensure binding, yet the simplicity of the potential enables a rigorous analysis of the quantum-mechanical problem. This approach has been popular and the physics of two-particle bound complexes in *translation invariant* lattices is now well understood, see for example [9–11] and the bibliography therein. Much less is known about non-translation–invariant cases. When defects or boundaries are present the two-body problem can no longer be reduced to a one-body problem, which significantly complicates analysis. In continuum physics, scattering of

(*) E-mail: bulatov@physics.orst.edu
(**) E-mail: pavel.kornilovich@hp.com

bound pairs was approached from the general *three-body* formalism [12–14], although no exact results were obtained beyond the one dimension with delta-function potentials. On a lattice, the previous research was limited to the surface excitonic effects [15, 16]. Bulatov [17, 18] developed a general theory and an efficient numerical procedure to obtain the energy spectra and wave functions of lattice excitons in the presence of a surface.

In this letter, we extend the method of [17,18] to the general scattering problem of lattice bound pairs. The method consists of calculating the full two-particle Green operator G and then acting with it on the wave function of an incident pair Ψ_V. The core feature of the method is the usage of two different decompositions of the Hamiltonian on a zero part and a perturbation. The first decomposition is applied to find G while the second decomposition is used to calculate the scattering amplitudes. The accuracy of the method scales exponentially with the number of lattice sites used to approximate the non-translation–invariant part of G. As the first application of the method we solve the problem of tunneling of a one-dimensional bound pair through a weak link on a chain. We find that the pair transmission at large lattice momenta is significantly *enhanced* in comparison with the transmission of a single particle. In fact, the transmission coefficient approaches unity at the Brillouin zone boundary.

Method. – The generic model consists of free motion of two particles H_0, interparticle interaction V (which is usually attractive), and single-particle scattering U:

$$\begin{aligned} H &= H_0 + V + U && (1)\\ &= H_V + U && (2)\\ &= H_U + V. && (3) \end{aligned}$$

Here we introduce *two* partial Hamiltonians, $H_V = H_0 + V$ and $H_U = H_0 + U$. Equations (2) and (3) define the two decompositions mentioned above. Using (2), the full wave function Ψ satisfies the Schrödinger equation:

$$\Psi = \Psi_V + G_V U \Psi, \tag{4}$$

where $H_V \Psi_V = E\Psi_V$, Ψ_V has the appropriate boundary conditions at infinity, $G_V(E) = (E - H_V + i\gamma)^{-1}$ is the Green operator of H_V, and $\gamma \to 0$. Three other Green operators G, G_0, and G_U are defined analogously. In the basis of localized lattice states the Green operators can be represented as ordinary matrices, albeit of infinite size.

Ordinarily, equations like (4) are used to develop perturbative expansions for Ψ from the knowledge of the partial Green operator G_V. Now suppose that the full Green operator G is known. Since $G = (1 - G_V U)^{-1} G_V$ and $\Psi = (1 - G_V U)^{-1} \Psi_V$, the last term in (4) is re-arranged as follows:

$$G_V U \Psi = G_V U (1 - G_V U)^{-1} \Psi_V = (1 - G_V U)^{-1} G_V U \Psi_V = G U \Psi_V \,, \tag{5}$$

so that, from eq. (4),

$$\Psi = \Psi_V + G U \Psi_V = (1 + GU) \Psi_V \,. \tag{6}$$

Thus if G is known, the full wave function can be found from the last equation by matrix multiplication.

Now comes an important observation. Since G is the full Green operator it does not matter how it is obtained. In particular, one is not obligated to use the same decomposition (2) that has led to eq. (6). For the scattering of bound pairs it is more convenient to use the decomposition (3), which yields

$$G = (1 - G_U V)^{-1} G_U \equiv A^{-1} G_U \,. \tag{7}$$

The advantage of this approach is that G_U is the Green operator of two non-interacting particles, both scattered off the potential U. Therefore G_U can be calculated as a convolution of two *one-particle* Green operators g_U:

$$G_U(\boldsymbol{r}_1\boldsymbol{r}_1';\boldsymbol{r}_2\boldsymbol{r}_2';E) = i\int_{-\infty}^{\infty}\frac{\mathrm{d}\epsilon}{2\pi}\, g_U(\boldsymbol{r}_1\boldsymbol{r}_1';\epsilon)g_U(\boldsymbol{r}_2\boldsymbol{r}_2';E-\epsilon). \tag{8}$$

