

On the theory of systems with substitutional non-Hermitian disorder

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A novel family of disordered systems is proposed. This family belongs to the class of systems containing random substitutional non-Hermitian impurities. We limit our consideration to a rather simple case when the presence of substitutional point defects results in the model Hamiltonian featuring a diagonal disorder. In contrast to known models of non-Hermitian impurities, the nonzero density of states for each isolated from the host impurity is restricted to a continuous band of finite width. A method to construct corresponding impurity Hamiltonians is provided.

Keywords: non-Hermitian impurity, locator, local density of states, disorder.

1. Over the past two decades, quantum systems that are described by non-Hermitian Hamiltonians were under intensive and sustained investigation [1–5]. Albeit real-world realizations of non-Hermitian systems can be thought of as quite exotic, their existence is not proscribed by any fundamental law [6–8]. Recently, examples of such systems began to propagate at a steady pace within certain metamaterials and optical lattices. The availability of nontrivial experimental data resurged the theoretical activity in this already well-established field.

Meanwhile, a novel shift of scientific interest happened in this sphere: attention to disordered non-Hermitian systems has been considerably increased. In particular, systems with non-Hermitian impurities got into focus [9–11]. Below we are making an effort to improve understanding of the main principles on which physically-consistent non-Hermitian impurity models should be devised.

Given that this study attempts to go beyond conventional impurity models for solid-state systems with the diagonal disorder, we dedicate it to Prof. Viktor Bar'yakhtar, who celebrates his 90th birthday in the August of this year, and whose contribution to the theory of crystal state has long been widely recognized beyond dispute.

2. To move on to substantive issues, consider a generic inhomogeneous system, which Hamiltonian \hat{H} can be divided into two parts: the host one $\hat{H}^{(h)}$ that represents the

initial clean system, and the impurity one $\hat{H}^{(d)}$ that contains the introduced disorder. So one has that

$$\hat{H} = \hat{H}^{(h)} + \hat{H}^{(d)}. \quad (1)$$

We presuppose that only off-diagonal elements in the matrix, which represents the separated above host Hamiltonian, are non-zero:

$$\hat{H}^{(h)} = \sum_{\substack{n,m \\ n \neq m}} t_{nm} c_n^\dagger c_m, \quad (2)$$

while the impurity part of the Hamiltonian consists exclusively of diagonal on-site operators:

$$\hat{H}^{(d)} = \sum_n \varepsilon_n c_n^\dagger c_n. \quad (3)$$

It should be pointed out that non-diagonal matrix elements t_{nm} remain intact between different realizations of the disordered system. In contrast, diagonal matrix elements ε_n do vary between them. Indeed, we will take for granted that the host Hamiltonian is Hermitian:

$$t_{nm} = t_{mn}^*. \quad (4)$$

When diagonal elements ε_n are all real, we are dealing, as a matter of fact, with a Hermitian full Hamiltonian. Usually, Hamiltonians of this sort are interpreted as a

spinless tight-binding model for a single isolated electronic band. In this particular case, c_n^\dagger and c_m stand for Fermi creation and annihilation operators, which indices n and m enumerate lattice sites of the underlying crystal structure. Respectively, non-diagonal matrix elements t_{nm} represent hopping integrals calculated between the n th and m th site, and the remaining ε_n 's are on-site potentials in this single-electron Hamiltonian. The values of on-site potentials usually are assumed to be randomly distributed in the crystal lattice. On-site potentials can take one of just two fixed values with a given probability, which corresponds to the model of a binary alloy with the diagonal disorder (also frequently named after Lifshitz) or are allowed to vary within a specified energy interval for each site (the Anderson model), etc.

Nevertheless, the mentioned detail in the spatial distribution or in imposed magnitude constraints for on-site potentials will have no impact on what follows, and thus we are not confined in this study to any specific type of available impurity models. For instance, even those models that take into account spatial correlations between on-site potentials are not excluded. Just to reiterate: no restrictions are enforced on the impurity model, except that the disorder is to be present only in diagonal matrix elements of the full Hamiltonian. Without any loss of generality, we can assume that the mean value of random on-site potentials meets the requirement

$$\sum_n \varepsilon_n = 0, \quad (5)$$

which is achieved by the proper choice of the energy axis origin.

In the impurity problem, the main objective is to calculate in one way or another the Green's function of the disordered system

$$\hat{G} = (\varepsilon - \hat{H})^{-1}, \quad (6)$$

which can be expressed through the host Green's function

$$\hat{G}^{(h)} = (\varepsilon - \hat{H}^{(h)})^{-1} \quad (7)$$

by means of the Dyson equation

$$\hat{G} = \hat{G}^{(h)} + \hat{G}^{(h)} \hat{H}^{(d)} \hat{G}. \quad (8)$$

As a consequence, the Green's function of the disordered system can be expanded into the following series:

$$\hat{G} = \hat{G}^{(h)} + \hat{G}^{(h)} \hat{H}^{(d)} \hat{G}^{(h)} + \hat{G}^{(h)} \hat{H}^{(d)} \hat{G}^{(h)} \hat{H}^{(d)} \hat{G}^{(h)} + \dots \quad (9)$$

Afterwards, the terms of the series are individually averaged over all possible distributions of on-site potentials in the actual crystal lattice, and a double partial summation of the resulting series is performed. In this stage, the translational invariance of the host Green's function $\hat{G}^{(h)}$ is commonly exploited as a simplifying factor. The restoration

of the translational invariance of the Green's function \hat{G} , which comes from the configurational averaging, is exercised as well [12]. It is worth mentioning here that the impurity part of the Hamiltonian $\hat{H}^{(d)}$ serves as a perturbation in this technique.

In effect, we are not going to take advantage of the translational invariance of the host Green's function $\hat{G}^{(h)}$ hereinafter. Therefore, the host Hamiltonian $\hat{H}^{(h)}$ can, in principle, represent a system that lacks translational invariance altogether. Moreover, it can be even assumed that the host Hamiltonian per se characterizes a system with a structural disorder.

On the other hand, there is an alternative approach to calculate the Green's function \hat{G} of the disordered system. In this method, the initial system is based on the impurity part of the Hamiltonian $\hat{H}^{(d)}$. Accordingly, the Green's function of the initial system reads

$$\hat{g} = (\varepsilon - \hat{H}^{(d)})^{-1}. \quad (10)$$

It is, indeed, diagonal in the site representation by the virtue of the diagonal character of the impurity Hamiltonian $\hat{H}^{(d)}$. Corresponding diagonal matrix elements

$$g_n(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_n + i0} \quad (11)$$

are often named locators. It is not difficult to express the Green's function of the disordered system \hat{G} through the locator Green's function

$$\hat{g} = \sum_n g_n(\varepsilon) c_n^\dagger c_n \quad (12)$$

with the help of the respective Dyson equation:

$$\hat{G} = \hat{g} + \hat{g} \hat{H}^{(h)} \hat{G}. \quad (13)$$

Subsequently, the Green's function of the disordered system can be expanded into a structurally different series:

$$\hat{G} = \hat{g} + \hat{g} \hat{H}^{(h)} \hat{g} + \hat{g} \hat{H}^{(h)} \hat{g} \hat{H}^{(h)} \hat{g} + \dots, \quad (14)$$

where, contrary to Eq. (9), the host Hamiltonian $\hat{H}^{(h)}$ is acting as a sort of perturbation.

It is readily understandable that within the locator method the disordered system under consideration is effectively comprised of separate subsystems, which are characterized by their particular Green's functions — the locators $g_n(\varepsilon)$, and are interacting with each other by the means of the hopping integrals t_{nm} that, in turn, make up the host Hamiltonian $\hat{H}^{(h)}$.