In turn, g_U follows from the solution of a one-particle scattering problem:

$$g_U = (1-g_0U)^{-1}g_0\,, \tag{9}$$

where $g_0 = (\varepsilon - H_0 + i\gamma)^{-1}$ is the one-particle Green operator of the translation-invariant system. The zero operator g_0 is most easily calculated from the spectral expansion

$$g_0(\boldsymbol{r},\boldsymbol{r}';\varepsilon) = \sum_{\boldsymbol{k}}\frac{e^{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}}{\varepsilon-\varepsilon_{\boldsymbol{k}}+i\gamma}\,, \tag{10}$$

where $\varepsilon_{\boldsymbol{k}}$ is the one-particle spectrum. G_U can also be calculated from the two-particle spectral expansion [19]. Thus the strategy of the present method is to use the decomposition (3) and the formulas (7)-(10) to obtain the Green operator G, and then use the decomposition (2) and the formula (6) to calculate the full wave function Ψ and the scattering coefficients of interest.

Calculation of $(1-G_UV)^{-1}$. – Once G_U is known, the main task is to invert the matrix $A \equiv 1 - G_UV$, see eq. (7). The way of calculating A^{-1} is the second key component of the present method. Observe that inverting $(1-G_UV)$ is analogous to inverting $(E-H)$, *i.e.*, to calculating the Green operator. Imagine a G_U that consists of a translation-invariant part G_U^0 and a perturbation $\delta G = G_U - G_U^0$ which is localized in real space. Then the translation-invariant part $(1-G_U^0V)$ plays the role of the translation-invariant part of $(E-H)$ while δGV the role of the localized perturbation. Performing the standard transformation one obtains

$$A^{-1} \;=\; (1-G_U^0V-\delta G\,V)^{-1} = (1-B^{-1}\delta G\,V)^{-1}\,B^{-1}, \tag{11}$$

$$B \;\equiv\; 1-G_U^0V. \tag{12}$$

Thus, inversion of A is replaced with two inversions. The first inversion is that of B. Since B involves only translation-invariant matrices, this is achieved by changing to the quasi-momentum representation in which B is block-diagonal with the block size equal to the range of V in relative coordinates [18]. The second inversion is that of $(1-B^{-1}\delta G\,V)$. The latter is the sum of the unit matrix and a matrix localized around the scattering region, which is due to the localization of δG. Therefore, only inversion of a finite-size matrix that contains the non-zero elements of $B^{-1}\delta G\,V$ is required. As a result, the abstract task of inverting the infinite matrix A is replaced with two easy-to-perform operations on finite-size matrices.

To summarize, the algorithm begins with the calculation of the Green matrix G_U from eqs. (8)-(10). Then G_U is separated into the translation-invariant part G_U^0 and the remainder δG. On the next step, A^{-1} is calculated according to eq. (11), and then the full Green operator is obtained from eq. (7). Finally, a free pair wave function Ψ_V is chosen and the scattered wave function is calculated from eq. (6). This formulation is non-perturbative and applicable to a variety of particular cases. One such problem is analyzed below.

Chain with a weak link. – Consider a one-dimensional chain characterized by the nearest-neighbor hopping matrix element $t > 0$ and the Hubbard-like attraction of strength $|v| > 0$.

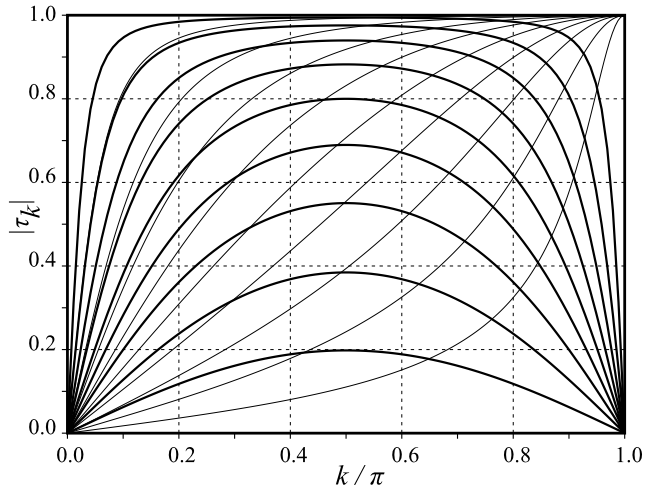

Fig. 1 – Bold lines: modulus of the single-particle transmission coefficient $|\tau_k|$ through the weak link, see eq. (14). From the top curve down: $t'/t = 0.1,\ 0.2,\ \ldots,\ 0.9$. Thin lines: the same quantity in the presence of a resonant state at the top of the single-particle band, see eq. (18).