3. In a kind of a thought experiment on the disordered system, nothing prohibits to gradually diminish all the values of hopping integrals simultaneously. Finally, we will get that $t_{nm} = 0, \forall n, m$. As a result, the disordered system at issue will break down into individual isolated subsystems that belong to their respective lattice sites. When on-site energies are real, these subsystems are simply repre-

senting energy levels of localized electronic states. At each site, the locator, as a sound Green's function, satisfies the causality condition,

$$\text{Im } g_n(\varepsilon) = -\pi\delta(\varepsilon - \varepsilon_n) < 0, \quad (15)$$

the local density of states is, as it ought to be, normalized to unity,

$$-\frac{1}{\pi} \int_{-\infty}^{+\infty} \text{Im } g_n(\varepsilon) d\varepsilon = \int_{-\infty}^{+\infty} \delta(\varepsilon - \varepsilon_n) d\varepsilon = 1, \quad (16)$$

and the Kramers–Kronig relation is obviously fulfilled:

$$-\frac{1}{\pi} \text{v.p.} \int_{-\infty}^{+\infty} \frac{\text{Im } g_n(\varepsilon')}{\varepsilon - \varepsilon'} d\varepsilon' = \frac{1}{\varepsilon - \varepsilon_n} = \text{Re } g_n(\varepsilon). \quad (17)$$

It has been suggested in Ref. 13 to assign random complex values to on-site potentials. Inevitably, the Hamiltonian of the corresponding disordered system becomes non-Hermitian. Indeed, the host Hamiltonian still remains Hermitian as in Eq. (2), while all the non-Hermiticity is contained in the impurity part of the Hamiltonian (compare with Eq. (3))

$$\hat{H}^{(d)} = \sum_n (\varepsilon_n - i\gamma_n) c_n^\dagger c_n, \quad \gamma_n > 0, \quad (18)$$

where γ_n is the broadening of the energy level residing at the n th lattice site, and all on-site potentials ε_n are real.

Since we will be concerned below only with the physicality of this non-Hermitian model, any particulars in the spatial distribution of its on-site parameters are irrelevant for our purposes. Usually, the presence of an imaginary part in the diagonal matrix elements of the Hamiltonian is attributed to the presence of dissipation of some kind. Let us look on the other side, employ once again the locator approach and switch off intersite interactions that are determined by the hopping integrals. Then, the disordered system will decompose into individual on-site subsystems, characterized by locators (compare with Eq. (11))

$$g_n(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_n + i\gamma_n}. \quad (19)$$

It appears that these subsystems despite featuring non-Hermiticity are physically consistent. Just as in the case of a Hermitian Hamiltonian (see Eq. (15)), the causality condition is, of course, met,

$$\text{Im } g_n(\varepsilon) = -\frac{\gamma_n}{(\varepsilon - \varepsilon_n)^2 + \gamma_n^2} < 0, \quad (20)$$

the local density of states, which possesses a familiar Lorentzian shape, is also (see Eq. (16)) normalized to unity

$$\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\gamma_n}{(\varepsilon - \varepsilon_n)^2 + \gamma_n^2} d\varepsilon = 1, \quad (21)$$

and the real and imaginary parts of each locator $g_n(\varepsilon)$, likewise in Eq. (17), are connected through the Kramers–Kronig relation:

$$\frac{1}{\pi} \text{v.p.} \int_{-\infty}^{+\infty} \frac{\gamma_n}{[(\varepsilon' - \varepsilon_n)^2 + \gamma_n^2](\varepsilon - \varepsilon')} d\varepsilon' = \frac{\varepsilon - \varepsilon_n}{(\varepsilon - \varepsilon_n)^2 + \gamma_n^2}. \quad (22)$$

Thus, we are dealing with a set of subsystems represented by energy levels, which are, as opposed to the conventional case, arbitrarily broadened. As long as we are concerned only with their respective Green's functions $g_n(\varepsilon)$, defined by Eq. (19), the isolated subsystems in question are behaving in a physically correct manner.

However, their local densities of states remain nonzero at all energies. Switching on the host Hamiltonian back will not spoil the disordered system. At that, finite in their values hopping integrals are transferring a collective excitation from one site to another, at which their inherent subsystems exhibit infinite spectra. In other words, there is a conflict between the finite bandwidth due to intersite hopping and the infinite bandwidths of unperturbed local densities of states. This brings up the question of whether the proper system of Wannier functions can be in principle devised for this particular model.

It is worth emphasizing, that complex on-site potentials are not unknown in the physics of disordered systems and naturally appear as the outcome of the coherent potential or average T-matrix approximations. The only distinction is that on-site potentials in these methods are not random, but are identical on all translationally invariant lattice sites. However, within the applicability restrictions of these approximations, the imaginary part of the on-site potential differs from zero only inside the resulting continuous electronic bands.

4. It would be desirable to modify the non-Hermitian model of the disordered system in such a way that the spectrum of each isolated subsystem will have a restricted bandwidth, which is comparable to the bandwidth generated by hopping integrals in the Hamiltonian with the exclusively Hermitian disorder. With this in mind, let us choose a single continuous band for the local density of states of each isolated subsystem. By way of an example, the mentioned local density of states can be shaped in a semielliptical manner that is frequently used for simplicity to model the host electronic band in a three-dimensional binary alloy problem:

$$\text{Im } g_n(\varepsilon) \sim -\sqrt{w_n^2 - (\varepsilon - \varepsilon_n)^2} < 0, \quad (23)$$

$$\varepsilon_n - w_n < \varepsilon < \varepsilon_n + w_n, \quad w_n > 0.$$

Outside of the site-dependent energy interval of width $2w_n$, the imaginary part of the locator is set to zero. Due to the dedicated shape, it is not so difficult to normalize the initial local density of states to unity,

$$\frac{2}{\pi w_n^2} \int_{\varepsilon_n - w_n}^{\varepsilon_n + w_n} \sqrt{w_n^2 - (\varepsilon - \varepsilon_n)^2} d\varepsilon = 1. \quad (24)$$

Thus, for the imaginary part of the locator, we finally get

$$\text{Im } g_n(\varepsilon) = -\frac{2}{w_n^2} \sqrt{w_n^2 - (\varepsilon - \varepsilon_n)^2}. \quad (25)$$

The real part of the locator can be reconstructed by resorting to the Kramers–Kronig relation,

$$\frac{2}{\pi w_n^2} \text{v.p.} \int_{\varepsilon_n - w_n}^{\varepsilon_n + w_n} \frac{\sqrt{w_n^2 - (\varepsilon' - \varepsilon_n)^2}}{\varepsilon - \varepsilon'} d\varepsilon' = \frac{2}{w_n^2} (\varepsilon - \varepsilon_n). \quad (26)$$

When energy falls inside the subsystem band, both preceding results combine to yield

$$g_n(\varepsilon) = \frac{2}{w_n^2} \left[(\varepsilon - \varepsilon_n) - i \sqrt{w_n^2 - (\varepsilon - \varepsilon_n)^2} \right], \quad (27)$$

$$\varepsilon_n - w_n < \varepsilon < \varepsilon_n + w_n.$$

Below the subsystem band, the proper expression for the locator can be obtained by analytic continuation:

$$g_n(\varepsilon) = \frac{2}{w_n^2} \left[(\varepsilon - \varepsilon_n) + \sqrt{(\varepsilon - \varepsilon_n)^2 - w_n^2} \right], \quad (28)$$

$$\varepsilon < \varepsilon_n - w_n.$$

One can proceed likewise for those energies that exceed the upper edge of the subsystem band. The resulting expression for the locator reads

$$g_n(\varepsilon) = \frac{2}{w_n^2} \left[(\varepsilon - \varepsilon_n) - \sqrt{(\varepsilon - \varepsilon_n)^2 - w_n^2} \right], \quad (29)$$

$$\varepsilon > \varepsilon_n + w_n.$$

At this stage of calculations, the construction of the illustrative locator should be considered as completed. Nonetheless, our main challenge is to devise a physically sound, but simultaneously non-Hermitian, impurity part of the Hamiltonian. This can be achieved by taking reciprocals of on-site locators:

$$\hat{H}^{(d)} = \sum_n \left[\varepsilon - \frac{1}{g_n(\varepsilon)} \right] c_n^\dagger c_n \equiv \sum_n v_n c_n^\dagger c_n, \quad (30)$$

where v_n is the corresponding, generally speaking complex, on-site impurity perturbation. It is straightforward to calculate each reciprocal due to the chosen semielliptic locator model.