The hopping amplitude between sites $n = 0$ and $n = 1$ contains an additional element t'. The resulting Hamiltonian reads

$$H = -t \sum_{\langle nn'\rangle\sigma} c^\dagger_{n\sigma} c_{n'\sigma} - |v| \sum_n c^\dagger_{n\uparrow} c_{n\uparrow} c^\dagger_{n\downarrow} c_{n\downarrow} + t' \sum_\sigma \left(c^\dagger_{0\sigma} c_{1\sigma} + c^\dagger_{1\sigma} c_{0\sigma} \right), \tag{13}$$

where $\langle nn'\rangle$ denotes pairs of nearest-neighbor sites. The value $t' = 0$ corresponds to the absence of any scattering, while $t' = t$ corresponds to two decoupled semi-infinite chains. A standard solution of the one-particle scattering problem yields the transmission coefficient:

$$\tau_k = \frac{(t'/t - 1)(e^{ik} - e^{-ik})}{e^{-ik} - (t'/t - 1)^2\, e^{ik}}, \tag{14}$$

where k is the one-particle momentum. The modulus of the transmission coefficient $|\tau_k|$ is shown in fig. 1 in bold lines. Note that $\tau_k = 0$ at $k = 0$ or $k = \pi$.

In the absence of scattering ($t' = 0$), two particles form a singlet bound state with an (unnormalized) wave function,

$$\Psi^\pm_V(n_1, n_2) = e^{\pm i \frac{K}{2}(n_1+n_2)} e^{-\lambda|n_1-n_2|}, \tag{15}$$

where $K \geq 0$ is the total momentum of the pair and $\sinh\lambda = |v|/[4t\cos(K/2)]$. The energy of the bound state is $E = -\sqrt{v^2 + 16t^2\cos^2(K/2)} < 0$. We choose to study the scattering of the pairs incident from the left with energy $E < -4t$ to prevent the processes of pair breaking in two free particles. At these energies the full wave function (6) has the asymptotic $\Psi \to \Psi^+_V + R\Psi^-_V$ at $n_1, n_2 \to -\infty$, and $\Psi \to T\Psi^+_V$ at $n_1, n_2 \to +\infty$. We are interested in the pair transmission coefficient T as a function of the pair momentum K and model parameters t' and $|v|$.

Determination of T begins with calculating G_U from eqs. (8)-(10) using as input $\varepsilon_k = -2t\cos k$ and U that has all the matrix elements zero except $u_{01} = u_{10} = t'$. The translation-invariant part of G_U can be obtained numerically by setting $t' = 0$. Alternatively, the

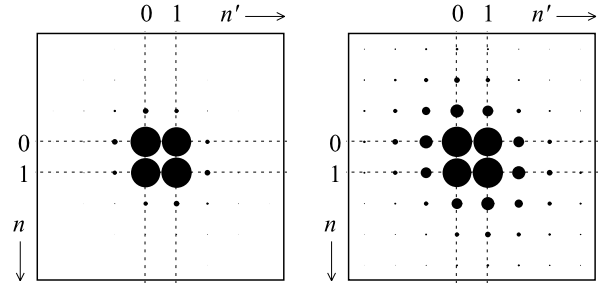

Fig. 2 – The non-translation–invariant part of the Green operator $\delta G(n,n')$ for $|v| = 4.1\,t$ and $t' = 0.3\,t$. The pair momentum is $K = 0.3\pi$ (left panel) and $K = 0.8\pi$ (right panel). The radius of the circle represents the modulus $|\delta G|$. Notice the high degree of localization around the weak link.

two-particle spectral expansion yields for G_U^0 at $E < -4t$ the following expression (for the model (13), only $n_1 = n_2$, $n_1' = n_2'$ matrix elements of G_U^0 are needed because of the locality of the Hubbard attraction):

$$\begin{aligned} G_U^0(n,n;n',n';E) &= \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{\mathrm{d}k_1\mathrm{d}k_2}{(2\pi)^2} \frac{\cos k_1(n-n')\cos k_2(n-n')}{E + 2t\cos k_1 + 2t\cos k_2} \\ &= -\int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\pi} \frac{\cos q(n-n')}{\sqrt{E^2 - 8t^2 - 8t^2\cos q}}\,. \end{aligned} \tag{16}$$

In accordance with the general scheme, the matrix δG is calculated by subtracting G_U^0 from G_U. $\delta G(n,n')$ is very localized around the weak link $n,n' = 0,1$, see fig. 2.