Indeed, the resulting expression for the on-site impurity perturbation depends on the relative energy position against the subsystem band. Since there is, be it recalled, a certain amount of disorder, the locator bandcenter ε_n , and the bandwidth $2w_n$ are both site-dependent. For those en-

ergies that are inside the band of the given subsystem at the n th site, the impurity perturbation has the form

$$v_n = \frac{1}{2} \left[(\varepsilon + \varepsilon_n) - i \sqrt{w_n^2 - (\varepsilon - \varepsilon_n)^2} \right], \quad (31)$$

$$\varepsilon_n - w_n < \varepsilon < \varepsilon_n + w_n.$$

At energies that are below the band bottom, for v_n one has

$$v_n = \frac{1}{2} \left[(\varepsilon + \varepsilon_n) + \sqrt{(\varepsilon - \varepsilon_n)^2 - w_n^2} \right], \quad (32)$$

$$\varepsilon < \varepsilon_n - w_n,$$

while above the locator band, the respective expression reads

$$v_n = \frac{1}{2} \left[(\varepsilon + \varepsilon_n) - \sqrt{(\varepsilon - \varepsilon_n)^2 - w_n^2} \right], \quad (33)$$

$$\varepsilon > \varepsilon_n + w_n.$$

It should be noted that on-site impurity perturbation appears to be energy-dependent. This feature of the on-site perturbation is not unique to non-Hermitian impurities and can be found in generic Hermitian impurity models [14]. More importantly, the impurity perturbation tends to a finite real on-site potential, as energy moves away from the locator band:

$$v_n \approx \varepsilon_n, \quad |\varepsilon - \varepsilon_n| \gg w_n. \quad (34)$$

Therefore, the impurity Hamiltonian under consideration behaves as fundamentally non-Hermitian one only when energy belongs to at least one of the locator bands. Outside of the energy interval that covers all those bands, the impurity Hamiltonian drops its non-Hermitian character. Consequently, at energies that are lying far outside of the energy domain encompassing all locator bands, the impurity Hamiltonian reduces to the commonly-used model with the diagonal disorder and random on-site potentials.

5. In essence, we have proposed above a consistent method of constructing non-Hermitian impurity models for inhomogeneous systems with the diagonal disorder. To summarize, we assume that the Hamiltonian of the disordered system can be expressed in the site representation, which automatically implies the presence of a certain underlying spatial structure. Substitutional impurities are treated as individual self-contained subsystems, each of which is entitled to exist independently, while a Hermitian hopping part of the Hamiltonian is not randomized and glue these subsystems together.

We do not provide any specifics of the internal structure of the aforementioned subsystems and acknowledge that they might be governed by some hidden quantum numbers. We characterize subsystems by locators — valid Green's functions that are diagonal in the site representation and belong to just one site.

To devise a dedicated type of locator, we postulate firstly the outline of its imaginary part, which can be confi-

gured according to any continuous function of energy that attains exclusively non-positive values. Then, the corresponding local density of states is to be normalized, and the real part of the locator should be restored through the Kramers–Kronig relation.

Following these three easy steps, a theoretically legitimate locator can be fully specified. At this point, we take advantage of the fact that the function, which defines the shape of the imaginary part of the locator, may be designed in a way to have nonzero values only inside a fairly narrow energy interval. At that, particular parameters of this function can be used to introduce disorder. Moreover, impurities can be modeled by mixing locators of qualitatively different types.

In this approach, the actual on-site impurity perturbations are obtained by calculating reciprocals of corresponding locators and, thus, are inevitably energy-dependent. Given that impurities in the proposed model are non-Hermitian only inside a sufficiently narrow energy window and are resembling conventional real random on-site potentials outside of this window, it is quite appropriate to place respective disordered systems in a separate family.

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До теорії систем з негермітовим безладом заміщення

Ю.В. Скрипник, В.М. Локтєв

Запропоновано нове сімейство неупорядкованих систем. Це сімейство належить до класу систем, що містять випадкові негермітові домішки заміщення. Розгляд обмежено досить простим випадком, коли наявність точкових дефектів заміщення призводить до модельного гамільтоніану з діагональним безладом. На відміну від відомих моделей негермітових домішок, ненульова густина станів для кожної ізольованої від основного кристалу домішки наявна лише у неперервній зоні кінцевої ширини. Наведено спосіб побудови відповідних домішкових гамільтоніанів.

Ключові слова: негермітова домішка, локатор, локальна густина станів, безлад.