The last thing we need is an expression for B^{-1}, see eq. (12). Again, only the matrix elements in the block $n_1 = n_2$ and $n_1' = n_2'$ are required. By diagonalizing the block by a Fourier transformation one can show that [17, 19]

$$B^{-1}(n;n') = \int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\pi} \frac{\cos q(n-n')}{1 - \frac{|v|}{\sqrt{(E+i\gamma)^2 - 16t^2\cos^2(q/2)}}}\,. \tag{17}$$

Numerical results. – The results obtained in the preceding section enable the calculation of the full two-particle Green operator, the exact pair wave function, and the scattering coefficients of bound pairs for the model (13). In fig. 3 we show the modulus $|\Psi_K|$ as a function of the particle coordinates n_1 and n_2 for $K = 0.3\,\pi$, $|v| = 4.1\,t$ and $t' = 0.3\,t$. Notice how reflection off the weak link creates interference between the incident and reflected waves. In contrast, the transmitted wave (in the lower right part of the graph) has a constant amplitude. In fig. 4 we show the pair transmission coefficient T_K. As a function of pair momentum, T_K behaves qualitatively different from the one-particle transmission τ_k, see fig. 1. τ_k first increases with the momentum but then decreases and vanishes at $k = \pi$. In contrast, T_K is a monotonically increasing function of the momentum, and reaches unity at $K = \pi$. Thus *at large lattice momenta a bound pair is transmitted through a weak link much easier than a single particle.* The likely physical reason for the anomalously high transmission is resonant tunneling through a two-body state localized at the weak link. Bulatov and Danilov [20] previously analyzed the two-particle spectrum of a semi-infinite Hubbard chain, *i.e.* model (13) with $t' = t$. They found that the chain boundary introduces a resonant state with $E = -|v|$, *i.e.* exactly at the top edge of the pair band. We conjecture that such a state exists for $t' \neq t$ as well, and facilitates efficient transmission through the weak link of pairs with energies close to the top of the band, *i.e.* with momenta close to π.

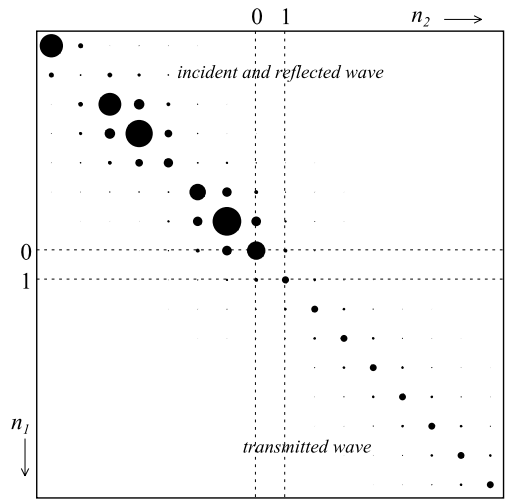

Fig. 3 – The pair wave function $\Psi_K(n_1, n_2)$ for $K = 0.3\,\pi$, $|v| = 4.1\,t$ and $t' = 0.3\,t$. The radius of the circle represents the modulus $|\Psi|$.

It is instructive to compare this effect with *one-particle* tunneling through the weak link in the presence of a resonant state. Such a state appears in the model (13) with $|v| = 0$ if an additional one-particle repulsive potential w is added at the two sites on either side of the weak link. At $w = t'$, the state has the energy of the top of the one-particle band, $E = 2t$. For those parameters, the transmission coefficient is [19]

$$\bar{\tau}_k = \frac{(1 - t'/t)(e^{ik} - e^{-ik})}{(e^{ik} - e^{-ik}) - 2(t'/t)(1 + e^{ik})}\,. \tag{18}$$

This function is shown in fig. 1 in thin lines. The resonant state qualitatively changes the transmission at large momenta. Instead of vanishing $\bar{\tau}_k$ approaches unity. The overall shape of the curves is remarkably similar to the pair transmission curves of fig. 4, which further

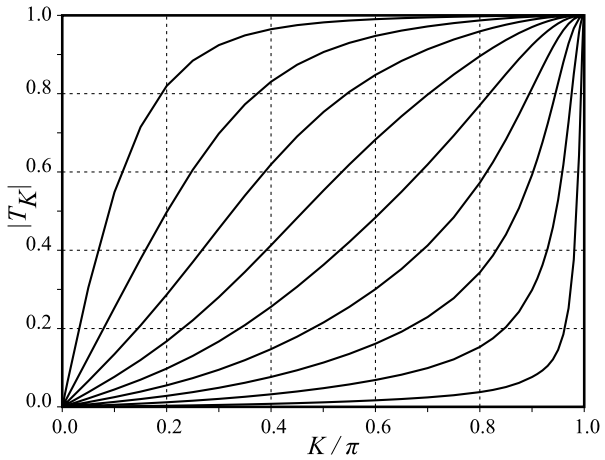

Fig. 4 – Pair transmission coefficient T_K for $|v| = 4.1$ and different t'/t. From the top curve down: $t'/t = 0.1,\ 0.2,\ \ldots,\ 0.9$.

supports our interpretation of pair tunneling as through a resonant state.

Enhanced transmission of *slow-moving* weakly bound pairs in a continuum model with a delta-function repulsive barrier was reported previously in [14]. We have not observed similar enhancement in our model at moderate binding potentials. Analysis of the extreme weak-coupling limit is not straightforward in our method because of the increasing extent of δG. In addition, the two models are quite different. This makes the comparison of the two effects an interesing but difficult task, which warrants a separate investigation.

Summary. – We have developed an efficient procedure of calculating scattering coefficients of bound pairs on a lattice. The key technical advance of the paper is the usage of two different decompositions of the Hamiltonian; one is used to calculate the full Green operator of the system while another to find the resulting wave function of the pair. Another important element is the method of inverting the matrix $(1 - G_U V)$, which is based on separating G_U into a translation-invariant part and a part localized around the scatterer, see eqs. (11) and (12). The numerical accuracy of the method scales exponentially in the number of basis states chosen to represent the localized part. The method is non-perturbative and general, enabling accurate investigation of a variety of scattering and tunneling problems. As the first application, we have studied transmission of bound pairs through a weak link on the one-dimensional chain. Contrary to simplistic expectations, we have found that at large momenta the pairs penetrate the barrier more easily than single particles. The anomalously high transmission has been identified with tunneling through a resonant pair state.

REFERENCES

[1] Davydov A. S., *Theory of Molecular Excitons* (McGraw-Hill, New York) 1962.
[2] Knox R. S., *Theory of Excitons* (Academic, New York) 1963.
[3] Mattis D., *The Theory of Magnetism*, Vol. **1** (Springer, Berlin) 1981.
[4] Davydov A. S., *Nonlinearity*, **2** (1989) 383.
[5] Brazovskii S. A. and Kirova N. N., *Pis'ma Zh. Eksp. Teor. Fiz.*, **33** (1981) 6 (*JETP Lett.*, **33** (1981) 4).
[6] Heeger A. J., Kivelson S., Schrieffer J. R. and Su W.-P., *Rev. Mod. Phys.*, **60** (1988) 781.
[7] Alexandrov A. S. and Mott N. F., *High Temperature Superconductors and Other Superfluids* (Taylor & Francis) 1994.
[8] Alexandrov A. S. and Kornilovitch P. E., *J. Phys. Condens. Matter*, **14** (2002) 5337.
[9] Mattis D. C., *Rev. Mod. Phys.*, **58** (1986) 361.
[10] da Viega P. A. F., Ioriatti L. and O'Carroll M., *Phys. Rev. E*, **66** (2002) 016130.
[11] Kornilovitch P. E., *Phys. Rev. B*, **69** (2004) 235110.
[12] Schwebel S. L., *Phys. Rev.*, **103** (1956) 814.
[13] Jasperse J. R. and Friedman M. H., *Phys. Rev.*, **159** (1967) 69.
[14] Alexandrov A. S., Bratkovsky A. M. and Kornilovitch P. E., *Phys. Rev. B*, **65** (2002) 155209.
[15] Hizhnyakov V. V., Maradudin A. A. and Mills D. L., *Phys. Rev. B*, **11** (1975) 3149.
[16] Gumbs G. and Mavroyannis C., *J. Phys. C*, **14** (1981) 2199.
[17] Bulatov V. L., *Fiz. Tverd. Tela*, **26** (1984) 2480 (*Sov. Phys. Solid State*, **26** (1984) 1501).
[18] Bulatov V. L., *J. Phys. C*, **20** (1987) 5421.
[19] More details will be described elsewhere.
[20] Bulatov V. L. and Danilov I. Yu., *Fiz. Tverd. Tela*, **36** (1994) 679 (*Sov. Phys. Solid State*, **36** (1994) 373).